

## The Journal for Chemical Information and Computer Scientists: A 25-Year Perspective

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How this Journal came to be and its evolutionary nature over the years are reviewed.

The introduction in 1961 of the *Journal of Chemical Documentation* by the American Chemical Society was a great moment in the evolving history of chemical information science and of chemical computer science. Since 1961, this Journal has served as the primary medium for the publication of papers that advance the art and science of these two disciplines of chemistry. Its achievement of 25 years of progressive growth and worldwide stature provides an auspicious opportunity to commemorate how it came about and what it came to be.

Four elements that characterize a scientific discipline are as follows: (1) a body of scientists engaged actively in the discipline, (2) a forum for the presentation of papers and interaction among the scientists, (3) a journal for the publication of papers that advance the scientific discipline, and (4) roots in the educational structure.

These four elements are historically continuous in which the first must occur before the second can materialize, then the third, and finally the fourth. Until well into the 20th century, information science was not a separate subject of interest in the historical evolution of chemistry. Systems and devices were developed, however, for collating, retrieving, interpreting, relating, and communicating the results of experimentation and scholarship. Such activities were an integral part of what most chemists did but in which only a very few specialized.

As chemistry slowly evolved during the 19th and into the 20th centuries toward becoming a science, a profession, an educational curriculum, and an industry, chemists directed considerable attention to areas we now call chemical information science. Along with their active roles in shaping chemistry into a discipline of science, these chemists laid the foundation for communication channels, most particularly with journals, education, and chemical societies, and for the development of a framework of paradigms, such as nomenclature, symbols, formulas, classification systems, indexing systems, and abstracting protocols. In retrospect, as they made the literature, they systematized it. Some who played an important role in the development of our paradigms were Lavoisier in nomenclature, Dalton for his atomic theory, Berzelius for symbols, formulas, and nomenclature, Gmelin for the inorganic "Handbuch", Beilstein for the organic "Handbuch", Kekule for tetravalent carbon and hexagonal benzene, Mendeleev for the periodic table, Remsen for *American Chemical Journal*, Gibbs for thermodynamics concepts, Fechner for *Chemisches Zentralblatt*, and Noyes for *Chemical Abstracts*.

Each of the above, among others, is a hero in chemistry. Yet the fame for most rests on accomplishments from their mastery of the information and knowledge of the chemical literature known during their scientific careers. Several of the above, but not all, made notable contributions from their experimental work. It would not be amiss, nor a case of hubris, for chemical information scientists to view them as their heroes and to emulate them.



Herman Skolnik has had a wide-ranging career as a chemical engineer, analytical chemist, organic chemist, and chemical information scientist. He was the major factor in the introduction of this Journal by the ACS in 1961, for which he served as editor for 22.5 years, and in the introduction of *Documentation Abstracts* (later *Information Science Abstracts*) in 1966, for which he served as its first chairman of the board. He was an abstractor for *Chemical Abstracts* (1946-1960) and has been Editor of its Terpenes Section since 1959. He obtained his B.S. in chemical engineering from Pennsylvania State University and his Ph.D. in organic chemistry from the University of Pennsylvania. He joined Hercules Inc. in 1942 as a research chemist and was appointed Supervisor, Literature Research Group, in 1947 and Manager of the Technical Information Division in 1952, the position he held until he retired in 1979. He has presented over 100 papers and chaired many symposia in 10 ACS divisions and has authored four books and over 200 papers in some 20 scientific journals. He has been the recipient of several awards, most notably the Patterson-Crane award and the ACS Division of Chemical Information award, which is named the Herman Skolnik award in his honor.

Segmentation of chemistry into disciplines of inorganic, organic, analytical, and physical occurred in the second half of the 19th century. With the rapid growth of the chemical industry during the 20th century, and especially since 1940, the increasing number of chemists needed to sustain the growth, and the phenomenal expansion of the chemical literature, segmentation of chemistry into new disciplines was further accelerated. Chemical information science, which emerged in the 1940s, was one of these new disciplines.

Actually, chemical information science became a segmented discipline of chemistry within the chemical industry as research and development programs became an integral part of the industrial complex in the early 1900s. By the 1940s, many chemists with unique skills and talents were employed in the chemical industry as editors, writers, translators, abstractors, indexers, literature searchers, and others. These people were called literature chemists, patent chemists, and library chemists. They were educated and trained as chemists, and gen-

erally their first industrial assignments were in the laboratory where their unique skills and talents were discovered and then transferred to assignments in which they functioned as chemical information scientists. They thought of themselves as chemists and as doing chemistry just as did those listed above. Indeed, from the time chemistry emerged as a science, all professional chemists devoted energies in several areas of what we today call chemical information science. Furthermore, by the 1940s there were several thousands chemists who were engaged full time in this phase of chemistry. These chemists, however, were a disparate community of individuals.

Papers on various aspects of the chemical literature were presented at ACS national meetings from almost the very beginning. In 1893, bibliography was one of nine groups of papers in the World's Congress of Chemistry cosponsored by the ACS. The first symposium in an area of chemical literature presented at an ACS national meeting was on "Chemical Libraries and Their Problems" at Buffalo, NY, April 1919. Thereafter, papers and symposia in chemical information science were presented at many ACS national meetings. One of the more significant papers was entitled "Problems of the Scientific Literature Survey" presented by G. Egloff, M. Alexander, and P. M. Van Arsdell at the Detroit ACS 1940 Spring national meeting in the Division of Chemical Education. The significance of this paper, which enjoyed a high attendance, was that it motivated a group in the audience to get together to plan for the 1943 Fall meeting a symposium on "Technical Library Techniques" under the leadership of N. C. Hill and the blessings of the Division of Chemical Education's executive committee. This well-attended symposium led to the formation of the Chemical Literature Group of the Division of Chemical Education.

This new group engineered well-attended programs and was rewarded by the ACS Council with divisional status beginning in 1949, becoming the 19th ACS division. The advent of the Division of Chemical Literature made possible for the first time a community of chemists with shared interests and objectives and a forum for the presentation of papers in chemical information science. With the papers presented by members of this community of chemists there evolved responsible authorities in various areas of chemical information science and an important body of technical papers.

Although 63% of the 149 papers presented before the Chemical Literature Group from 1943 to the end of 1948 was published, the publications were dispersed among numerous journals and books. For the 12-year period, 1949 to the end of 1960, only 36% of the 1013 papers presented before the Division of Chemical Literature was published in over 25 different journals and 12 books (Table I).

Quite a few ACS divisions have been concerned with the dispersal of their published papers among many journals, especially among those that are not related to the scientific and technical interests of their members. Five divisions, consequently, have opted for preprints for their papers in the absence of a proper publication medium. Impetus to the ACS for expansion of its stable of journals has come from several divisions not served adequately nor specifically by existing journals. This was the approach taken by the Division of Chemical Literature and its Publication Committee beginning in 1955, and which culminated in the introduction of this Journal by the ACS in 1961.

On launching this Journal, we estimated and hoped for a minimum of 1000 subscribers by the end of the first year. To keep the potential deficit as low as possible, we decided to have two issues per year. By the time we put out the second issue of Volume 1, the number of subscriptions exceeded 1500. The Journal not only could be published on a financially sound basis for the two issues planned but could be expanded to three issues

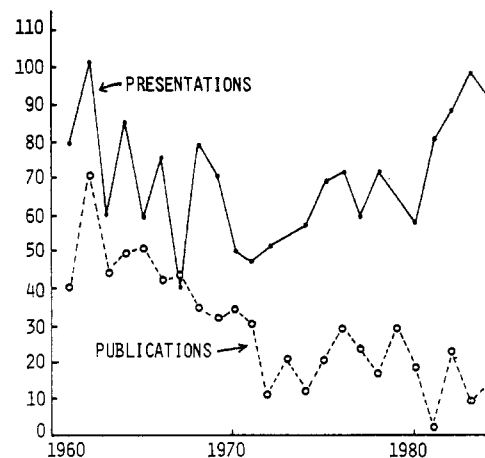


Figure 1. Number of DCI papers published in JCICS vs. DCI papers presented from 1960 to 1984.

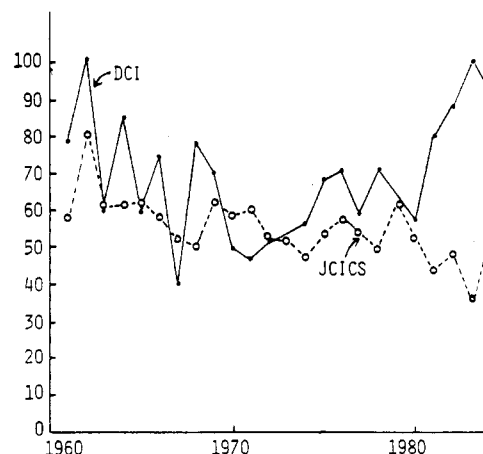


Figure 2. Number of DCI papers presented vs. total papers published in JCICS from 1960 to 1984.

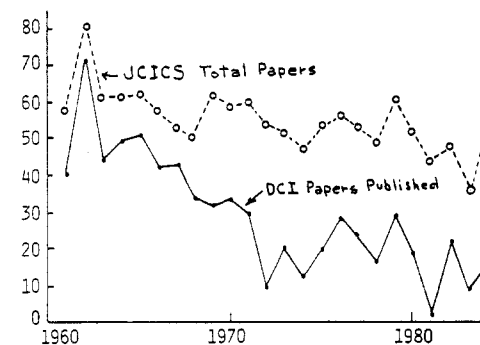


Figure 3. Number of DCI papers published in JCICS vs. total papers published in JCICS from 1960 to 1984.

for the introductory year, a rare event for a new journal, and to four issues per year thereafter. This was fortunate as the flow of good papers through the peer review system was such that we needed the four issues to handle the demand.

A total of 59 papers was published in the three issues of the first volume, of which 40 had been presented in Division of Chemical Literature programs, one as early as 1950. In the second volume, 71 of the 81 papers published had been presented in the division's programs. Until 1971, a relatively high percentage of the papers from the divisional programs was published in this Journal (Figure 1). Thereafter, the number of divisional presentations published dropped precipitously. As shown in Figure 2, the number of papers presented in the divisional programs far exceeded, except for a few years, the number of papers published in this Journal from all sources.

Table I. DCI Papers: Presented vs. Published

publication	presentation period			
	1943-1960		1961-1964	
	presented	published	presented	published
<b>books</b>				
ACS <i>Advances in Chemistry</i>				
No. 4 (1951), "Library Techniques"		25		
No. 30 (1961), "Library Techniques"		36		
No. 8 (1953), "Nomenclature"		13		
No. 10 (1954), "Market Literature Sources"		59		
No. 16 (1956), "Pharmaceutical & Medical Literature"		25		
No. 17 (1956), "Training Literature Chemists"		7		
No. 20 (1958), "Petroleum Literature"		22		
No. 46 (1964), "Patents"		4		
"Punched Cards"; Casey and Perry (1951)		4		
"Information Processing Equipment"; Doss (1955)		9		
"Technical Editing"; Weil (1958)		17		
"Advances" in Documentation and Library Science"; (1956)		13		
<b>Journals</b>				
<i>Journal of Chemical Documentation</i>		44		194
<i>Journal of Chemical Education</i>		82		
<i>Chemical &amp; Engineering News</i>		23		
<i>Industrial and Engineering Chemistry</i>		17		
<i>American Documentation</i>		16		1
<i>Tappi</i>		31		3
23 other journals		31		3
<b>total</b>	<b>1162</b>	<b>455</b>	<b>334</b>	<b>198</b>

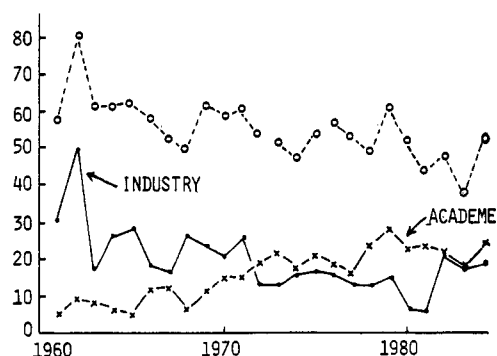


Figure 4. Sources of papers published in JCICS from 1960 to 1984: industry vs. academe.

The effect of this downward trend is shown in Figure 3.

Whereas the impetus for the introduction of this Journal came from the Division of Chemical Literature, papers presented in its programs over the past decade no longer dominate the contents of this Journal, despite the fact that the number of papers presented in the division has been maintained at a high level.

In harmony with the increasing number of papers received and published that were concerned with computers and with the formation in 1974 of the ACS Division of Computers in Chemistry, the name of this Journal was changed in 1975 from *Journal of Chemical Documentation* to *Journal of Chemical Information and Computer Sciences*. Also, in 1975, the Division of Chemical Literature changed its name to Division of Chemical Information to reflect the increasing involvement of its members with computer operations. Although the Division of Computers in Chemistry has had programs in ACS national meetings, the majority of papers from these programs have not been submitted to this Journal. Most have been in the *ACS Symposium Series*. Members of the division have been submitting papers not given at any meeting.

Inasmuch as the great majority of the members of the Division of Chemical Information are employed in the chemical industry, it is not surprising that this became the major source for papers presented and published. As shown in Figure 4, since 1972, papers from academe took over as the primary source. Many of the papers from academe have been in the

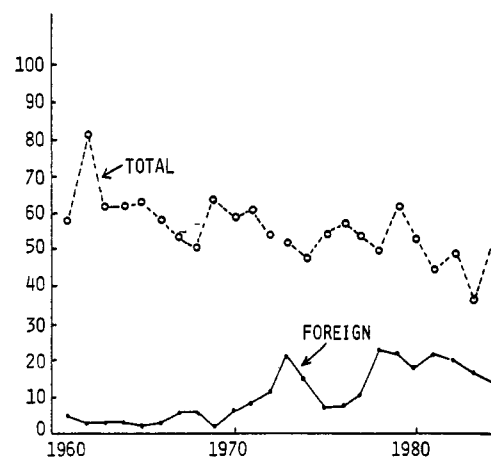


Figure 5. Number of non-U.S. papers published in JCICS from 1960 to 1984.

area of computer science. With the journal's change of name, the subject content of the published papers became about equally divided between chemical information science and computer science. Also, members of the Advisory Board were appointed equally from the two disciplines of chemistry.

Two other significant changes occurred. Almost from the very beginning, this Journal attracted papers from those written specifically for publication with no association with a previous scientific or technical meeting. Since the 1970s, these papers accounted for between 30% and 55% of the total papers published in this Journal. Also beginning in the 1970s was the relatively large number of papers from 15 different nations—these papers in recent years have accounted for close to 50% of the total papers published (Figure 5).

Although a symbiotic relationship exists with the ACS Divisions of Chemical Information and Computers in Chemistry, this Journal has become the international medium for the best papers in chemical information science and computer science. As long as these two disciplines of chemistry flourish, this Journal should continue to be their premier communication medium on which succeeding generations will build their knowledge base.

This Journal has played an important experimental role for the ACS Journals Department's research and development

programs in new publication methods. From the very beginning, Volume I was offset printed without right justification. Although this typography had general acceptance, feedback was such as to prompt a change to photocomposition for Volume II with right justification for aesthetic reasons. In researching computer-assisted photocomposition by the ACS Publications Research and Development Group, four papers in the November 1965 issue were processed via computer and offset printing. In 1966, this Journal became the first to be produced by computer-assisted photocomposition. By 1976 all ACS publications were computer-assisted photocomposed.

Author and subject indexes for the 1969 issues were computer processed by A. E. Petrarca and W. M. Lay, Department of Computer and Information Science, Ohio State University, by a modified version of the Double-KWIC Coordinate Index. In the mid-1970s, annual author and keyword subject indexes have been produced by CAS from its computer data bank of journal articles.

It has been a great privilege to serve as this Journal's editor for its first 22.5 years. From my perspective, I see a great future for it and for those who practice the art and science of the two disciplines of chemistry this Journal serves.

## Computer Hardware and Software in Chemical Information Processing<sup>†</sup>

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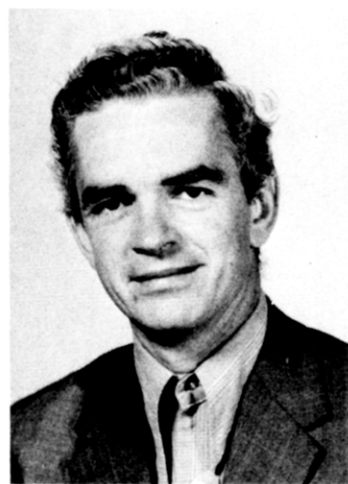
This paper examines the progress of chemists in using computer systems (hardware and software) to sustain, expand, and manage what is perhaps the world's most successful information distribution system, albeit one of many parts. Beginning with the days before stored-program computers—the "mechanization" era—this paper presents an overview of developments in computing and the application of computer and related technology to the handling of chemical information.

### INTRODUCTION

The field of chemistry is blessed with perhaps the most comprehensive record of progress of any field of scientific endeavor. Chemists have always been in the van in respect to development and application of modern techniques and technologies for organization and management of chemical information. From the development of regularly published journals (e.g., *Philosophical Transactions of the Royal Society*, 1665), to present-day on-line retrieval systems, chemists have been instrumental in developing, adapting, and using a wide range of techniques and technologies to help facilitate the process of discovery and practice in chemistry and allied fields.

The purpose of this paper is to provide a brief glimpse of the progress chemists have made in handling chemical information during just the past 40-50 years. This period is noteworthy for many reasons. Nearly the whole of polymer chemistry developed during this period, as did nuclear chemistry. The wealth of discoveries in organometallic compounds, the development and application of new analytical tools (e.g., infrared, ultraviolet, and nuclear magnetic resonance spectroscopies and chromatography), important discoveries in biochemistry, great progress in space travel, and much more has occurred during the past 4 or 5 decades. I want to examine just one facet of this exciting period, namely, the development, adaptation, and use of computers in chemical information processing.

Chemical information comprises the entire record of progress in chemistry. Processing of this information has the purpose of organization, coordination, and correlation so as to facilitate further research, development, and practice in chemistry. Chemical information processing may be divided into two broad categories, that which deals with representations of chemical substances and that which deals with nonstructural or textual descriptions of substances and with processes and phenomena related thereto. Since other authors in this issue examine both of these areas in some detail, I will treat them only from the perspective of significant work related to the



James E. Rush received his B.S. in chemistry and mathematics from Central Missouri State University in 1957 and his Ph.D. in chemistry from the University of Missouri in 1962. He is President and a principal shareholder of James E. Rush Associates, Inc. (an Ohio Corp.). He was Director of Research and Development at OCLC, Inc. (1973-1979), and their Director of Research and Coordinator of the Office of Planning and Research (1979-1980). Prior to that, he was an Associate Professor (1968-1973) and is now Adjunct Associate Professor, in the Department of Computer and Information Science at The Ohio State University. In 1980, he was also appointed Adjunct Professor of Library Science at the University of Illinois. He was associated with Chemical Abstracts Service (1962-1968) as an Assistant Editor in the Organic Index Editing department, Assistant Head in the Chemical Information Procedures department, and Technical Liaison Officer. He is actively engaged in research and has numerous publications to his credit on chemical information handling, computing, library automation, and other topics in the field of information storage and retrieval, including two books coauthored with Charles H. Davis.

adaptation and use of computers. I will first review developments in the computer field and then will address some of the significant milestones in both structural and textual in-

<sup>†</sup> Presented in part before the first Computer Secretariat, 189th National Meeting of the American Chemical Society, Miami Beach, FL, April 30, 1985.