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Information Chemistry in Japan

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A brief history of the abstracting services for journal articles in Japan, starting with *Kagaku Soran* in 1927 and leading to the recent development of the nationwide on-line information service system of TOOL-IR, is given. Current activities in information chemistry in Japan are also reviewed. The importance of the basic terms in science and technology is stressed in relation to the promotion of better exchange of chemical information. It is also observed that the old Asian documents may be considered as a kind of database of chemical substances. Although Western chemical science grew as an analytical science, presently it relies on the databases of chemical information. The latter fact may be considered as the merging of the standpoints of chemistry in the East and the West.

INTRODUCTION

Historical Sketch. In the past few decades, enormous developments have been achieved for chemistry through the use of computers. They have occurred in the fields of computational chemistry, chemical information, and physicochemical measurements. The latter include access to data, control of samples, instrument interfaces, and data handling such as accumulation, fast Fourier-transform analysis, and other sophisticated data manipulations. More recently, computers have been widely used for the generation of bibliographic databases and for the retrieval of information.

Those active in the fields cited above organized meetings that dealt with topics of computational chemistry and chemical information. The former were oriented more to the software problems of chemical information and the latter more to the studies of the database management system (DBMS) or to the problems of retrieval of chemical information.

Apparently both phases of activity cited above are equally concerned with chemical information, although each has a somewhat different purpose. Recently, it has been recognized that activities in computational chemistry and in chemical information could be merged into one, because both overlap with and rely on each other. Thus, the division of information chemistry was formed within the Chemical Society of Japan in 1983 with Prof. S. Sasaki as the chairman. Its annual meeting in 1984 was considered the seventh. That took into account the number of previously held meetings on chemical information.

The abstracting service for the journal articles was first started in 1927 by Prof. Toshiyuki Majima at Tohoku University. He built Kagaku Kenkyukai, which published *Kagaku Soran* (*Complete Abstracts of Japanese Chemical Literature*).[1] Prof. Shinichiro Fujise continued the work of Prof. Majima until 1963. Kagaku Kenkyukai was succeeded by the Japan Information Center of Science and Technology (JICST) in 1963. The latter is an organization fully supported by the Japanese government. Kagaku Kenkyukai is still active in the promotion of information chemistry, such as granting fellowships or research funds to young scientists.

Shizuo Fujiwara graduated from the Department of Chemistry, Faculty of Science, University of Tokyo, in 1944 and obtained his Dr.Sc. degree in 1949. He was appointed assistant professor at the University of Electro-Communications in 1949 and full professor in 1956 and moved to the University of Tokyo as professor of analytical chemistry in 1960. He served there as director of the Research Center for Spectrochemistry (1977–1979), the Research Center for Information and Library Sciences (1978–1981), and the Central Library (1978–1981). He retired from the University of Tokyo and moved to the Chiba University as chemistry professor in 1981. He served as a titular member of the Interdivisional Committee on Machine Documentation in the Chemical Field (1969–1976) and of the Commission on Atomic Weights (1969–1976) of IUPAC and as a council member (1979–1981) and vice-president (1981–present) of FID. He is now president of the Japan Society for Analytical Chemistry and editor of *Analytical Sciences*.

The Science Council of Japan (SCJ), started in 1949, maintains a national committee on information. That committee had two divisions before the reorganization of SCJ in 1984, one on information of documentation and the other on numerical data. The first division has been concerned with the problems of journal publication, standardization of articles, management of libraries, and codings. It also acts as the

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national committee for the Fédération Internationale de Documentation (FID). The second division has been concerned with the problem of numerical data and acts as the Japanese national committee for the Committee on Data for Science and Technology (CODATA). Since November 1984, these two bodies have been reorganized into three national committees: on information science concerned with its general basis, on information of documentation with the function to work as the national committee of FID, and on numerical data with the function as the national committee of CODATA. Those three national committees are expected to work effectively for the organization and policy making of information science in Japan. A symposium on information is held annually by SCJ with the participation of those three committees. Most of the Japanese researchers in information chemistry are directly involved in the activities of those three committees either by direct association with the operation of the board or by participation in the projects. The Chemical Abstracts Service (CAS) of the Americal Chemical Society has cooperated with the Japanese chemists for a long time. Prof. Hideki Chihara started contribution to CAS with respect to the preparation of the abstracts of chemical articles in Japan in 1954. The Chemical Society of Japan helped in that work and formed the Japan Association for International Chemical Information (JAICI).

As to the academic activities in the field of information chemistry, the following may be listed. Annual meetings on computational chemistry and chemical information started around 1970 with the Chemical Society of Japan as the main host besides several other learned societies. As explained above, the seventh annual meeting in 1984 took place under the name of Information Chemistry. At that meeting, about 400 scientists participated, and 48 papers were presented.

Activities in computational chemistry mostly rely on the application of computers of high speed and large capacities. The earliest research by high-speed computer can be traced back to the building of the PL-1 computer at the University of Tokyo around 1953. Many chemists conducted investigations using that computer as well as the PL-2, the successor of the PL-1. T. Shimanouchi and his co-workers calculated molecular force constants and other terms in structural chemistry. I also performed the analysis of multispin nuclear magnetic resonance spectra, for example, that of the six-spin system of monofluorobenzene in 1956.[2]

Around 1960, efforts were made by the university scientists to build computer centers to support their research. The first one was built at the University of Tokyo, then at Kyoto and others. Now, we have seven large computer centers that can be used by all the university scientists at the national level. The computers that were installed in the centers worked well to support the laboratory experiments in one-line mode as well as in batch modes. The large-scale computer files provided the basis for the information services to retrieve bibliographic and factual data. I created with my colleagues TSIR-1 (Todai Scientific Information Retrieval),[3] which was the first on-line information retrieval system. It led to the development of TOOL-IR (Tokyo University On Line Information Retrieval System). Its characteristics are listed in Table I,[4] as it existed in 1974. That system led in turn to the development of the information center with the help of the Ministry of Education and is providing a nationwide service.

Since 1980, a project has been undertaken to build a network of databases of factual information. The Agency of Science and Technology has defined its scope and made the financial arrangements with participation of 10 governmental and private organizations. The names of the participating organizations are listed in Table II. The scope of the project covers a wide range of interests such as chemical, physicochemical, environmental, pharmacochemical, medical, and so on. The important goal of the project is to coordinate the activities of all the participants, with chemical compounds as they key to the coordination.

Table I. Characteristics of the University of Tokyo Computer Center in 1974

CPU	HITAC 8800 (two), average instruction execution time = 200 ns
	HITAC 8700 (two), average instruction execution time = 800 ns
buffer memory	for 8800, 32 kB each, cycle time = 60 ns
	for 8700, 16 kB each, cycle time = 210 ns
main memory	3 MB, cycle time = 0.9 μs
disc	233 MV (four)
	400 MB (three)
TSS	22 terminals (200 Baud, 2400 Baud)
RJE	11 terminals (2400 Baud)
numbers of jobs	45 277/month (as of January 1974)
number of users	2496 (registered), 2148 (active) (as of January 31, 1975)

Although chemists become gradually accustomed to the use of those new tools and systems in the early 1970s, it was still found that they were not well aware of the potential of the new systems, of minicomputers, microcomputers and large computers, and of the feasibility of cooperation between the information scientists and chemists.

Thus, the joint Japan–U.S. seminars on "Computer-Assisted Chemical Research Design" have been organized by H. B. Mark, Jr., and myself, the first in July 1973 in Honolulu and the second in August 1976 in Washington, D.C.[5] Leading scientists from both countries presented papers and exchanged views on various topics of common interests.

The activities in this field have kept growing and it is difficult to describe all of them in a brief article. Some of them, particularly those of JICST and JAICI and of some individual researchers, are listed below.

INSTITUTIONAL ACTIVITIES

Some of the research activities done at the universities have been mentioned already. The achievements of individual researchers will be described in a later section. Here, some other institutional activities are identified.

Since 1983, research has been carried out by the Science and Technology Agency in order to produce a distributed database system of chemical substances and bibliographic information linked by a computer communication network. The project is directed by the Research Promotion Committee, which is responsible for the programming of the project as a whole, and by two subcommittees on the design and the coordination of the member institutions, as listed in Table II, and on the setting of the protocol for the network database sharing. I chair the former.

The project aims at an integrated database system for chemical substance information. The features of the project are various, but chemical compounds are links between the different databases. Databases of different institutions—governmental, industrial, or academic—are to be coordinated together. The goal is not to remain on the level of research and development but to form an integrated database system of real usefulness, which offers information services to domestic and foreign users. Because the project takes chemical compounds as the basis of coordination, it may be referred to as an activity of information chemistry. The databases that are included in the project cover some fundamental information on chemical substances such as spectral data and thermophysical and thermochemical data, as well as environmental data, toxicity test data, production and shipment data, and legal regulation data. The names of 10 institutes that participate in the project are shown in Table II.

Table II. Chemical Databases Produced by the 1984–1985 Project of the Science and Technology Agency of Japan

	database	abbreviation	producing organization	main data elements included
1	Chemical Substance Database	DC	The Japan Information Center of Science and Technology, Japan Association for International Chemical Information	substance names, structures, database locators
2	Agricultural Chemical Substances Database	BC	National Food Research Institute, The Ministry of Agriculture, Forestry and Fisheries	biological, chemical physical, and industrial data on fertilizers, food additives, enzymes, and so on
3	Mutagenicity, Carcinogenicity, Teratogenicity Database	BL	National Institute of Hygienic Sciences	test data of chemical substances such as mutagenicity, carcinogenicity, and teratogenicity
4	Environment Database	EN	National Institute for Environmental Studies	analytical methods and data and physical and chemical property data of environmental chemicals
5	Pharmaceuticals Database	PH	Japan Pharmaceutical Information Center	name (trade name, common name, abbreviated name), ingredient, composition, usage, manufacturer, and distributor of drugs
6	Japanese Chemical Regulation Laws Database	SF	Japan Chemical Industry Ecology-Toxicology and Information Center	regulatory and legal information of Japan for potentially hazardous chemical substances
7	Spectrum Database	SP	National Chemical Laboratory for Industry, Board of Industrial Technology	IR, ^1H NMR, and ^{13}C NMR spectral data of fundamental standard substances
8	Thermophysical and Thermochemical Property Database	TH	The Japan Information Center of Science and Technology	thermophysical and thermochemical data of substances in three or less component systems
9	Pesticides Database	PE	Japan Agricultural Chemical Industry Association	active ingredient, usage, formulation type, dosage, production, and shipment data of pesticides
10	Poison Database	TX	Japan Pharmaceutical Information Center	ingredient, toxicity, clinical effect, treatment, and case reports of poisoning for commercially available substances that may cuase acute poisoning

The Chemical Substance Database System works as a central key for the databases of the member institutes. It consists of two subdatabases, the Stereochemical Accurate Registry of Substances (STARS)[6] and the CAS Registry file. STARS is searchable by using data elements such as Japanese chemical names, stereochemical structure, and components of mixtures or molecular compounds as well as those included in other existing chemical substance databases. It is noted that the Japanese names of compounds either in Kana or Kanji can be referred to here.

The system is a kind of distributed database system in which the Chemical Substance Database and the component databases are logically connected with each other. Arrangements have been made to establish an advanced technique by which distributed databases on different computers can be used efficiently.

For this purpose, a standard protocol has been defined with Data Communication Network Architecture (DCNA),[6] which has been developed by NTT (the Nippon Telephone and Telegramme Public Corp.) as the basis. By use of this protocol, the databases mentioned have become accessible through any computer center.

JAICI is working as an institute producing a bibliographic database of chemical literature, *Kagaku Shoho* (*Chemical Abstracts of Japan*), and providing a selective dissemination of information (SDI) service in addition to participating in the Chemical Database project of the Science and Technology Agency.

JICST has also made efforts to produce a database of the Japanese scientific and technological literature. English-translated titles of the Japanese literaure, at present, number 470 000, including foreign articles.

INDIVIDUAL RESEARCHES

Reference will be made to some of the papers presented at the seventh annual meeting of the Information Chemistry Division in November 1984. At that meeting, the various chemical databases produced in Japan were described (Table I). In particular, Y. Fujiwara (University of Tsukuba) in context of the Chemical Substance Database (DC) described the dictionary of chemical compounds that allows compound generation from names in Japanese and in English and also from structures on the basis of his BCT (the Block-Cutpoint Tree)[7] scheme, while the Thermophysical and Thermochemical Property Data (TH) was introduced by J. Osugi (Kyoto University).[8] T. Hiraishi and O. Yamamoto introduced their Spectrum Database (SP) and indicated the usefulness of having a database of full spectra, mass spectra, and nuclear magnetic resonance spectra.

T. Oshima introduced the Japanese Chemical Regulation Laws Database (SF). Features of the SF are as follows. The regulation on the use of chemical compounds is basically local. By local we mean that the regulation is usually very specific with respect to the area of application. It varies depending on the purpose of regulation, such as concern for environment, safety, or toxicity, and more than that depending on the geological conditions of the city, county, or state or whether it applies to private or institutional organizations. The application of chemical compounds is thus much limited by the legal regulations. The SF file aims at the compilation of the legal regulations for chemical compounds and at the coordination with bibliographic and factual or numerical data. In order to achieve that, enormous efforts must be expended with the cooperation of everybody, people in academia, industry, and government, as well as those involved in chemistry and information sciences. The latter work becomes the concern of the research scientists of information chemistry.

Papers of more theoretical nature were presented by H. Hosoya[9] (Ochanomizu University), M. Uchino[10] (Tokyo Institute of Tech.), K. Maeda (IEE), K. Iizuka[11] (Gakushuin University), and others.

Design or estimation of chemical reactions is another important subject of information chemistry, which has been investigated extensively by Y. Yoneda[12] (formerly University of Tokyo, now Tokai University), S. Sasaki (Toyohashi Technical University), and others.[13] It must be mentioned that

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1) 魏伯陽(漢), “周易参同契” (～100)
2) 張華(晋), “博物志 (10 巻)” (～300) (“増訂漢魏叢書” 所収)
3) 陶弘景(斉), “神農本草集註 (7 巻)”, 永元 2 (500)
4) 藤原時平, “延喜式 (30 巻)”, 延長 5 (927)
5) 李時珍(明), “本草綱目 (52 巻)”, 万暦 24 (1596)
6) 貝原益軒, “大和本草”, 宝永 5 (1708)
7) 小野蘭山, “本草綱目啓蒙 (48 巻)”, 文化 3 (1806)

Figure 1. Names of the books in Table V in Chinese characters.

Table III. Terms of General Nature That Were Most Frequently Cited (Top 10) in More Than Two CA Sections in 1977 and 1978

action	compound	material	purification
activity	determination	metabolism	reaction
agent	development	natural	reagent
analysis	effect	new	review
blood	energy	part	structure
book	gas	phase	study
brain	growth	plant	synthesis
cell	heat	preparation	system
characterization	high	product	total
composition	liquid	property	water

those activities were also presented at other meetings on molecular design.

Individual efforts to produce databases have been made so far by Y. Fujiwara and others for ^{13}C NMR data,[14] by Y. Yoneda for chemical reaction data (EROICA),[15] by S. Sasaki for multisource spectral chemical data (CHEMICS-F), and others. The databases are being maintained by them.

PERSONAL VIEWS ON INFORMATION CHEMISTRY

I have reviewed thus far the history and current status of the information chemistry in Japan. Next, my personal view will be presented. At this stage of the growth of information chemistry and the increased number of the people engaged in it, when the large computers, minicomputers, microcomputers and institutional or personal computers have fairly well been developed, what should we do now? The first thing to promote is the cooperation between the scientists of different fields with respect to the discipline, the geographical location, or the institutional environment.

The second thing is to recognize the great potential of the computer with increasing capacity. The large capacity of computers has so far been demonstrated by either their speed of operation or the size of the files. For example, high speed has been utilized in physicochemical calculations and the large-scale files in the information handling. However, large files are now also essential for the large-scale calculation, since memory is needed for the retention of the intermediate results of calculation. High speed, on the other hand, is good for information retrieval. Thus, large computers offer new vistas in the age of information chemistry. At the same time, the microcomputer is able to handle almost the same work as that previously handled by the old computer center. Thus the work formerly needing a large computer can now be done at the bench, which may change radically the chemical laboratory. In order to be prepared for such a situation, appropriate education courses and training must be arranged.

Table IV. Basic Terms Chosen by More Than 13 Learned Japanese Societies and Their Fields

term	no.[a]	term	no.[a]	term	no.[a]	term	no.[a]	term	no.[a]	term	no.[a]
aging	18	carrier	16	division	14	inversion	23	phase	16	shell	14
analysis	13	cell	16	drift	16	isotope	15	pole	14	stability	23
arm	13	chance	16	excitation	13	joint	19	quenching	21	strut	19
base	23	chart	23	exposure	21	key	15	radiation	17	torsion	19
beam	17	clamp	16	filter	19	level	17	range	15	track	15
bearing	16	condenser	21	frame	14	lift	16	reduction	16	transition	14
bellows	15	core	23	frequency	19	line	13	resonance	18	transmission	14
bond	14	counter	15	grain	17	load	19	scale	23	viscosity	16
brace	13	density	13	grating	15	matrix	23	sampling	16	weight	20
bridge	15	deviation	19	head	15	noise	15	screen	16		
calibration	16	diaphragm	20	indicator	18	oscillation	15	section	18		
capacity	14	dimension	20	interference	16	permeability	18	setting	15		

field	Japanese	English	field	Japanese	English
Zoology	2046	2169	Spectroscopy	2098	2108
Nuclear Engineering	3707	3607	Odontology	596	535
Aeronautics	3120	3195	Meteorology	1751	1841
Botany	2579	2667	Mechanical Engineering	9204	10272
Chemistry	9848	9977	Architectural Engineering	6373	5841
Electrical Engineering	10030	10116	Logic	735	803
Library Science	3963	4846	Oceanography	2378	2414
Mathematics	1624	1644	Civil Engineering	5761	6027
Instrumentation Technology	2542	2684	Geography	1857	1720
Physics	3902	4033	Genetics	1821	1846
Seismology	2451	2475	Astronomy	2177	2214
Naval Architecture and Marine Engineering	8412	9232	total	88975	92266

[a] Number of societies that chose the term.

Table V. Some Database Books of Chemical Substances in Old China and Japan

no.	name of book	author	period
	In Chinese Pronounciation		
1	"Zhou Yi Can tong chi"[a]	Wei Bo Yang	Han
2	"Bo Wu Zhi"[b]	Zhang Hua	Jin
3	"Shen Nong Ben Cao ji Zhu"[c]	Tao Hong Jing	Qi
5	"Ben Cao Gang Mu"[d]	Li Shi Zhen	Ming
	In Japanese Pronounciation		
4	"Engi Shiki"[e]	Fujiwara Tokihira	
6	"Yamato honzō"	Kaibara Ekiken	
7	"Honzō kōmoku keimō"	Ono Ranzan	

[a] The textbook of Taoism in which preparation of the acrogenic drugs is described. It is considered as the oldest book that has referred to the chemial substances. [b] Encyclopedia of the natural products. It is referred to as the oldest data file of the chemical substances. [c] The oldest handbook of the pharmacological and food materials. [d] The most comprehensive encyclopedia of the natural products, where the inorganic, botanical, pharmacological, and other products in nature are described with systematic classification. [e] A comprehensive classification of the social (governmental) positions and the responsibilities in old Japan is given in this book, in which ways of handling of all kinds of natural products are covered.

The third thing to be noted is the importance of the basic terms in chemistry or, more generally, in science and technology. Professors H. Chihara and Akira Yamasaki[16] (University of Electro-Communications) made useful studies on the chemical terms to be used for access to chemical information. It is very necessary and important to establish the basic terms in science and technology for the cooperation of scientists and for their education. I did some work on the study of basic terms.[17,18] The results of my work are reproduced in Tables III and IV.

Table III is a list of basic terms that have been chosen by the frequency analysis of 10 million keywords provided for 600 000 articles in *Chemical Abstracts* (CA). Table IV is a list of the basic terms that are commonly used by more than 13 Japanese learned societies. It is interesting to note that the terms given in Tables III and IV seem to refer to the basic elements of human intellectual activities in science. This may suggest that the contents of Tables III and IV form the basis of cooperation of scientists and that of education.

Lastly, one view on the trends of the East and West in information chemistry will be presented. Observations have been made that the characteristic feature of Western science, particularly that of modern Western science, is its analytical approach, whereas that of the Eastern science or older Asian science is synthetic or inductive. However, the opposite situation seems to be developing when one observes the recent trends of Western science. Science in old Asia started with the preparation of the list of substances in nature, which is somewhat analogous to the production of a file or database of chemical substances.[19] The oldest one and some other typical works are shown in Table V and Figure 1. The book listed as 5 in the table is the first translated into Japanese and is considered as the most comprehensive compilation. Both 4 is the first one to which the products of Japan have been added. Books 6 and 7 contain classification systems of Japanese concepts.

The important point to be noted here is that modern Asian science, which is becoming an analytical science having followed the Western science in the 19th century, was semantic in the old times. Western science is now approaching the ways of the old Asian science in the sence that databases of chemical substances are generated semantically and rely on the knowledge and information.

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