Two National Bureau of Standards Data Centers: Chemical Kinetics and Mass Spectrometry*

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Received December 5, 1966

Two current information retrieval centers, one for chemical kinetics, the other for mass spectrometry, are described. The methods and philosophies of operation of these programs are compared. The role of specialized information systems in promoting data evaluation, the evaluation of their usefulness as sources for reference material, the choice of techniques, and possibilities for intercenter coordination are discussed.

This paper describes two data and information centers operating in close proximity at the National Bureau of Standards. Both deal with various types of collision processes. Of particular interest is the fact that the two centers function in terms of different philosophies and use different techniques. These differences are a continuing subject for discussion.

The element in common to both is the objective: to obtain quickly specific answers to specific questions about rates of reactions (kinetics) and ionization phenomena (mass spectroscopy). The tacit assumption, shared with other modern information systems, is that resort to the classical abstract journals is too time consuming to be done haphazardly and repeatedly by research scientists. This is felt to be particularly true when the problem is (hopefully) to find all relevant quantitative information on a subject.

Ideally one would consult a new "International Critical Tables" which is comprehensive, up-to-date, and within easy reach. Such a mega-volume does not, and is unlikely to, exist.

The National Standard Reference Data Program of the National Bureau of Standards offers an alternative. Its purpose is to coordinate and support efforts leading to the compilation of critically evaluated reference data in the physical sciences. In the area of concern here the present mechanism is to sponsor a series of review monographs in which data evaluation will be emphasized. The two data centers are part of this program. Their principal function is to lift from the shoulders of the authors of these reviews the task of finding, collecting, and codifying the material they need. Hopefully they will then be able to devote their time and energies to analysis.

In addition to this function these centers serve as information sources for the public. Their resources are available to all. A letter or a telephone request is sufficient. A request to one center will invoke the services of both. There is no charge for the service.

* Presented in part 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

CHEMICAL KINETICS INFORMATION CENTER

This center is part of the Elementary Processes Section, Institute for Basic Standards, NBS. It provides a bibliographic service, both in answer to specific requests from the public and in support of the National Standard Reference Data System's "critical review" program. The types of questions that now can be answered are these:

What work has been done on determining the rate and mechanism of a specific reaction?
For example:

$$O + NO_2 \rightarrow NO + O_2$$
$$H_2 + C_2H_4 \rightarrow C_2H_6$$

What work has been reported on a class of reactions?
For example:

Recombination of alkyl radicals.
Hydrolysis of benzoic acid esters.
Reactions of the nitrogen oxides with N, O, O_2, O_3, and with themselves.

The answers are in the form of lightly annotated bibliographies. Two sample formats used are shown in Figure 1. Data evaluation is not part of this program; the Kinetics Center does not issue recommended numbers. The answers are based on a search of the collection of papers at the

D. Husain and R. G. W. Norrish
Proc. Roy. Soc. **A273**, 145 (1963). "The Explosive Oxidation of Ammonia and Hydrazine Studied by Kinetic Spectroscopy."

$$N_2H_4 + h\nu \rightarrow 2NH_2\cdot$$
$$N_2H_4 + O_2 \rightarrow N_2 + H_2O$$
$$N_2H_4 + 2O_2 \rightarrow 2NO + 2H_2O$$

Figure 1, *A*. Typical entry in a bibliography issued by the Chemical Kinetics Information Center.

$N + NO \rightarrow N_2 + O$	Clyne + Thrush	NATUA-1961-189-56
$N + NO \rightarrow N_2 + O$	Clyne + Thrush	PRLAA-1961-261-377
$N + NO \rightarrow N_2 + O$	Herron, J.	JCPSA-1961-35-1138

Figure 1, *B*. Typical entries in a bibliography based on the Institute for Defense Analyses compilation.

MASS SPECTROMETRIC DATA INFORMATION CENTER-NBS

ION	REACTANT	OTHER PRODUCTS	IP or AP	METHOD	YR	DOC NO
CN^+	CNI	I	18.1±0.1	SP	60	00073
CN^+	CNBr	Br	18.3±0.1	SP	60	00073
CN^+	CNCl	Cl	18.3±0.2	SP	60	00073
CN^+	CH_3NO_2	?	19.15±0.09	IB	55	00090
CN^+	CH_3NO_2	?	33.6±1.0	IB	55	00090
CN^+	CN		14.5±0.2	SP	61	00154
CN^+	CN		14.5±0.5	SP	61	00154
CN^+	C_4N_2	C_3N	19.2±0.3	SP	61	00154
CN^+	HC=C-CN	C_2H	19.8±0.2	SP	61	00154
CN^+	C_6N_2	C_5N	20.0±1.0	SP	61	00154
CN^+	$(CN)_2$	CN	21.5±0.3	SP	61	00154

TERM DESIGNATION

SP=SEMILOG PLOT
IB=INITIAL BREAK

REFERENCES

00073 Herron, J. T. and Dibeler, V. H., "ELECTRON IMPACT STUDY OF THE
00073 CYANOGEN HALIDES", J. Am. Chem. Soc. 82, 1555(1960)
00090 Kandel, R. J., "APPEARANCE POTENTIAL STUDIES. II. NITROMETHANE,"
00090 J. Chem. Phys. 23, 84(1955)
00154 Dibeler, V. H., Reese, R. M. and Franklin, J. L., "MASS
00154 SPECTROMETRIC STUDY OF CYANOGEN AND CYANOACETYLENES", J.
00154 Am. Chem. Soc. 83, 1813(1961)

BRIEF REFERENCES

DOC NO	JOURNAL CODEN	VOL	PAGE	YR	FIRST AUTHOR
00073	JACS	82	1555	60	HERRON
00090	JCPH	23	0084	55	KANDEL
00154	JACS	83	1813	61	DIBELER

Figure 2. Typical output of the Mass Spectrometry Data Center showing appearance potentials determined for the CN^- ion in three studies.

center. Custom searches of the chemical literature are not undertaken.

Scope. The scope of the center is homogeneous reaction kinetics. The term is interpreted liberally to include measurements on the dynamics of collision processes, such as energy transfer, photochemistry, and chemical kinetics.

Resources. The resources of the center, at present, include about 11,600 indexed research papers, reports, and theses. About 4500 of these were provided, and indexed, by the Institute for Defense Analyses. These were collected under the direction of A. Hochstim for a forthcoming bibliography of atomic cross sections and rates of light molecule reactions. About 9100 papers (partially overlapping the IDA work) have been collected at NBS from reprint collections of NBS staff members and searches of the current literature. About half of the papers were published after January 1, 1959. For the older literature, the center draws upon NBS Circular 510 and Monograph 34, "Tables of Chemical Kinetics—Homogeneous Reactions" and unpublished material collected during the preparation of these volumes (*1*).

Organization. The main collection has been arranged as a coordinate subject index. Papers are indexed in terms of keywords drawn from a prescribed, but open-ended, subject vocabulary and in terms of the reagents and products of the reactions. The information is stored on optical overlay cards (*2*). No data are extracted. The unit of storage is the document. The IDA collection is indexed in terms of the specific reaction and broad categories. This material is on magnetic tape. The unit of storage is the reaction.

The present input to the center is almost entirely from the current literature. There are no plans to capture the older work. Instead, the center will rely on bibliographies developed in the preparation of review articles sponsored by NBS.

MASS SPECTROMETRY DATA CENTER

This center is part of the Mass Spectrometry Section, Institute for Basic Standards, NBS. It is prepared to answer the following types of questions:

> What is the ionization potential of molecule A?
> What is the appearance potential of ion B?
> What information is available on (a specific) ion-molecule reaction?

In the first two cases the answers include the reference, the numerical values, with error limits (as reported in the source), the method used, and the details of the process studied. In the third case a bibliography is provided.

Scope. This center operates by defining a limited subject for which compilation and data extraction appear desirable. These subjects are drawn from the research areas exploited mainly by mass spectroscopists. As a result,

the scope, as defined by the available output, changes radically with time.

Resources. In developing the ionization and appearance potential file, the search was restricted to the years since 1955 because of the availability of the compilation by Field and Franklin (*3*). The file was built, initially, from the bibliographies of the ASTM E-14 Subcommittee II, the compilation of Kiser (*4*), reference lists in "Advances in Mass Spectroscopy,"and review articles. References in articles cited in these sources were also added when applicable. At present the input is based on searches of *Physics Abstracts*, *Current Contents*, and checks of literature citations. This collection contains about 2000 indexed documents. The ion-molecule bibliography covers the years 1900–1966 and lists about 450 references. Numerical data in this field should be available shortly.

Organization. All numerical and bibliographic information is stored on punched cards, which also contain sorting codes. Answers to inquiries are prepared by selection of cards from the file and printing the information by means of a typewriter controlled by punched cards. Sample output is shown in Figure 2.

COMPARISON

The groups are physically located next to each other. Some of the same scientists search for and analyze papers for both systems. The Kinetics Center provides the clerical services for the Mass Spectrometry Center. The collections overlap in the three areas reviewed to date by the Mass Spectrometry group. The Kinetics Center has larger total holdings in mass spectrometry and related areas (ionization and appearance potentials, ion-molecule reactions, instrumentation, isotope abundances, photoionization) than does the other; but these papers, although indexed, have not been analyzed in detail.

The approach of the two centers to their function of supporting the NSRDS program illustrates the philosophies of operation. The Kinetics Center is a broad-gage project that aims to collect the available current literature in kinetics and then to draw upon this bank to supply authors with most of what they need. It also collects material for them based on their search lists. This is a service function appropriate for a technological field that spans several research disciplines. The Mass Spectrometry Center uses the custom search approach. It selects a topic believed ripe for review, collects the material, codifies it, and then uses the result to persuade the expert that the project is manageable. This is a "forcing" function. It has been successful in bringing about a revision and updating of the compilations on ionization and appearance potentials. The service offered by the Kinetics Center has had a similar effect.

The two centers differ sharply in their approach to literature coverage. The output demands for material for a review in chemical kinetics require input from research papers in several disciplines—*e.g.*, physical and organic chemistry, photochemistry, radiation chemistry, and mass spectrometry. The literature search must be broad, and inevitably, much more material will be put into the system than will be delivered for use. The Mass Spectrometry Center operates with the conviction that certain areas need to be assessed carefully now, that these should be examined in depth and prepared for analysis. In the future, after other prime areas have been so treated, the time will come to update topics treated earlier. This approach appears to be eminently practical for a center with a small, carefully defined scope.

These two attacks lead to different indexing requirements. The Kinetics Center needs to identify a wide range of phenomena studied, many types of quantitative results, and must provide for cataloging and retrieval of a vast number, seemingly unlimited, of compounds and intermediates. The Mass Spectrometry Center's indexing can be limited and closely keyed to each topic examined. Indeed, close definition of the topic eliminates the need for elaborate indexing. This in turn, provides time for data extraction.

GENERAL DISCUSSION

Information systems such as the two discussed here aim to provide a limited body of technical knowledge to the consumer. They hope to offer it in a more palatable form than when it is buried in abstract journals and articles. They also hope to provide only the pertinent material, profiting from direction and control by research scientists familiar with the areas. These features, reduction in bulk, selectivity, and pertinence, appear to be advances over the large, comprehensive abstracting systems. Nevertheless, the question must be asked: Is the result worth the effort?

If, by offering this service, these centers can promote the rapid accumulation of a body of critically evaluated physical data, the answer is yes—relative to the National Standard Reference Data Program. In relation to the general technical community the answer is as yet unknown. The centers are too new for us to be able to tell. Here the determinant is the acceptability of the product. There appears to be only one simple test of this: Is the use of the system increasing, and can the product be obtained more efficiently than by classical means? The evaluation of the answer will, of course, be difficult, but the facts concerning usage, when available, must be displayed prominently in any assessment of modern information systems.

Use also plays another role. Feedback is important for a large system. Critical, contributing, users are needed to keep a system viable.

Priorities for information systems are also important; the effort that can be expended is limited. The Mass Spectrometry Center has settled this matter by a policy of selective, sequential treatment of limited topics. Analogous priorities exist for the broader field of chemical kinetics. These are the topics of the current NSRDS critical review series, which include elementary gas phase reactions, unimolecular reactions, heavy isotope effects, solvent effects, reactions of the nitrogen oxides, and bond dissociation energies. For the larger center, it is merely the method of meeting these priorities (and the anticipated increased tempo of review production) that is different. It is not clear which approach will prove to be more successful.

Efficiency of operation of such systems deserves mention. For the user they are efficient (although they require

a change in work habits). The major part of the work of locating, collecting, and codifying the reference material can be done by clerical personnel. But efficiency can be improved beyond this point. It is suggested that for a field as broad as kinetics the input task can be subdivided by research areas—that is, it could be handled by centers devoted to gas-phase kinetics, photochemistry, solution kinetics, etc. The material collected should then be shared. This approach seems preferable either to strict, exclusive definitions of areas for several centers or to the creation of a central scientific documentation system. Initially, duplication of effort may be severe. Some duplication of effort is advisable—goals are different, material may be missed, correspondence of indexing with need may be minimal. However, the trading of information and mutual evaluation of performance offers the best current route to future reduction of duplicate efforts.

In turn, this plan for information trading makes more important the use of machine-readable records. Their advantage at the collection and proofreading stages is apparent. For transfer they are almost mandatory. Another factor in favor of machine records is that information systems outgrow their techniques; an easy conversion path is needed, or the clerical load becomes unbearable. We believe that any well-tagged set of machine-readable records can be merged or converted more economically than can hand-processed material.

In summary, we have presented two case histories of solutions to the "information explosion." The problems that we have sought to solve have been formulated on the basis of our professional experience in these particular scientific areas. The mechanics of these solutions are not elegant but appear to be both adequate and applicable to a large number of such problems.

LITERATURE CITED

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(2) Wildhack, W. A., Stern, J., Ch. 6, "The Peek-A-Boo System—Optical Coincidence Subject Cards in Information Searching," in "Punched Cards," Casey, Perry, Kent, and Berry, 2nd ed., Reinhold, N. Y.; NBS Tech. News Bull. **45**, 113 (July 1961), "A New Microcite Machine for Large Scale Information Searching."

(3) Field, F. H., Franklin, J. L., "Electron Impact Phenomena," Academic Press, New York, N. Y., 1957.

(4) Kiser, R. W., U. S. Atomic Energy Commission, Office of Technical Information, Report No. T1D-6142, June 30, 1960, and Suppl. June 20, 1962, "Tables of Ionization Potentials."

The Radiation Chemistry Data Center*

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Received November 7, 1966

All possible sources of data from radiation chemistry are being collected. The information is indexed by keywords, and the numerical values reported for measurements of chemical and physical properties of the irradiated systems are recorded. The data file is now a manual operation but future plans include the transfer of data to machine-searchable form.

The Radiation Chemistry Data Center is a specialized data center under the chemical kinetics program of the National Standard Reference Data System, and is supported jointly by the Division of Technical Information of the Atomic Energy Commission and the National Bureau of Standards. Radiation chemistry data include rates of elementary processes and yields of products and intermediates formed by the action of ionizing radiation on definable chemical systems. Radiation chemistry may involve experimental measurements of various properties of irradiated chemical systems and deduction of reaction mechanisms, or may be a theoretical study of model irradiated systems.

The Radiation Chemistry Data Center was established for the purpose of bringing together all information on radiation chemistry and providing a means of making selected and evaluated data readily available to scientists throughout the world. One of its main objectives is to act in a service capacity to radiation chemists. There is an urgent need for critical reviews and there are experts in many laboratories uniquely qualified to make the

* 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 Radiation Laboratory of the University of Notre Dame is operated under contract with the U. S. Atomic Energy Commission. This is A.E.C. Document No. COO-38-518.