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.

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The Radiation Chemistry Data Center*

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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

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reviews. But in most cases these scientists cannot spare the time to search the literature, obtain the papers, and organize and tabulate the data therefrom, before undertaking the truly scientific task of evaluation and critical review.

The Data Center will take over the preliminary tasks and will provide bibliographies and tabulated data to individuals or groups who are able to contribute their talents to the evaluation of the data. The evaluated data will be made available either by publication, under the authorship of the experts who have reviewed it, or on request in answer to specific inquiries that come to the Center.

Scientists often review data; the first step is to compile all the published values and methods by which they were obtained. The scientist must then evaluate the published values and select the best value. Hopefully, his selection will be made available to others. All too often, the individual scientist's efforts have remained in his own file. Data centers must make themselves well-known to all potential users, so that they can help the individual reviewer by providing the initial compilations of data from the literature, or at least the references. The data centers should then receive the critical evaluations as input for their systems, as well as assist with publication of selected data. The data centers must be more than clearinghouses for such occasional efforts; they must persuade the experts to carry out evaluations and critical reviews in the fields where they are most competent.

It is impossible to draw sharp lines to encompass the interests of radiation chemists; other groups under the National Standard Reference Data Program are compiling and evaluating data in related fields which are very important to radiation chemists, such as mass spectrometry, gas and solution kinetics, and molecular spectroscopy. The cooperation between data centers or individual scientists undertaking compilations is essential. Good communications with other centers are valuable in extending the range of service which can be provided by any one center. The ultimate goal of a nationwide network for rapid communication between data and information centers, libraries, and individuals deserves our best efforts toward its implementation.

RADIATION CHEMISTRY LITERATURE

The published literature which contains radiation chemistry information is estimated to amount to a current yearly accumulation of about 1000 papers, reports, theses, etc. Its growth has been fairly recent; only a few papers per year appeared on the subject prior to the early 1950's. The Radiation Chemistry Data Center will record all the useful data from that literature, and store the references and data so that they can be made quickly available, and arrange for evaluation and dissemination of selected data. The literature is acquired by scanning journals, abstracts, and lists of publications from major laboratories carrying on radiation chemistry research, and by receipt of reports and reprints directly from many individuals and organizations. The selection of items from which data are to be stored is made by an experienced scientist on the staff. The bibliographic description will be stored on magnetic tape and programs written to search for authors, reference, year, laboratory, language, report number, and secondary references.

KEYWORD INDEX

Papers are indexed by keywords so that general information such as review articles, papers on methods, theory, etc. can be found; the keywords will be stored on magnetic tape along with the bibliographic description. The authors' assistance in choosing appropriate keywords for their papers is solicited whenever possible. Arrangements with several groups in foreign countries have been made whereby they send to the Radiation Chemistry Data Center their reprints on radiation chemistry together with a list of keywords which they have selected.

There is a gradually increasing acceptance of the idea of publishing indexing terms with the journal articles or technical report. In many domestic journals the abstracts and titles which authors provide for their papers have become much more informative during the last few years. The improvements have come about primarily through the insistence of journal editors. Some journals also require submission of a selection of keywords or other indexing aids by the author to assist in categorizing the information in the paper. In one case the authors provide a concise description of all properties measured (*1*). The information and data centers may encourage publication of author-aided indexing terms but the responsibility for instituting and enforcing such a requirement will be with the publishing media.

Publication of index terms should be of value to current awareness journals (in which the papers are listed by category), abstracting journals, information centers, and data centers. From the point of view of the data center, general categories would be useful, but so also would be the specific types of data reported. For example, a specific property such as extinction coefficient or half-life of a particular intermediate might be an appropriate indexing term; such information might not have been included in the abstract.

RADIATION CHEMISTRY DATA FILE

The keyword index will provide for the person seeking general information. Much more detailed information will be included in the radiation chemistry data file (Figure 1). The data file will be searchable and will contain specific terms describing the irradiated chemical system and the results of the measurements which were made.

Chemical compounds of all types have been irradiated. The compounds have been studied in many physical states: gaseous; liquid; aqueous or nonaqueous solutions; crystalline; glassy; gas or liquid adsorbed on a solid; or colloidal. The products and intermediates of the radiation-induced reactions include not only neutral molecules, but also atoms, ions, or radicals in the ground state, or any of these species in an excited state. Reactants and products range from the simplest molecules, such as H_2, to polyfunctional organic compounds. The data file of chemical species will include not only molecular formulas and chemical names, but also the designation of such characteristics

BIBLIOGRAPHIC DESCRIPTION

KEYWORDS

SECONDARY REFERENCES

DATA:

Chemical System
- State
- Temperature
- Pressure
- pH
- Concentration

Source
- Radiation
- Energy
- Dose and dose rate

Intermediates and Products

Elementary processes

Chemical and physical properties

Figure 1. Information included in the radiation chemistry data file.

as charge and electronic state. Certain structural information can be obtained from searching the molecular formulas and charge type. Also, a limited number of descriptors, such as heterocyclic, three-membered ring, steroid, will be used in the chemical data file to make it possible to search for certain structural features. However, it is not planned to attempt detailed structure searches.

The elementary processes for which specific rates or other data have been reported will be included, and also to a limited extent, reactions which are postulated to occur but for which no data are reported. In searching for elementary processes all the reacting species and products must be represented by identifiable formulas and a useful method must be found for classifying the reactions. Each species must be distinguishable from all others, including the designation of charge state, excitation state, oxidation state, isotopic substitution, and atomic, spatial, and electronic arrangement to the extent that they have been reported. A machine-searchable file of elementary processes will be useful to scientists studying reaction mechanisms. Searches for a particular reaction have heretofore ranged from difficult to impossible. We plan to make it possible to search for a particular reaction, or a particular reaction type, such as the example in Figure 2.

Reaction type: $A\cdot + BH \longrightarrow AH + B\cdot$
Hydrogen abstraction

Reaction: $\cdot OH + CH_3COOH \longrightarrow H_2O + \cdot CH_2COOH$

Figure 2. Searching elementary processes.

No data have yet been stored on tape, pending the acquisition of an input device and printer with an expanded character set including super- and subscripts and other essential symbols. A card file containing extracted data is being created in the following way. Current papers are read by staff scientists and all data within our scope are recorded on data cards or worksheets. Radiation yields (G) of products from a particular system are recorded on cards and filed by main reactant. Specific rates for elementary processes are recorded on cards which are filed by reaction. The chemical system is described along with other parameters such as temperature, radiation, and method of measurement. Activation energy and frequency factor are also recorded. Other data for products of radiation reactions, such as absorption bands, emission bands, half-life, ion mobility, etc., are recorded on a worksheet for eventual inclusion in the data file along with the information on the cards.

SOURCES OF ERROR

The problem of recording errors, whether systematic or simply typographic, is acute (2). Chemical kinetic data are subject to sizeable errors. It is extremely helpful when the authors estimate the error range for a particular value. Lacking an actual estimate, a listing of probable sources of error is helpful for the compiler-reviewer. It is the author's responsibility to give as completely as possible any information he can provide on the reliability of his data (especially when a new method is used), and to state any assumptions made in obtaining the numerical data he reports.

The restrictions on authors imposed by space limitations preclude the publication of all data and complete descriptions of methods. However, the necessity for brevity in published papers should not excuse the presentation of an incomplete or biased description and interpretation of results. In many cases the compiler will need to obtain further information from the author. It is hoped that the originally measured numerical values will be available when necessary. Specialized data centers may be suitable repositories for fragmentary or extensive tables of numerical data unsuitable for publication.

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