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Public/Private Cooperation in Planning and Developing Reference Data Programs*

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Received January 18, 1973

The National Standard Reference Data System relies heavily on the advice of experts in special subject-areas of science and technology to plan and develop programs for compilation and evaluation of quantitative data. Advisory panels provide a means of bringing together generators and evaluators of data to define needs, recommend specific projects, determine priorities, and coordinate new activities with those already in process. Such advisory panels are the natural basis for the development of cooperative programs, not only for data compilation and evaluation, but also for improvement in the quality of original experimental work, standardization of techniques, and agreement on formats for the presentation of, e.g., spectroscopic data. While such panels are sponsored by the Federal Government, the panel membership includes people from universities, private industry, professional societies, and consultant organizations. The cooperative nature of the undertakings fosters attention to user needs and public benefits.

In a symposium concerned with cooperative efforts, it is highly appropriate to give some consideration to those kinds of cooperation which cross the interface between the public and the private sectors. In so many of the relationships between Government agencies and private individuals or groups, there exists a one-way-only action. For example, Government may take things (via taxes, the draft, etc), or provide them (roads, flood relief); it may buy (through contracts or cash purchase); or sell (books from the Government Printing Office). In more sophisticated relationships, Government agencies call upon individuals or groups to give advice which the agency may then unilaterally follow or modify. But this also is a one-way-at-a-time activity—the advice is requested, then it is given, and then follow-up action may be taken.

What I intend to describe is a truly two-way relationship in which public and private parties work together actively toward a commonly defined set of goals. This type of relationship can, and does, lead to situations in which everyone benefits.

BACKGROUND

To provide a background for this discussion of cooperative activities, it may be worthwhile to spend a few minutes describing the National Standard Reference Data System (NSRDS), its mission, its scope, and its organizational approaches. This description will be brief, since details have been presented at an earlier symposium sponsored by this Division[1-3] and written descriptions are readily available in many publications.[4,5] The primary mission of the NSRDS is the provision of reliable, critically evaluated, numerical data in the physical sciences, in a convenient and accessible form for the use of the scientific and technical community. The technical scope of the program is restricted to well-defined physical and chemical properties of substances and systems which are well characterized. The organizational approach utilized in seeking the goals of the NSRDS is a decentralized activity comprising many projects, with coordination furnished by a program office (the Office of Standard Reference Data, OSRD) in the National Bureau of Standards.

The scope of the NSRDS, encompassing all of the physical sciences, is too broad to permit any small group of people to be knowledgeable and expert in either operating all of the projects or in managing the program as a whole. Moreover, the program is both government-wide in that it includes many agencies of the Federal government, and national in the sense that it seeks to improve the capabilities of *all* segments of the country's science and technology to perform their defined tasks effectively. Not only is the technical scope too broad to permit expert operation by any small group, but also the diverse uses and needs for standard reference data are too varied and wide ranging for full appreciation by the central program office alone.

Accordingly, it is essential that the OSRD obtain a great deal of advice of many different kinds.

* Presented before the Division of Chemical Literature, 164th Meeting, ACS, New York, N. Y., Aug. 27, 1972.

STRUCTURE OF ADVISORY SERVICES TO THE NSRDS

The formal advisory structure for the National Standard Reference Data System is organized under the sponsorship of the National Academy of Sciences–National Academy of Engineering–National Research Council. These bodies have established a Numerical Data Advisory Board under which a number of more specialized advisory and overview responsibilities are subsumed, as indicated in Figure 1. The Numerical Data Advisory Board consists of a Committee on National Programs, with an evaluation panel for the Office of Standard Reference Data, plus three other major committees of less immediate concern to the topic under discussion.

At the next level, focussing on increasingly specific interests, the Committee on National Programs of NDAB. maintains technical advisory panels for some of the seven program subject areas of the National Standard Reference Data System. This substructure is shown in Figure 2. It is the function of these area panels to provide a review of the scope of that area, to suggest specific programs and projects, to assign priorities, and to indicate competent experts to undertake tasks in project areas as needed. Individual members of the Advisory Board also assist from time to time by reviewing the outputs of some of the projects.

At a still more specific level, subpanels are set up as needed, usually on an ad hoc basis, to study needs and define the precise scope of projects on individual topics.

In addition to the formal advisory structure, the Standard Reference System receives valuable continuing advice from other interested organizations, from members of the technical staff of the National Bureau of Standards, and from individual experts in the scientific and technical community who are involved in and concerned with research relevant to specific projects.

Except for the number of levels of participating bodies, there is nothing unusual in this kind of an advisory structure. Many Government agencies get advice from panels. However, as indicated earlier, the advice which these panels provide does not stop at the discussion level, nor is it limited to a once-a-year meeting. It extends over into the planning and development of individual projects. These specialized ad hoc panels are in fact the focal point for interaction of the National Standard Reference Data System with the concerned audience of users of reliable reference data throughout the community. These ad hoc panels, in other words, are key elements of the cooperative planning and development of the System.

There is no uniform procedure for the development or activities of the ad hoc panels advisory to the National Standard Reference Data System. The ad hoc nature of the groups and the wide variety of user communities which are concerned makes it appropriate to organize the work of each individual panel in accordance with the problem at hand. In spite of this fact, certain characteristic steps have been taken by several of the subpanels concerned with the several types of molecular spectroscopy. Some of these steps will be discussed in more detail.

The general pattern of panel activities leads us to take a look at the Joint Committee on Atomic and Molecular Physical Data (JCAMP), an organization which has no formal structural links with the Numerical Data Advisory Board, but which, at the working level, has evolved into a valuable source of expert specialized assistance and program guidance for the Office of Standard Reference Data. The development of the cooperative activities of this Joint Committee with the National Standard Reference Data System are primary illustrations for the present discussion. To complete the background picture, let us see how JCAMP came into existence.

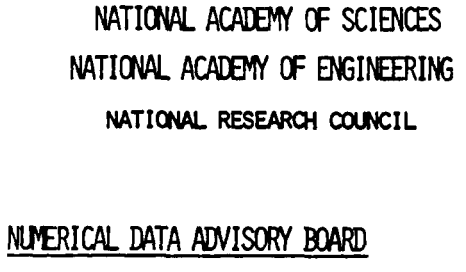

Figure 1. Numerical data Advisory Board

JOINT COMMITTEE ON ATOMIC AND MOLECULAR PHYSICAL DATA

The National Standard Reference Data System was established in 1963 by issuance of a Federal Policy Statement from the Federal Council for Science and Technology. Project operations concerned with data compilation and evaluation began during the first half of 1964.

One of the early projects at that time focussed on the collection and evaluation of existing infrared spectra of the type used for analytical chemical purposes. This project was undertaken with the goal of providing public accessibility to the useful content of several collections of infrared reference spectra maintained at a number of government and private laboratories, with no proprietary interest or security consideration which might restrict their publication. The NSRDS project was designed to provide a machinery by which such spectra could be solicited, collected, evaluated, and where appropriate, published in a convenient manner.

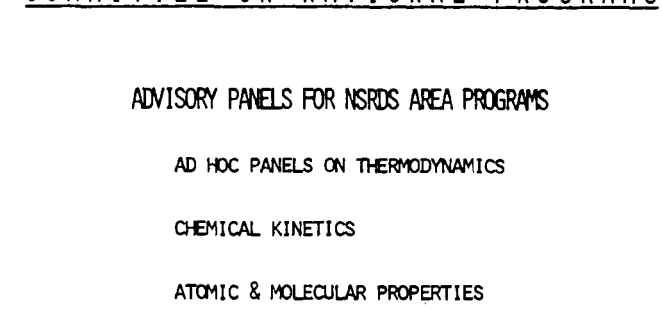

Figure 2. Committee on National Programs

To evaluate the reference spectra collected, project workers found that they needed technical specifications by which the spectra might be classified. The Office of Standard Reference Data commissioned the Coblentz Society to define specifications for publishable spectra. It developed that such criteria would be useful to other spectroscopists setting standards in their own laboratory. The resulting specifications were published in *Analytical Chemistry* in August 1966. Spectra were classified according to their purpose and quality. Very briefly, a Class I Spectrum is defined as a spectrum completely independent of the spectrometer—in other words, a physical constant of the material (no Class I Spectra have yet been produced, but Fourier transform spectrophotometers may make such spectra a reality within the next few years). A Class II Infrared Spectrum, or research quality analytical spectrum, is defined as a spectrum of a pure material produced on a good grating spectrometer using good technique and run under optimal conditions. A Class III Spectrum, or approved analytical spectrum, is one produced on defined substance using good sampling techniques with a high quality sodium chloride prism instrument or a grating instrument not meeting Class II standards.

The concept of Class I, II, and III spectra was accepted by the National Standard Reference Data System, was discussed and employed by the people doing evaluation of spectra, and has proved to be applicable to many other kinds of numerical data as well. The operators of the project also found that their work also called for the assistance and participation of major professional and technical organizations concerned with molecular spectroscopy. It was with the intention of providing such participation that the Joint Committee on Atomic and Molecular Physical Data was formed in 1966.

The stated purpose of the Committee was to "generate, collect, evaluate data; approve the publication and encourage the distribution of atomic and molecular data in suitable form to serve as references for pure compounds and mixtures." The original focus was on infrared spectroscopic data, although the language used was deliberately more general. With some foresight, the members of the Joint Committee recognized that the time might come when they would wish to broaden their horizons. The original sponsoring organizations which made up the Joint Committee included the American Petroleum Institute, the American Society for Testing and Materials, the Coblentz Society, the Manufacturing Chemists Association, the Society for Applied Spectroscopy, and the Spectroscopy Society of Canada (at that time named the Canadian Association for Applied Spectroscopy). The American Chemical Society and the American Society for Mass Spectrometry joined as sponsors at a later date.

When the time came for decisions on a publication channel for the spectra, it was concluded that the Joint Committee should serve as the sponsor. The Coblentz Society (which had been publishing good quality contributed spectra for a number of years) undertook to use the opportunity to publish only evaluated spectra, at least 90% of which met Class III standards or better. With these conditions, the spectra resulting from the NSRDS project were turned over to the Coblentz Society for publication. The Office of Standard Reference Data, following advice that it should avoid allocating too large a fraction of its resources to spectroscopic data of intermediate quality, terminated its financial support of the project.

Thus was set the pattern for a range of cooperative and collaborative efforts in the area of molecular spectroscopic data which has expanded in subsequent years. In this particular instance, a number of professional societies, each concerned with a different aspect of the availability of good quality reference data, shared the responsibilities for various phases of the work which NSRDS had begun. But beyond the specific project, the impact of the program on the technical community was greatly increased by the participation of the sponsor societies.

The publication of spectra by the Coblentz Society has continued and 4000 such spectra have been published in this new regime, without additional support from the National Standard Reference Data System.

In addition, a pilot study for collecting and generating Class II Spectra has been started. Both the Coblentz Society and the American Society for Testing and Materials provided initial funds to the JCAMP to support the study.

EXPANSION OF DATA COMPILATION ACTIVITIES

There has been substantial impact, both nationally and internationally, resulting from the spectral data project described above. On the basis of this experience, the National Standard Reference Data System and the Office of Standard Reference Data felt that further ventures into data compilation activities in the areas of molecular spectroscopy should commence with an assessment of the state-of-the-art in each of the spectral areas concerned, with particular reference to the capabilities for providing reference spectra at various quality levels, and user needs for data of such quality. Ad hoc Advisory Panels have been established in three specific areas, nuclear magnetic resonance spectroscopy, microwave spectroscopy, and Raman spectroscopy. These Advisory Panels, working on behalf of the National Standard Reference Data System, have focussed their attention on questions of quality, availability and need for spectra rather than urging the Office of Standard Reference Data to undertake major compilation projects. At the same time, these Panels have related themselves, because of common interest, to the Joint Committee on Atomic and Molecular Physical Data. Members selected from the ad hoc Advisory Panels have formed subcommittees of the Joint Committee in the parallel subject areas. As a result, the over-all structure of interactions takes on the configuration shown in Figure 3.

Addressing only the area of Atomic and Molecular Properties, the Atomic and Molecular Advisory Panel has thus established four subpanels concerned with three areas of spectroscopy and the area of interatomic distances. Each of these advisory groups has been instrumental in shaping and developing the activities of the Office of Standard Reference Data in the appropriate subject areas. Similarly, under the Joint Committee on Atomic and Molecular Physical Data, there is a subcommittee for each of five areas of molecular spectroscopy. However, the parallel is not 100%, because there is no data compilation project on mass spectrometry nor is there an NDAB Advisory Panel on mass spectrometry. Similarly, OSRD supports a microwave data project, and there is a microwave subcommittee under the Joint Committee but no NDAB Advisory Group on that subject. Furthermore, as might be expected, the Joint Committee has not established a subcommittee on interatomic distances, since it does not at present anticipate any direct involvement in the area. The societies which the Joint Committee represents have no direct focus on interatomic distances data such as they do in the other areas.

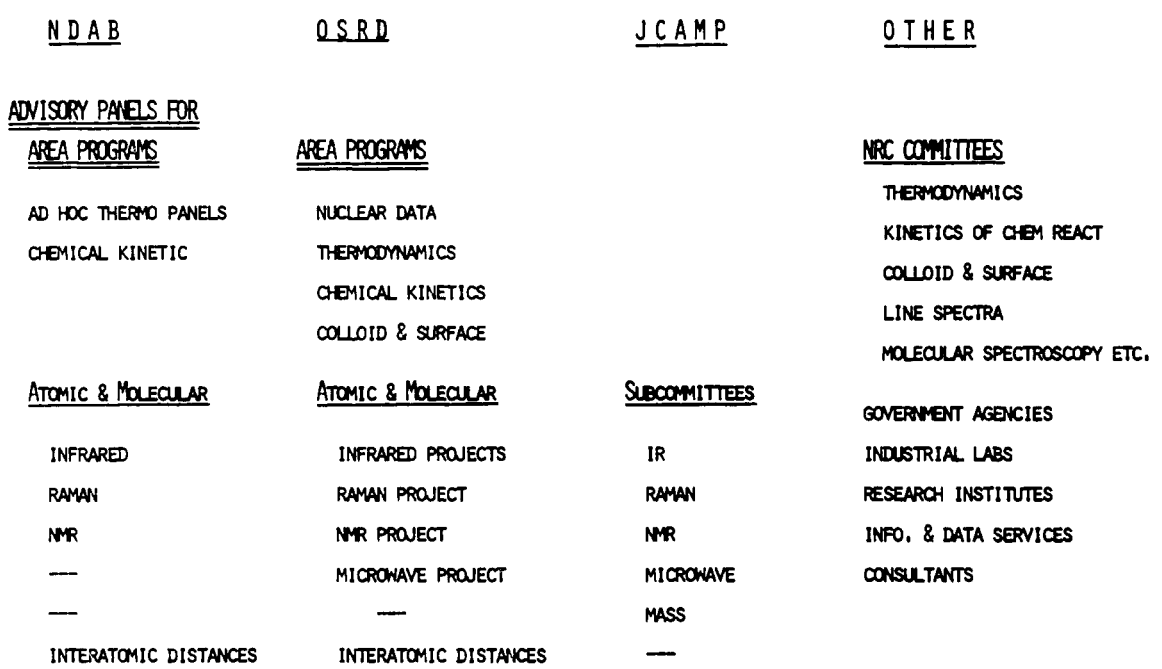

Figure 3. Parallel structure of advisory and operational data groups

The degree of overlap and interaction among these three organizations is most advanced in the area of infrared spectroscopy. Here, the Office of Standard Reference Data has had a number of different specialized projects, the first of which started in 1964. At present, the Standard Reference Data commitment to infrared spectroscopy consists of two projects, the first is a long standing compilation program concerned with fundamental vibration frequencies as derived from infrared, Raman, and microwave spectral data. The results of this project have been published in the NSRDS-NBS Series and more recently in the *Journal of Physical and Chemical Reference Data.*

The second NSRDS project is a small exploratory undertaking, mentioned earlier, which seeks to develop a collection of perhaps 200 or 250 infrared spectra of Class II quality. The goal of this project is a usable trial collection of data to furnish a basis for determining the applicability of the spectra in the solution of applied problems. The relatively high precision of such spectral data may facilitate computerized searching of reference collections. In this Class II Spectral undertaking, the Joint Committee on Atomic and Molecular Physical Data has played an important role as have the Coblentz Society, the American Society for Testing and Materials, one of the original sponsors of the Joint Committee, along with a number of individual scientists in Government, industrial, and academic laboratories. The Office of Standard Reference Data has supplied funds to cover a fraction of the expenses of obtaining some of the samples and confirming the fact that the spectra run have achieved Class II specifications. However, a major fraction of the total costs have been borne by the individuals and organizations who have cooperated in the program.

The existence of the Joint Committee has been invaluable in providing a well-defined basis for such contributions of time and effort. The Joint Committee has also provided links between the infrared and Raman spectroscopy communities, in efforts to formulate criteria for the presentation of Raman spectra. These criteria have been presented to the International Union of Pure and Applied Chemistry and now have international recognition.

Similarly the Joint Committee program for NMR spectroscopy, closely associated with the OSRD NMR project, has resulted in a set of tentative standards which have been submitted to the International Union of Pure and Applied Chemistry and formal adoption is expected in the near future.

To complete the list of participants in these spectral data activities, I wish to call attention to the role of the private-sector people. Three groups from private industry are concerned. The first includes spectroscopists in industrial laboratories, whose time and efforts are supported by their employers. The second provides the vigorous participation of the companies which make spectroscopic instruments. Their active efforts to improve the level of spectral reference data have been of great help to the whole program. The third is the "information and data industry," the people whose livelihood comes from the generation and sale of technical information. One aspect of their participation is illustrated by the Sadtler Research Laboratories as the distributor of the Coblentz Society spectra.

In summary, what has evolved is a free-form set of interactions of advisory and problem-solving groups, each rather small in number, each composed of experts in a special field of science, and each reflecting the interests of their peers. These groups work within a general framework which helps to maximize the impact of their advice and efforts. With the general goal of assuring that in each speciality, the *numerical data* activities are as closely matched as possible to what the user community needs. The limitation on all these efforts is the supply of funds to support data activities. The advice and professional leadership and working manpower are assured.

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