important technical topics, although the level of effort needs to be increased to meet the rapid rate of appearance of new data. Greatly increased effort on newer kinds of solid state data (energy levels, band structure, interaction with radiations, etc.) has been recommended by the solid state advisory panel.

In the field of chemical kinetics the first stage of the program has been the preparation of a series of critical reviews of the state of quantitative knowledge in selected aspects of the field. The activities in the area of colloid and surface properties are the result of a cooperative relationship with the National Academy of Sciences-National Research Council Committee on Colloid and Surface Chemistry, which had been planning an extensive program of data evaluation prior to the establishment of the National Standard Reference Data System. A preliminary critical survey of the field of mechanical properties has been carried out in order to determine appropriate activities.

Continuing efforts have been initiated to establish and promote effective working relationships with program officers in other government agencies (such as Atomic Energy Commission, Department of Defense, National Aeronautics and Space Administration, National Science Foundation, National Institutes of Health, and others) in order that the National Bureau of Standards' program might be responsive to the needs of these agencies. In some cases jointly funded projects have been established. In others, Office of Standard Reference Data staff members have served as a means through which program officers in other agencies were able to locate the competent staff needed to undertake the compilation activities required for their missions. Steps have been taken to ensure that persons working in closely related areas are fully aware of each other's activities. The search for competent technical people willing to undertake data compilation and evaluation projects continues.

A summary report describing the status of the program has been prepared and is available from the Government Printing Office (6).

FUTURE OUTLOOK

The program of the National Standard Reference Data System is regarded by the National Bureau of Standards and its other participants and proponents throughout the Federal Government as a permanent feature of the nation's future technical activity. The pace of scientific and technological progress shows no sign of slackening; the need for systematic data evaluation can only increase. With the support and participation of the technical community and of the United States Congress, the National Standard Reference Data System can make a vital contribution to the health and efficiency of our entire national technical effort.

LITERATURE CITED

- See, for example, "Science, Government, and Education,"
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 D. C., 25 cents.
- (2) See, for example, "Report on the Conference on Critical Tables of Thermodynamic Data," March 1963; National Academy of Sciences-National Research Council, Washington, D. C.
- (3) See, for example, the reports of the Joint Army-Navy-Air Force thermodynamic data compilation project under the direction of Dr. Daniel Stull, Dow Chemical Co., Midland, Mich.
- (4) The policy statement establishing the National Standard Reference Data System is given as Appendix A in the report "National Standard Reference Data System Plan of Operation" by E. L. Brady and M. B. Wallenstein; Superintendent of Documents, Washington, D. C., 15 cents.
- (5) "Information Handling in the National Standard Reference Data System," F. L. Alt, NBS Technical Note 290, July 1, 1966; Superintendent of Documents, Washington, D. C., 25 cents.
- (6) "Status Report National Standard Reference Data System,"
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 Superintendent of Documents, Washington, D. C., 50 cents.

Needs of American Chemical Society Members for Property Data*

HERMAN M. WEISMAN
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The mission of the National Standard Reference Data System is to provide the American technical community with critically evaluated data in the physical sciences. To fulfill its mission of administering the NSRDS, the NBS Office of Standard Reference Data has recognized

* 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.

it must tune its operations to the needs of the users of data. In its early planning stages, the Office of Standard Reference Data sought advice and counsel for this purpose from a small number of specialists. It was always evident that it would be important to obtain input from large cross sections of the technical community—for example, from the membership of the American Chemical Society. Such information would be valuable in determining prior-

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In August 1965, the American Chemical Society, on behalf of the NBS Office of Standard Reference Data, sent a questionnaire to its membership asking for information on their needs for compilations of critically evaluated data. Approximately 16,000 replies were received. Overwhelmingly, response was that present compilations of data satisfy poorly or at best only moderately the requirements of the membership of ACS. The survey identified the properties which ACS workers most often sought in the literature as well as those compilations most often consulted by respondents. Many worthwhile comments and suggestions were contributed as to approaches taken, compilation priorities, and techniques of format and presentation.

ities for the program and also in locating interest and competence for the conduct of compilation and evaluation projects.

Our office sought and was happy to obtain the cooperation of the American Chemical Society in surveying its membership for information on their needs for compilations of critically evaluated data. In late August of 1965 a survey was mailed to the membership of the ACS. Figure 1 shows the explanatory transmittal letter and the survey form. The Office of Standard Reference Data paid for the entire mailing. A stamped, addressed envelope was provided for convenient return of the survey. The questionnaire, which was first tried out on the entire NBS professional staff, was constructed to enable the respondent to provide the essential information our Office needed in a minimum of time. Most respondents could reply in 10 minutes or less.

The questionnaire was sent to the entire membership in the latter part of August 1965; approximately 100,000



AMERICAN CHEMICAL SOCIETY

8. R. STANIASON Executive Secretary 1155 SIXTEENTH STREET, N.W., WASHINGTON, D.C. 20036, Republic 7-3331

August 1965

Dear Professional Colleague:

The American Chemical Society is cooperating with the National Bureau of Standards by conducting a survey of the needs of its members for compilations of critically evaluated data.

The information obtained from this survey will be used to guide the activities of the National Standard Reference Data System, a government-wide effort to provide to the technical community of the United States optimum access to the quantitative data of physical science, critically evaluated and compiled for convenience.

This program was established in 1963 by the President's Office of Science and Technology, acting upon the recommendation of the Federal Council for Science and Technology. The National Bureau of Standards has been assigned responsibility for administering the effort.

The general objective of the System is to coordinate and integrate existing data evaluation and compilation activities into a systematic, comprehensive program, supplementing and expanding technical coverage when necessary, establishing and maintaining standards for the output of the participating groups, and providing mechanisms for the dissemination of the output as required.

More information on the plans and method of operating of the National Bureau of Standards' Office of Standard Reference Data may be found in CHEMICAL AND ENGINEERING NEWS August 9, 1065

Sincerely yours,

BR Stanerson

questionnaires were mailed. There were approximately 16,000 returns. About 12,000 replies arrived within the first six weeks, and, over the next five-month period, an additional 4000 came in. Approximately 2000 respondents indicated that they were either retired or in a type of activity not requiring critically evaluated data.

Response to Question 2 indicated, overwhelmingly, that present compilations of data either satisfy poorly or, at best, only moderately, data requirements of the membership of the American Chemical Society.

About 1000 of the respondents answered Question 5, indicating that they were either themselves compiling or knew of compilers of data not now conveniently accessible to the American technical community. These 1000 replies were carefully sifted. Those replies which were vague or which indicated that the compilations were in a classified area or were in a company proprietary or confidential area were eliminated. About 300 compilers were filtered through. These 300 were further scrutinized by Office

AMERICAN CHEMICAL SOCIETY

Survey of Needs for Critical Data Compilations

- Which physical, chemical, and mechanical properties of substances and systems do
- which physical, chemical, and mechanical properties of substances and systems of you seek most often in the literature? Please list properties and types of substances, e.g. free energies of formation of hydrocarbons, infrared spectra of pesticides, transition probabilities in light atom spectra, etc.
- How well do existing compilations of data satisfy your needs?
 Completely Moderately Poorly
- Which data compilations do you consult most often? Please list small, highly specialized compilations as well as more extensive compendia.
- 4. Which properties would you like to see made the subject of a comprehensive <u>critically evaluated compilation?</u> Please list properties and types of substances. Please consider properties that are computed from experimental data and functions that are used in the quantitative interpretation of experimental data, as well as compilations of such experimental data themselves.
- Are you now preparing any such compilation yourself or do you know of any already
 in existence or in preparation that are not now conveniently accessible to the American
 technical community? If so, please identify the compiler, his address, and the subject of his compilation.
- 6. Please use reverse side for additional comments.

BB No. 41-6536

Figure 1. Covering letter (left) and questionnaire (right) sent to ACS members.

NEEDS OF AMERICAN CHEMICAL SOCIETY MEMBERS FOR PROPERTY DATA

of Standard Reference Data personnel and a follow-up survey was sent asking for further details of their data compilation work. These returns indicated that the Office of Standard Reference Data was fully aware of the vast majority of these data compilation activities. There were very few instances of critical compilation activities within the technical scope of the present program of which the Office or its Advisory Committees were unaware. There were some instances of workers at different institutions duplicating or overlapping compilation work. These workers were apprised of the others' activity and the Office suggested that they get together and keep each other informed. The follow-up survey revealed that there were almost 30 compilers previously unknown whose work was significant to present and future directions and activities of the National Standard Reference Data Program. Lest anyone think that this number is small and unimportant, let me point out that the present program of the NBS Office of Standard Reference Data includes only 57 compilation projects.

The survey identified the properties which the respondents most often sought in the literature. About 1600 properties were so identified. A breakdown of the properties most often used by chemists in the United States follows (Table I), in order of frequency listed and identified by the Office of Standard Reference Data category of technical program area.

The responses also identified those properties which respondents desired to be made the subject of a comprehensive critically evaluated compilation. In this category there were almost 1000 properties. A breakdown of most frequently identified properties follows (Table II).

While there is some variation in individual ratings, there is correspondence between the types of properties chemists

Table I

Property	Times Listed	Office of Std. Ref. Data Technical Program Area
Boiling Point	2990	Thermodynamic & Transport Properties
Melting Point	2767	Thermodynamic & Transport Properties
Solubilities	2495	Thermodynamic & Transport Properties
Infrared Spectra	2126	Atomic & Molecular Properties
Thermodynamic Properties: Heats of	1786	Thermodynamic & Transport Properties
formation, etc., enthalpies, resis-		
tivities, conductivities, etc.		
Ultraviolet Spectra	1449	Atomic & Molecular Properties
Nuclear Magnetic Resonance Spectra	1021	Atomic & Molecular Properties
Physical Properties: Specific Gravities &	910	Thermodynamic & Transport Properties
Densities	500	3.6 1 1 173 41
Mechanical Properties	728	Mechanical Properties
Free Energies	721	Thermodynamic & Transport Properties
Equilibrium Constants	679	Thermodynamic & Transport Properties
Viscosities	660	Colloid & Surface Properties
Heat Capacities	638	Thermodynamic & Transport Properties
Refractive Indexes	606	Atomic & Molecular Properties
Chromatographic Data	591	Thermodynamic & Transport Properties
Toxicity	449	(Not within scope of program)
Thermal Conductivity	418	Thermodynamic & Transport Properties
Molecular and Atomic Weights	402	Atomic & Molecular Properties
Thermochemical Data	333	Thermodynamic & Transport Properties
Phase Relations	323	Thermodynamic & Transport Properties
Corrosion Data	312	(Not within scope of program)
Crystallographic Data	281	Solid State
PVT Data	276	Thermodynamic & Transport Properties
X-ray Data	253	Atomic & Molecular Properties, also Solid State
Kinetic Rate Data	228	Chemical Kinetics
Chemical Reaction Data	226	Chemical Kinetics
Optical Rotation Data	224	Atomic & Molecular Properties
Stabilities	212	Thermodynamic & Transport Properties
Entropies	204	Thermodynamic & Transport Properties
Visible Spectra	200	Atomic & Molecular Properties
Electric Resistivity Data	177	Solid State
Diffusion Data	177	Thermodynamic & Transport Properties
Azeotropic Data	158	Thermodynamic & Transport Properties
Structure Data	146	Atomic & Molecular Properties
Mass Spectra	141	Atomic & Molecular Properties
Decay Data	126	Nuclear Data
Absorptivity	101	Atomic & Molecular Properties

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HERMAN M. WEISMAN

Table II

Property	Times Listed	Office of Std. Ref. Data Technical Program Area
Thermodynamic Properties: Heats of	1637	Thermodynamic & Transport Properties
formation, etc., enthalpies, resis-		
tivities, conductivities		
Infrared Spectra	1125	Atomic & Molecular Properties
Solubilities	1084	Thermodynamic & Transport Properties
Boiling Point	897	Thermodynamic & Transport Properties
Ultraviolet Spectra	672	Atomic & Molecular Properties
Free Energy	631	Thermodynamic & Transport Properties
Melting Point	621	Thermodynamic & Transport Properties
Nuclear Magnetic Resonance Spectra	593	Atomic & Molecular Properties
Heat Capacities	557	Thermodynamic & Transport Properties
Specific Gravity and Densities	552	Thermodynamic & Transport Properties
Equilibrium Constants	549	Thermodynamic & Transport Properties
Chromatographic Data	470	Atomic & Molecular Properties, also
		Thermodynamic & Transport Properties
Vapor Pressure	402	Thermodynamic & Transport Properties
Refractive Indexes	383	Atomic & Molecular Properties
PVT Data	378	Thermodynamic & Transport Properties
Mechanical Properties	311	Mechanical Properties
Crystallographic Data	289	Solid State
Dielectric Constants	280	Atomic & Molecular Properties
Entropies	268	Thermodynamic & Transport Properties
Viscosity	255	Colloid & Surface Properties
Mass Spectra	181	Atomic & Molecular Properties
Glass Transition Temperature	165	Mechanical Properties
Thermal Stabilities	164	Thermodynamic & Transport Properties
Electrical Properties (resistivity)	163	Solid State
Dispersion Data	159	Atomic & Molecular Properties
Modulus of Elasticity	157	Mechanical Properties
Physical Properties	152	Thermodynamic & Transport Properties
Kinetic Rates	150	Chemical Kinetics
Thermal Conductivity	130	Thermodynamic & Transport Properties
Polarographic Half-wave Potential	121	Thermodynamic & Transport Properties
Extinction Coefficients	121	
Diffusion	114	Thermodynamic & Transport Properties
Absorption Spectra	114	Atomic & Molecular Properties
Atomic and Molecular Weights	100	Atomic & Molecular Properties

in the ACS work with and the properties they consider most important to be the subject of critically evaluated compilations. It would have been surprising if it were otherwise. The survey clearly revealed that properties within the Office of Standard Reference Data categories of Thermodynamic and Transport Properties and Atomic and Molecular Properties are those they most work with and need. The survey confirmed the priority judgments made by the Office of Standard Reference Data and its Advisory Committees on the direction of our program's compilation efforts. The resources of the Office of Standard Reference Data have and are continuing to concentrate on Thermodynamic and Atomic and Molecular fields, with some activity in lessening sequence in Chemical Kinetics, Solid State, and Colloid and Surface Properties.

Mechanical Properties—somewhere down the lower middle among properties worked with and required by ACS members—has presented special problems to our office. The Advisory Panel in this area has seen the need for critically evaluated data on mechanical properties of materials, but, at the same time, has recognized that some areas of the field are not well enough advanced theoretically or experimentally to warrent their inclusion within the present guidelines of the NSRDS.

Interest in nuclear properties is out of scope for the vast majority of the ACS members. This factor probably accounts for its low listing in this survey. The AEC supports large-scale efforts in this field.

The survey also identified those data compilations most often consulted by respondents. They are listed in the order of descending frequency (Table III).

There were about 500 distinct entries. These entries revealed very few surprises to the Office of Standard Reference Data. There were very few critically evaluated sources not previously within the data file of the Office of Standard Reference Data and these, of course, were ordered to be acquired. It is interesting that the majority of compilations receiving the greatest use by the ACS members were criticized the most for containing inaccuracies and gaps, and for lagging behind currently available data.

Many respondents offered worth-while comments and suggestions, not only on the needs, but on the implementation of the program to fulfill these needs for the technical

NEEDS OF AMERICAN CHEMICAL SOCIETY MEMBERS FOR PROPERTY DATA

Table III

rable in	
O	Times
Compilation	Mentioned
"Handbook of Chemistry & Physics" (Chemical Rubber	1705
Co.) Chemical Abstracts	1735 952
International Critical Tables (Washburn)	952 801
Beilstein's Handbuch	691
Perry, "Chemical Engineering Handbook"	431
Heilbron and Bundury, "Dictionary of Organic	401
Compounds"	402
API Project 44	303
Lange, "Handbook of Chemistry"	263
JANAF: Thermochemical Tables	254
Sadtler: Catalog of Infrared Spectra	242
Merck Index	231
Modern Plastics Encyclopedia	203
Tables of Experimental Dipole Moments	199
ACS Monographs	190
Seidell, "Solubilities"	185
ACS Special Series	179
ACS Publications	175
Landolt-Börnstein Tabellen	171
NBS Circular 500: Selected Values of Chemical	
Thermodynamic Properties	127
U. S. Pharmacopeia	101
Tables of Identification of Organic Compounds	85
Herschenson: Compilations of Absorption Spectra	84
NBS Circular 589: Tables of Dielectric Dispersion Data	00
for Pure Liquids and Dilute Solutions	80 79
Seidell: Table of Spectral Lines Varian NMR Spectra Catalog	79 77
Dana, "Mineralogy"	74
Chemisches Zentralblatt	70
Analytical Chemistry	68
NBS Monograph 53: Experimental Transition Probabil-	00
ities for Spectral Lines of 70 Elements	68
Technology Journals	68
Tables of Semiconductor Properties	65
Table of Nuclides	60
Advances in Catalysis	58
ASTM	56
ASTM X-ray Diffraction Data Card File	54
ASTM Diffraction Patterns of Solid State Compounds	
and Alloys	50
U.S.F.D.A. Publications	50

community. A few of the more significant comments, typical of or synthesizing the suggestions and opinions of the respondents, will be quoted. Comment A is from the editor of an industrial chemical company data handbook. His comments are as follows:

A. "I believe this to be an area where the ACS and NBS could make an important contribution. As you know, the International Critical Tables were published in 1926—40 years ago, and much has been learned since that time. Also, many of these tables are presented in such a manner that many a user has given up in desperation, even though he knew the data he needed were buried there. We have had such an instance happen more than once in our own library.

"When I critically reviewed the values for the physical properties of the elements for the handbook, I was astounded at the wide variation in the reported values of well-known elements, such as aluminum and copper. As a result of this investigation, you might be interested to know, I changed the b.p. of copper from 2336° C. to 2595° C. and the b.p. of aluminum from 2057° C. to 2467° C.—a difference of almost 400° C. In the case of aluminum there was such a wide varia-

tion between various reported and measured values that in desperation I wrote the Research Dept. of the Aluminum Co. of America. I was told that they were not satisfied with any of the values and they had made their own measurements. I adopted their value as a result, for I thought it to be the most reliable of any I had found.

"One of the greatest problems that plagues a compiler of handbook data is that of choosing a good value from a number of independent measurements. It ultimately resolves down to the problem of trying to determine which experimenter was the most careful in doing his work and reporting it. In some cases a review of the literature showed variations of as much as 100% in the physical properties of the elements. An example is cerium. In light of new information I was compelled to change the reported density in the handbook from 3.92 to 6.67 to 8.23 (depending on the allotrope).

"I would like to cite just one more example to show how the handbook values that are in common use are incorrect.

"William R. Mott published an article in the Transactions of the American Electrochemical Society in 1918, entitled 'Volatilities of Refractory Materials.' On page 287 of this paper a table was given which since has been widely copied, recopied, rerecopied, etc. It was an excellent article for its time. In this, Mott gives a value for the melting point of scandium, and a calculated boiling point. As far as I can determine there is not one shred of evidence where he got his values for this element—but I suspect he got an inkling from Moisson or one of the other pioneers. Scandium was not isolated until recently; nevertheless, Mott's values for scandium have appeared in well-known references, including the handbook until 1964 when I revised the value. I chose a value obtained from Dr. Spedding, who has done so much work on the rare earths at Iowa State.

"I am sure that many of the values we are using from day to day in our 20th century technology are incorrect and should be reinvestigated in light of our new knowledge. We should know, for example, what is the heaviest known element, but we don't. Crystalline osmium has been made, but no one has yet taken the trouble to determine accurately its density, as far as I can learn.

"I would like to see the ACS review the literature critically to see if the data in common use have been obtained from reliable sources or if original measurements were discordant. In cases where the data are discordant, the NBS could step in and make some reliable, original measurements. I am sure this would keep these agencies busy for many years."

- "Although I may be unduly pessimistic, I have found several major drawbacks to compilations of data in chemical physics and physical chemistry.
 - (1) They are never current, and probably cannot be.
 - (2) They are often not critical enough, so that one cannot be certain with what reliability the data can be used.
 - (3) I have found it very difficult to locate desired data in compilations, since I do not usually know a priori which compilation contains a particular datum.
 - (4) I often find it more expedient to try and locate the necessary information through Chemical Abstracts than through compilations, or by obtaining the necessary experimental data myself, albeit in a cruder form than might be found in a critical survey."
- C. "Most compilations are too big and expensive to be readily available. Even some large companies won't buy them, choosing to work on a library cooperation basis. This can mean a loss of two or three days or more. Such delay is frustrating, if nothing more when one is trying to get a job done.

"Data centers where one could telephone and get replies by teletype would be most helpful. Engineering and industrial design and problem solving could be speeded considerably."

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D. "The Kelley Bulletin and Circular 500 were fine in their time. But this effort must be continuing. The API and Manufacturing Chemists Projects would be wonderful if not so limited in scope.

"In thermodynamics and thermochemistry some large efforts are very badly needed. Who knows how much money is wasted daily because data are lost in the literature or used uncritically? Unnecessary experiments are run. Plants are built to wrong specifications, opportunities are by-passed, all because the data are not at hand when needed..."

- E. "Present compilations usually present conflicting data, not critically evaluated. *Parsons Handbook* is a good source but gives no reference as to sources and hence no evaluation can be made of applicability of figures. Virtually no compilation exists on information from nonaqueous electrochemists."
- F. "The key word is critically evaluated. Except for the National Bureau of Standards Thermochemical Compilations, hardly any sizeable bodies of data on any physical property are available. There is a real need for such compilations."
- G. "It is remarkable that the common compilations are as good as they are. However, some of the omissions are equally remarkable. For example, the vapor pressure of boric oxide has been determined twice in recent years and is of importance in semiconductor processing, yet this quantity is not listed for this simple compound in either the *Handbook of Chemistry and Physics* or in the American Institute of Physics Handbook. Up-to-the-minute compilations are of utmost importance today and the NBS effort will be invaluable."

While the vast majority of the returns were favorable and enthusiastic about the purposes of the National Standard Reference Data Program as indicated in the questionnaire forwarded to the membership, there were a few that were negative. It would be only fair to give this viewpoint as well. The tenor of the comments is indicated in the following two opinions:

- A. "This is ridiculous! I think the ACS dues should be reduced before our money is used on this junk."
- B. "Any questionnaire originating from the U.S. Gov't., its agencies, or the ACS is expected to be asinine. This is no exception.

"There are no good data compilations and never will be. A data compilation is only good if it contains the information you want. If you are doing decent research, the work is too new to be found in compilations. If you are doing industrial work, the compilations will undoubtedly be too finite, or, as in International Critical Tables, wrong.

"Any working chemist or engineer can usually find his own data—pertinent to his exact problems—faster by use of the lab than by use of questionable references, which, incidentially, were often provided by alchemists of the 1800's (favorite source of compilers).

"In my opinion, skip it.

"I'm sure you'll get erudite answers—more to your liking—from incompetants [sic] who expect to find the answer to their research in recorded history. I'm equally sure you'll happily listen to these hacks rather than to the working members of this Society."

The purpose of our survey questionnaire, of course, was to provide a vehicle whereby we could listen to the thoughts, desires, and experience of the working members of the ACS.

Let me end on a more positive note, and one that might bring a little cheer to some of the members of the ACS—provided there is truth in the following lament from one of the responding members:

"... Societies and associations have been timid or tardy in providing coordinated data and evaluation thereof. I picture a day when society dues could be increased to finance more of these efforts because the members would no longer need to buy so much liquor to drown the despondency of scientific frustrations."

The purpose of the National Standard Reference Data System is to provide coordinated and critically evaluated data; perhaps the day is not too far away, if our program can stay viable, when members of the American Chemical Society need no longer "drown the despondency of their scientific frustrations in drink." If most of the ACS membership is like the few I know, they will drink only for the pleasure of it.