

plexes. The relative swing from *Acta Cryst.* to chemical journals is presumably influenced by a recent change in the nature of organic crystallography. Nowadays, fast computers and powerful structure-solving techniques have created a situation where many crystal structure analyses are only part of a more comprehensive study. Thus, the emphasis is shifting from the crystallographic to the chemical nature of the problem.

FUTURE DEVELOPMENTS

The development projects in which the Centre is actively engaged come under three categories:

- (a) Input
- (b) Substructure Search
- (c) Data Base Extension

Input. From economic and other considerations, it would be advantageous if optical character recognition (OCR) could be utilized for input to the files. Trials have been conducted using Scan Data hardware to read bibliographic records, and these tests have been highly satisfactory. Over the next few months, it is intended to input material both by OCR and punched cards and switch entirely to the former as soon as the system is fully tested.

Substructure Search. As indicated earlier, certain search queries are not easily answered in terms of our classification scheme, and a deeper search capability is obviously needed. To this end, we are at present examining the possibility of encoding compounds in the Wiswesser Line Notation (WLN) and in the form of connection tables. Because of the wide range of compounds in our file, the WLN approach presents many problems in areas where rules have not yet been formalized.

Data Base Extension. The data base is being extended to cover molecular structures determined in the gas phase. A file is currently being set up to include structures studied by microwave and gas-phase electron diffraction studies. The first output from this file will be a bibliography, and it is planned to publish this as part of the series "Molecular Structures and Dimensions."

The data base is also being extended to protein structures, and the establishment of a Protein Data Bank has just been announced.⁶

ACKNOWLEDGMENT

We thank the Office for Scientific and Technical Information for their support of the activities of the Crystallographic Data Centre and individual staff members for their advice and helpful discussion. Space for the Centre was provided by Cambridge University and computing facilities by the Institute of Theoretical Astronomy. We are grateful to INSPEC and especially to P. Simmons for the use of their computer typesetting program. We thank R. S. Cahn and the Nomenclature Division of the Chemical Abstracts Service for advice on nomenclature, also P. Baker and his colleagues at ICI Pharmaceuticals Division for their assistance with the WLN system.

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SSIE—An Information Center Which Stores Foresight*

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Received November 11, 1971

In June 1971, the Smithsonian Science Information Exchange (SSIE) adopted the fourth official name it has borne in its 22-year history. These changes in name have been made to reflect expansions in the Exchange's coverage of subject matter or changes in administrative or fiscal structure. During this same period, the Exchange's methods of operation have undergone improvement and modernization, and it now has a much wider spectrum of services to offer the scientific and engineering community than ever before. The new, nonprofit organizational structure now in effect is shown in Figure 1.

*Presented at the American Chemical Society Northeast Regional Meeting, Buffalo, N. Y., October 12, 1971.

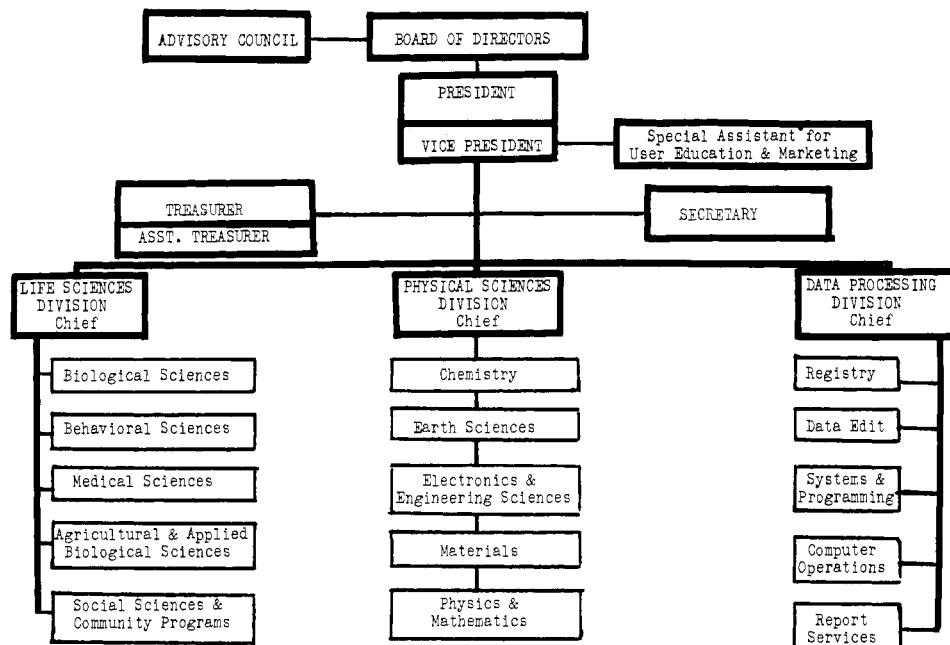
Since its founding in 1949, the SSIE and its predecessor organizations have been working in a unique field of information dissemination. The primary mission of the Exchange is to facilitate more effective planning, management, and coordination of the scientific research and development sponsored or supported by U.S. Government agencies. This is done by:

Developing and maintaining an up-to-date, comprehensive inventory of all types of ongoing, unclassified research projects.

Providing means and services to assist research and development administrators and other research and development personnel in obtaining and using the information stored.

The Smithsonian Science Information Exchange (SSIE) is the only single source that chemists and chemical engineers can turn to for information on 80,000 to 100,000 research projects annually which are still in progress and thus not yet published. SSIE operations have become increasingly automated, its range of services has been expanded, and more people than ever before have complete access to its file of information. But its basic mission has remained unchanged: to store and retrieve information about ongoing research projects as early as possible *before* they are completed and published. To do this, many thousands of projects are being registered, indexed, and computer-stored as they are received from hundreds of cooperating sources of support.

Figure 1. Organizational chart of Smithsonian Science Information Exchange, Inc.



Thus is the case of any ongoing research activity, although few if any results have been obtained, and no publications have emanated from the work, it may nevertheless be possible through SSIE to ascertain the direction and goals of the project, to learn who is supporting it, the name of the principal investigator, and where the work is being done. Thus if a paper in a journal or one presented at a meeting can be considered primary publication, then SSIE's information is available at a "preprimary" stage. The Exchange might justly be called "The Information Center Which Stores Foresight," since most other sources can store only hindsight—that is, information on projects which have already been published. Figure 2 illustrates a typical Notice of Research Project, SSIE's documentary way of presenting the data elements available.

The purposes of this early-bird assemblage of information are many and varied. The first and foremost function of SSIE's data bank has been to help Federal agencies to keep track of the projects under way in a given field, so as to aid in preventing unknowing duplication of effort. Granting agencies, both Federal and private, have been enabled to keep tabs on their own programs, which are frequently so massive as to require computerized access. The services provided by the Exchange were at first used primarily by Federal government agencies; some of the services were formerly not available at all to private requesters. But in the past few years, not only have all existing services been made available to any requester, but the number and variety of information products and services have been increased. Some of these innovations are mentioned later in this paper.

Since the Exchange is the National Registry of Research in Progress, it has comprehensive input on ongoing research information from every Federal agency with a research program of significant size, plus input from numerous foundations, universities, state and municipal agencies, some private companies and a few foreign sources. Of special interest in chemistry, for example, projects are registered from the Petroleum Research Fund and the Robert Welch Foundation. Altogether, the Exchange has been registering and storing between 80,000 and 100,000 project summaries annually, from the many different research-supporting organizations which cooperate with SSIE. With so many projects coming into SSIE throughout the year in every field, it is often surprising to find just how many different organizations are supporting research on a specified subject. As an example of this, the results of an actual request topic which SSIE's staff worked on recently are tabulated in Figure 3. In this case SSIE, retrieved more than the average number of project summaries, a total of over 500. If the requester had *not* come to SSIE for this information, but had instead dealt directly with the individual supporting organizations, he would have had quite a task. It would have been necessary to deal with 21 bureaus of 11 Federal agencies, plus 26 non-Federal organizations! Not surprisingly, the Environmental Protection Agency and the Interior Department support many projects in this field. But to obtain their project information alone would mean *missing more than half* of the ongoing work registered at SSIE.

The increasing scope of the Exchange's coverage can be seen in Figure 4, where the growth of holdings is shown

SSIE—AN INFORMATION CENTER WHICH STORES FORESIGHT

SCIENCE INFORMATION EXCHANGE SMITHSONIAN INSTITUTION 1730 M STREET, N.W. PHONE 202 381 5311 WASHINGTON, D.C. 20036		SIE NO GFP-1354-2
NOTICE OF RESEARCH PROJECT		
SUPPORTING AGENCY ATOMIC ENERGY COMMISSION RESEARCH DIVISION	AGENCY NUMBER(S) CONTRACT AT (04-3)-326, #28	
TITLE OF PROJECT NITRIDE FORMING REACTIONS IN LIQUID URANIUM ALLOYS		
PRINCIPAL INVESTIGATOR, ASSOCIATES AND DEPARTMENT(S) SPECIALTY: PROP NA PARLEE MINERAL ENGINEERING RN ANDERSON		
RECOMMENDATION STANFORD UNIVERSITY SCHOOL OF EARTH SCIENCES PALO ALTO - STANFORD, CALIFORNIA 94305		
PERIOD FOR THIS WORK 6/71 TO 5/72 FY71 FUNDS \$11,872		
SUMMARY OF PROJECT <p>The kinetics of UN and U sub 2 N sub 3 forming reactions in liquid uranium-tin alloys are being experimentally studied using a Sieverts type apparatus to measure the pressure and quantity of absorbed nitrogen. The physical characteristics of the nitride precipitate formed in the liquid are being studied to elucidate the cause of the hysteresis found in the reaction; 2U plus 3/2N sub 2 (g) equals U sub 2 N sub 3 (s) which occurs in the 600-1500 degrees C temperature range. This hysteresis is not observed in the reaction; U plus 1/2 N sub 2 (g) equals UN (s) which has been investigated in the 1500-1600 degrees C temperature range.</p> <p>To complete the basic thermodynamic study, the formation of UN at higher alloy concentrations than 18% uranium (by weight) and higher temperatures than 1600 degrees C is being investigated. The thermodynamics of nitride precipitation of uranium-tin alloys in the presence of such nitride formers as Zr, Nb, Ta and Th are being investigated to provide information on the potential of the nitride reactions as a metallurgical separation process. Solvents other than tin are being studied.</p> <p>Results: The thermodynamics of reactions of nitrogen with liquid uranium-tin alloys have been considerably elucidated for U sub 2 N sub 3 and UN. The equilibrium constants, interaction parameters, and activities of uranium in liquid tin have been determined.</p> <p>The low temperature kinetics of U sub 2 N sub 3 formation have been considerably investigated.</p>		
SUMMARY		

Figure 2. A typical notice of research project

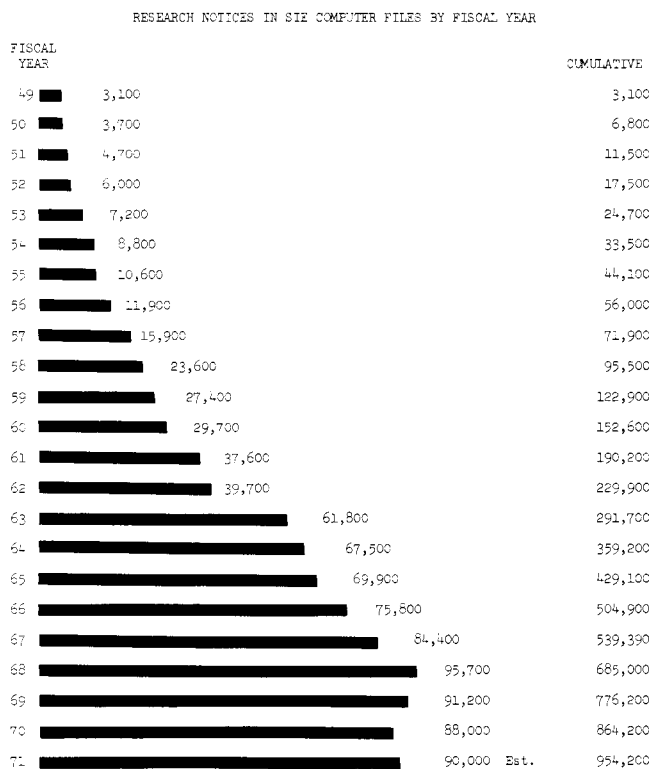


Figure 4. Growth of SSIE holdings

Subject Request #3351—Instrumentation for Pollutant Measurements

507 Projects Retrieved

Federally Supported	No. Projects	Non-Federally Supported	No. Projects
Dept. of Interior (7 Bureaus)	156	Universities (7)	12
Environmental Protection Agency	82	State Governments (12)	15
Dept. of Health, Education & Welfare	56	Private Companies (4)	4
National Science Foundation	38	Foreign Organizations (3)	17
Dept. of Defense (3 services plus ARPA)	37	No Formal Support Reported	5
Atomic Energy Commission	26	Total, 26 Non-Federal Sources	53
National Aeronautics & Space Adm.	20		
Dept. of Commerce (4 Bureaus)	20		
Dept. of Transportation	2		
Dept. of Justice*	1		
Total, 11 Federal Agencies	454		

* For detecting heroin in presence of other pollutants.

Figure 3. Tabulated results of a subject request

since 1949. At this time, almost a million projects have been registered at the Exchange during the years of its existence.

To cope with this mass of ever-changing information, SSIE's system has been improved by the addition of on-line video terminals and a high-capacity data cell. SSIE's man-machine system works to utilize this equipment while still providing requesters with scientist-to-scientist communication. The computer search strategy for each question asked of SSIE is formulated by a scientific staff member and each outgoing package of search results receives the scrutiny of an engineer, a chemist or another scientist

in the appropriate field. This system is working well, and further improvements on it are anticipated in the future.

Another change instituted is the storage of all project information, including text, on the computer, so that it is no longer necessary to maintain hard-copy files to answer requests. This has resulted in better legibility and faster response time—as well as in a significant reduction of floor space at SSIE.

Screening of the computer output is now performed only when the SSIE scientific staff deems it necessary; it is then done without extra charge. This procedure yields some time-saving and helps to keep down costs.

All registered project Notices are now available to requesters from any country; certain Notices were previously limited to distribution within the United States only. Perhaps this is one reason that, in the past year there has been an increase in the number of foreign requesters who are making use of SSIE services. The Exchange has also been in negotiation with several overseas organizations who wish to act as intermediaries, or wholesalers, in helping to make SSIE services more readily available abroad. In some of these countries such as England and Czechoslovakia there are information centers interested in having magnetic tapes transferred periodically from SSIE to them. These promising possibilities are being actively explored, while SSIE is simultaneously serving individual requesters in these countries. In Japan and France, SSIE services are made available through contractual intermediary organizations.

The Exchange updates its computer facilities from time to time as better hardware becomes available. The next major improvement in this respect is scheduled for Fiscal Year 1973, when it is planned to replace the present IBM 360/40 with the IBM 370/135. The new machine will be a slightly lower cost one, with 200,000,000 additional bytes of random storage over the present equipment.

The Exchange is also studying the possibility of adding systems which will permit frequent users to search all or part of SSIE's records at their own installation. Implementation of such systems will depend on the funding made available.

Among the products and services of special usefulness to chemists and engineers, two might be mentioned in some detail. First, a chemical company, university, or laboratory interested in polymer syntheses on a continuing or long-range basis, for example, can subscribe to SSIE's selective dissemination service. In this way the concerned staff members can keep up-to-date automatically on the projects in that field, as they are received and registered at SSIE. Planning executives and researchers alike can benefit from this regularly-updated "profile of interest" mailing. Company and agency libraries can handle the accessions in a way very similar to any journal subscription. SSIE has recently begun offering this current awareness facility on a monthly plan to those who need that frequency, but most requesters still prefer a quarterly updating.

The SSIE results for each quarter can be routed to all the chemists and engineers in that laboratory who have an interest in that particular subject matter. The initial search in such a quarterly series includes all of the relevant research summaries thus far accumulated during the two current fiscal years. Subsequent mailings include only the summaries received during the latest three months.

A one-time search at SSIE would provide exactly the same results as an initial search in a quarterly series. But if the one-time search were to be requested a *second* time a few months later, many of the same project summaries would be retrieved as before, rather than just the newly-registered summaries. Thus the one-time search is more useful in special circumstances such as when a literature search is made just prior to beginning a new project of

limited duration. As indicated before, granting agencies also sometimes make one-time subject searches at SSIE before giving final approval to grant applications.

Below are listed some examples of requests which might be suitable for either single-time searches or quarterly-updated searches, depending on the short-term or continuing needs of the requester. The first three topics listed involve only scientific subject matter, while the others also include search parameters such as location or supporting organizations. Thus the latter are called subject-administrative questions. Both types are handled the same way on SSIE's computer.

Examples of topics searched:

1. Mechanisms and Kinetics in Radiation Induced Polymerization Reactions
2. Reverse Osmosis and Electrodialysis in Desalination Processes
3. X-Ray Fluorescence Spectroscopy in Chemical and Physical Analysis
4. Air Pollution Studies Active in the State of California During FY 1971
5. Organic Chemistry Research Tabulated by Agency Support
6. A List of Current Research in all Aspects of Energy Conversion Which Identifies the Source of Support in A Certain Geographical Area

Because of the variety of question types which can be handled, SSIE services find application from the inception of a project on into the marketing stage. Among the uses which are being made by chemists and engineers of SSIE computer files, these should be noted:

1. For current awareness and to help avoid unknowing duplication of effort
2. To help prepare proposals for grants or contracts, and to aid in finding possible sources of grant support
3. To compile invitation lists for symposia and conferences and to identify prospective discussion leaders
4. To aid in planning visits and tours by foreign scientists
5. To learn what a certain investigator is working on, or what work is being done in a certain laboratory
6. Bibliographic leads
7. To compare and coordinate projects and programs among agencies with overlapping interests
8. To aid in locating consultants
9. To compile market research information

All these are actual uses which have been made of SSIE services by individuals as well as by large and small organizations.

In addition, such services and products as magnetic tape interchanges, catalog preparation, and specially-negotiated tabulations arranged by location, supporting agency, or other parameters, which are of interest mainly to associations, government agencies, and some private companies, are also available to any requester.