A Bibliometric Study on Chemical Information and Computer Sciences Focusing on Literature of *JCICS*

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A bibliometric approach was used to survey the state-of-the-art of research in the field of chemical information and computer sciences (CICS). By examining the *CA* database for the articles abstracted under the subsection "Chemical information, documentation, and data processing", *Journal of Chemical Information and Computer Sciences* (*JCICS*) was identified to have been the top journal in this subsection for the last 30 years. Based on this result, *CA* subsections and controlled index terms given to *JCICS* articles were analyzed to see trends in subjects and topics in the CICS field during the last two decades. These analyses revealed that the subjects of research in CICS have diversified from traditional information science and computer applications to chemistry to "molecular information sciences". The *SCISEARCH* database was used to grasp interdependency between *JCICS* and other key journals and also the international nature of *JCICS* in its publications and citedness.

1. INTRODUCTION

A bibliometric analysis of literature in a particular subject field often effectively reveals progress, trends, and other features of the research and development in that field. The methodologies used in this approach are based on counting and statistical processing of keywords, classification codes, author names, citations, and other bibliographic items available from a reference collection on the subject field (usually constructed by retrieval of one or a few bibliographic database(s)). Many bibliometric studies have been made in various fields, with the purposes of (1) structuring a subject field (including identification or finding of principal, or active, subfields and topics; interrelating the topics; and analysis of temporal change in the field structure), (2) identification of influential actors (individuals, organizations, countries, and journals) in a subject field and measuring connectivities among the actors, (3) assessment of the scientific activity and impact of a specific country or organization in a subject field, and (4) evaluation of an information source (database) for bibliometric analysis of a subject field from the viewpoint of comprehensiveness of information or adequacy of indexing.

The main works published within the last years[1−26] are shown in Table 1 together with their purpose and applied subject field.

In the field of chemical information and computer sciences (CICS), however, few attempts have been made on research trend analysis by means of the bibliometric approach. Only one related work which addressed applications of computers in chemistry was reported by Tsay,[27] but the areas it dealt with differ from CICS, though some areas might overlap. Moreover, his analysis does not go beyond showing the outline of the distribution of papers among document types, journals, authors, and languages. This article tries to deal macroscopically with the research trends and features in the CICS field over the last two decades on the level of subject matter.

Table 1. Recent Studies on Research Trends in a Subject Field Using Bibliometric Methods

purpose of the study	subject field
1. subject field organization (including temporal trend analysis)	neural network;[1] laser;[2] condensed matter physics;[3,4] fullerenes[5] enzyme engineering;[6] welfare[7,8]
2. subject field organization (at a fixed time period)	research impact assessment;[9] chemistry;[9] near-earth space science;[10] hypersonic and supersonic flow;[11] fullerenes;[12] R&D management;[13] nanotechnology;[14] climate;[15] migraine headaches[16]
3. actors identification (including temporal trend analysis)	vaccines;[17] laser;[2] fullerenes;[5] enzyme engineering;[6] welfare [7,8]
4. actors identification (at a fixed time period)	nanotechnology;[14] climate;[15] laser;[18,19] microbiology[20]
5. activity assessment for a country/organization	alkaloid chemistry;[21] health and environment;[22] AIDS [23,24]
6. source evaluation	plant proteins;[25] microbiology[26]

2. ITEMS INVESTIGATED AND METHODS

In this paper the following questions are dealt with through bibliometric approaches: (1) What are core journals in the CICS field? (2) To what other fields in chemistry does the CICS field have a close relation? (3) How have the research topics in this field changed for the last two decades? (4) What are the interdependency relationships between *Journal of Chemical Information and Computer Sciences* (*JCICS*), the most principal journal in this field, and other journals? (5) Is *JCICS* more international than other journals published by the American Chemical Society?

The bibliographic data necessary for analyses of these questions were collected from the databases on STN

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Table 2. Ranking of Materials by the Number of Articles Abstracted under *CA* Subsection 20-5 in Different Periods[a]

(a) 9th and 10th *CA* CI Periods (1972−1981 of *CA*)

rank	material name	country of publication	no. of articles
1	*J. Chem. Inf. Comput. Sci. (J. Chem. Doc.)*	(USA)	431
2	*Nauchno-Tekh. Inf., Ser. 2*	(SUN)	47
3	*Nauchno-Tekh. Inf., Ser. 1*	(SUN)	42
4	*J. Inf. Processing Manag.*	(JPN)	37
5	*J. Chem. Educ.*	(USA)	36
6	*ACS Symp. Ser.*	(USA)	24
7	*Anal. Chem.*	(USA)	21
8	*Proc. Int. CODATA Conf.*		20
8	*Zh. Vses. Khim. O-Va.*	(SUN)	20
10	*Vopr. Inf. Teor. Prakt.*	(SUN)	18

(b) 11th to 14th *CA* CI Periods (1982−2001 of *CA*)

journal publication year: 1981−1985				journal publication year: 1986−1990			
rank	material name	country of publication	no. of articles	rank	material name	country of publication	no. of articles
1	*J. Chem. Inf. Comput. Sci.*	(USA)	137	1	*J. Chem. Inf. Comput. Sci.*	(USA)	169
2	*Proc. Int. CODATA Conf.*		35	2	*Tetrahedron Comput. Methodol.*	(GBR)	44
3	*Symp. Chem. Inf. Comput. Sci. (3rd)*	(JPN)	23	3	*ACS Symp. Ser.*	(USA)	37
4	*Comput. Handl. Generic Chem. Struct., Proc. Conf.*	(GBR)	18	4	*Proc. Int. CODATA Conf.*		27
5	*Chem. Nomencl. Usage, [Pap. Symp.]*	(GBR)	16	5	*J. Mol. Graphics*	(GBR)	25
5	*Zfi-Mitt.*	(DDR)	16	6	*Nauchno-Tekh. Inf., Ser. 2*	(SUN)	23
5	*Zh. Vses. Khim. O−Va.*	(SUN)	16	7	*Terminol. Biotechnol., Multidiscip. Probl., Proc. I*		21
8	*Nauchno-Tekh. Inf., Ser. 1*	(SUN)	14	8	*J. Chemom.*	(GBR)	20
9	*Am. Lab. (Fairfield, Conn.)*	(USA)	11	9	*Chem. Inf.*	(DEU)	19
9	*Drug Inf. J.*	(USA)	11	10	*Proc. Int. Chem. Inf. Conf.*		18
9	*J. Inf. Processing Manag.*	(JPN)	11	10	*Comput. Appl. Biosci.*	(GBR)	18
				10	*Hwahak Kwa Kongop Ui Chinbo*	(KOR)	18

journal publication year: 1991−1995				journal publication year: 1996−2000			
rank	material name	country of publication	no. of articles	rank	material name	country of publication	no. of articles
1	*J. Chem. Inf. Comput. Sci.*	(USA)	384	1	*J. Chem. Inf. Comput. Sci.*	(USA)	216
2	*Comput. Appl. Biosci.*	(GBR)	99	2	*Nucleic Acids Res.*	(GBR)	104
3	*J. Mol. Graphics*	(GBR)	71	3	*Bioinformatics*	(GBR)	65
4	*Spec. Publ. − R. Soc. Chem.*	(GBR)	53	4	*J. Inf. Sci. Tech. Assoc.*	(JPN)	52
5	*Methods Mol. Biol. (Totowa, N. J.)*	(USA)	51	5	*Proc. Int. Chem. Inf. Conf.*		40
6	*Chem. Struct. 2 Proc. Int. Conf., 2nd*		39	6	*Genome Inf. Ser.*	(JPN)	34
6	*J. Chemom.*	(GBR)	39	7	*Pharmaceut. Libr. Bull.*	(JPN)	31
8	*ASTM Spec. Tech. Publ.*	(USA)	36	8	*Nachr. Chem., Tech. Lab.*	(DEU)	24
8	*Genome Inf. Ser.*	(JPN)	36	9	*Methods Mol. Biol. (Totowa, N. J.)*	(USA)	22
10	*Proc. Int. Chem. Inf. Conf.*		31	10	*Pac. Symp. Biocomput. '98*	(USA)	20

[a] The figures are based on *CA* as of August 31, 2000.

International. *Chemical Abstracts* (*CA*) was used for items (1), (2), and (3) above-mentioned, while *Science Citation Index* (*SCISEARCH*) was used for items (4) and (5).

The ANALYZE command of STN International was very effective for counting and sorting field terms contained in the search results.

3. RESULT AND DISCUSSION

3.1. Core Journals in the CICS Field. To identify the core journals in the CICS field, we first have to define articles belonging to that field. As an initial (and rather narrower) definition, I take the articles classified under the subsection 20-5 "Chemical information, documentation, and data processing" in *CA*.

CA classifies every articles it abstracts into 80 "sections" and, more specifically, into their "subsections". In *CA*, a considerable portion of the articles in the CICS field should be concentrated under the subsection 20-5, although, of course, the articles in this field, or those relating to this field, might scatter over the entire range of *CA* sections/subsections. Therefore, it would be adequate to identify the core journals in the CICS field based on the occurrences of articles classified under the subsection 20-5.

By the way, the subsection code for "Chemical information, documentation, and data processing" has been 20-5 since *CA* volume 96 (1982) (corresponding to the *CA* 11th Collective Index (CI) period and later) but was 20-4 from *CA* Volume 76 (1972) to Volume 95 (1981) (corresponding to the *CA* 9th and 10th CI periods). Though this survey covers through all these periods, in this article we use a subsection code 20-5 to refer to both subsection codes 20-4 in earlier volumes and 20-5 in later volumes.

Table 2 shows the transition of the most productive 10 journals in this subsection for the last 30 years. In this table,

Table 3. Share Statistics of Journals in *CA* Subsection 20-5[a]

	9−10 CI periods	journal publication year in 11−14CI periods 1981−1985	1986−1990	1991−1995	1996−2000
total number of articles	1960	981	1448	2204	1889
JCICS articles	431	137	169	384	216
JCICS share (%)	22.0	14.0	11.7	17.4	11.4
articles of the no. 2 journal	47	35	44	99	104
the no. 2 share relative to *JCICS*	0.109	0.255	0.260	0.258	0.481
total number of journals	560	307	365	489	539

[a] The figures are based on *CA* as of August 31, 2000.

statistics are divided into five periods; the first covers the *CA* 9th and 10th CI periods (1972−1981 of *CA*) and the latter four correspond to each 5-year interval by the publication year of articles in the *CA* 11th CI period and later. We can easily find the following two facts from this table: (a) *Journal of Chemical Information and Computer Sciences* (*JCICS*) has continued to be the outstanding journal in this subsection and (b) the rankings of other journals or materials are very unstable. Thus, no journal other than *JCICS* appears in more than three periods. *Proceedings of International CODATA Conferences* and *Proceedings of International Chemical Information Conferences* appear three times, another eight materials two times, and another 26 appear only once.

In addition, as shown in Table 3, the share of *JCICS* in the subsection 20-5 has always been far over 10%. The number of articles for the no. 2 journal (it changes from time to time) was only about a quarter of that for *JCICS* for a long time, though *Nucleic Acid Research* reaches a half of *JCICS* just in the recent period.

From these findings, the outstanding productivity of *JCICS* in the CICS field is evident. Accordingly, hereafter I will discuss research trends in this field mainly by analyzing bibliometric features of the articles published in *JCICS*, assuming these articles represent literature in the CICS field.

3.2. Subject Fields Closely Related to the CICS Field. Articles published in *JCICS* are abstracted under various subsections as well as the subsection 20-5. This leads us to expect that investigating the distribution of *JCICS* articles among *CA* subsections might be the simplest way to know what subject fields in chemistry are closely related to CICS.

Figure 1 shows the main feature of *JCICS* article distribution among the *CA* sections/subsections for each 5-year interval of publication years since the *CA* 11th CI period. The subsection 20-5, in which most typical CICS articles are thought to be abstracted, accounted for 70% of all *JCICS* articles through the 1980s, but thereafter articles in the subsection 20-5 have rapidly decreased their share, from about 50% in the 1991−1995 period to about 30% at present.

Instead, sections 1 (pharmacology), 22 (physical organic chemistry), and 65 (general physical chemistry) have been significantly increasing their shares. Under those sections, the following subsections have noticeably grown: (1) 1-1 “pharmacology; methods” [0.0%→2.9%], (2) 1-3 “pharmacology; structure−activity” [0.5%→12.7%], (3) 22-1 “physical organic chemistry; general” [0.0%→2.9%], (4) 22-2 “physical organic chemistry; theoretical organic chemical concepts, including quantum and molecular mechanical studies” [2.0%→11.1%], (5) 22-13 “physical organic chemistry; other reactions, processes, and spectra” [0.0%→4.8%],

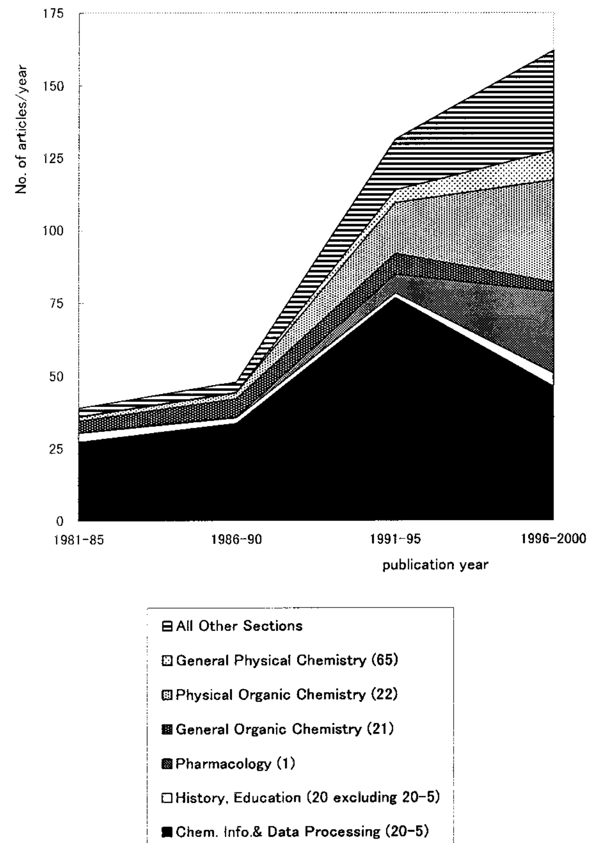

Figure 1. *CA* section distribution in *JCICS* articles.

and (6) 65-5 “general physical chemistry; atomic and molecular properties” [0.5%→2.9%]. (The two figures in each bracket mean the share percentages by the subsection in *JCICS* articles during 1981−1985 and during 1996−2000, respectively.)

The subject fields which are dealt with by all these subsections relate to molecular structure and properties and relationships between them from theoretical views. Thus, observation of the *CA* subsection distribution of *JCICS* articles tells us of a remarkable trend of the CICS field in the recent decade. This is that the main concern of the field has extended, from traditional chemical information science and computer applications to chemistry, to the inclusion of theoretical (or calculational) molecular chemistry.

One might suspect that the remarkable change in the shares by *CA* subsections could mainly be due to a change in *CA*’s classification policy. Indeed, while the description of *CA Subject Coverage Manual* indicated until 1991 that an article on “computers and computer programs related to the chemistry covered in a specific section” should be placed

Table 4. Statistics on *CA* Subject Index Terms (CT) Indexed to *JCICS* Articles[a]

		whole period since 11CI	breakdown by publication year 1981−1990	1991−1995	1996−2000
number of articles (A)		1850	435	658	757
total CT occurrences (B)		7593	1528	2534	3531
CTs per article (B/A)		4.10	3.51	3.85	4.66
number of different CTs (C)		1053	253	395	773
average occurrences per CT (B/C)		7.21	6.04	6.42	4.57
cumulative percentage of occurrences by CTs with *n* or more occurrences and the number of the corresponding CTs (in parentheses)	$n = 10$	74.6% (111)	69.8% (27)	70.1% (39)	58.6% (64)
	$n = 5$	83.6% (224)	80.1% (51)	80.6% (80)	74.7% (154)
	$n = 2$	92.5% (480)	91.0% (115)	91.6% (182)	87.5% (330)

[a] The figures are based on *CA* as of August 31, 2000.

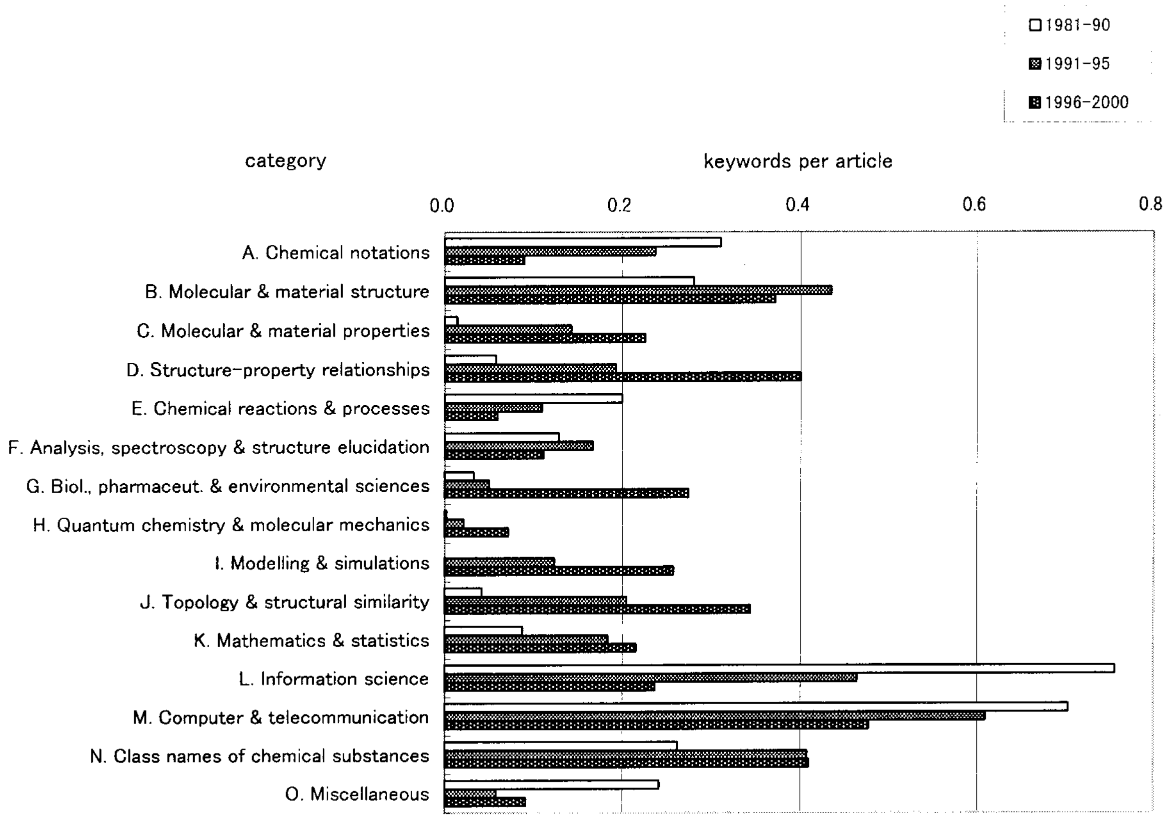

Figure 2. CT distribution in *JCICS* articles.

under an appropriate subsection other than the subsection 20-5, since 1992 the manual has changed the indication as an article on "chemical information and computer applications related to the chemistry covered in a specific section" and also on "nomenclature rules for specific substances or classes" should be placed under a subsection other than the subsection 20-5.

However, this revision, though it may have some influence, seems to be minor judging from the following facts. (1) The proportion of *JCICS* articles assigned to the subsection 20-5 was examined for each *CA* volume within 6 years before and after the revision. From this observation, the move of *JCICS* articles from this subsection to others is estimated to be at most 20% of the articles which would be placed under there without the revision. Thus, the proportion of articles placed under 20-5 might be at most about 60% in 1991−1995 and below 40% in 1996−2000 even if the manual indication had remained unchanged. (2) The *CA* subsection distribution was also examined for articles published in another journal specifically oriented to information science and technology, *Nauchno-Tekhnicheskaya Informatsiya* (series 1 and 2). The proportion of the articles under the subsection 20-5 to all articles of this journal abstracted in *CA* is 78% during 1986−1990 and 77% during 1991−1995, before and after the change of the manual description, respectively. The decreasing rate in this proportion is much lower than that for *JCICS*.

Consideration of (1) and (2) above supports the hypothesis that the subject areas *JCICS* covers have rapidly extended from traditional ones into theoretical molecular chemistry since early in the 1990s.

3.3. Topics in the CICS Research and Their Change. Every article abstracted in *CA* is assigned several controlled subject index terms (general subject index terms). The *CA* controlled terms (hereafter abbreviated as CTs) indexed to *JCICS* articles for over 20 years were examined for a deeper

Table 5. Journals Frequently Cited by *JCICS* Articles[a]

rank	by *JCICS* published in 1997–1998: journal name	no. of citing *JCICS* articles	no. of citations	by *JCICS* published in 1981–1985: journal name	no. of citing *JCICS* articles	no. of citations
1	***J Chem Inf Comput Sci***	244	1283	***J Chem Inf Comput Sci***	153	651
2	***J Am Chem Soc***	171	412	*J Chem Doc*	84	274
3	*J Comput Chem*	91	169	***J Am Chem Soc***	70	253
4	***J Med Chem***	85	287	***Anal. Chem***	34	141
5	*J Math Chem*	53	109	*ACS Symposium Ser*	34	45
6	*J Phys Chem A*	53	96	***Anal. Chim Acta***	33	71
7	*J Chem Phys*	52	146	***Science***	32	53
8	*Croat Chem Acta*	52	109	*J Org Chem*	23	38
9	***Science***	52	77	*Chem Inf Sys*	22	22
10	*Theochem-J Mol Struct*	49	86	*Comput Representat*	20	21
11	*Chem Phys Lett*	49	83	*Wiswesser Line Formu*	20	21
12	*Quant Struct-Act Rel*	48	74	***Tetrahedron***	19	41
13	***Anal. Chim Acta***	47	103	*Chem Eng News*	19	32
14	***Anal. Chem***	46	125	***J Med Chem***	18	67
15	*J Comput Aid Mol Des*	46	77	*J Chem Educ*	18	64
16	*Int J Quantum Chem*	45	90	*Angew Chem*	18	30
17	***Tetrahedron***	38	54	*J Am Soc Inf Sci*	17	26
18	*Nature*	35	51	***Comput Chem***	16	20
19	*Chem Graph Theory*	34	39	*Graph Theory*	16	18
20	*Chemometr Intell Lab Sys*	33	61	*Database*	13	19
	Angew Chem Int Edit	33	43			
	Comput Chem	33	38			

[a] The boldface journals appear in both periods.

Table 6. Journals Frequently Citing *JCICS* Articles[a]

rank	1997–1998 publications: journal name	no. of articles citing JCICS	1981–1985 publications: journal name	no. of articles citing JCICS
1	***J Chem Inf Comput Sci***	244	***J Chem Inf Comput Sci***	155
2	*Acta Cryst C*	48	***J Comput Chem***	21
3	***Tetrahedron***	31	*Anal. Chem*	17
4	***J Med Chem***	30	*Int J Quantum Chem*	16
5	*Theochem-J Mol Struct*	30	***Anal. Chim Acta***	14
6	***J Am Chem Soc***	29	***Computers & Chemistry***	11
7	*J Comput Aid Mol Des*	28	*J Chem Educ*	11
8	*Quant Struct-Act Rel*	24	***J Am Chem Soc***	11
9	***J Comput Chem***	23	*J Organic Chem*	10
10	*Acta Cryst B*	22	*Mutation Res*	9
11	*J Chem Soc-Dalton*	22	*Theor Chim Acta*	9
12	*Inorg Chem*	21	*ACS Symposium Ser*	8
13	*Organometallics*	21	***Croat Chem Acta***	8
14	*Perspect Drug Discov Design*	21	*Pure Appl Chem*	8
15	***Croat Chem Acta***	19	*Environ Health Perspect*	7
16	*Chemometr Intell Lab Sys*	17	***J Med Chem***	7
17	*J Organometal Chem*	17	*J Mol Graphics*	7
18	***Anal. Chim Acta***	16	*Anal.Chim Acta-Comput Tech Opt*	6
19	***Computers & Chemistry***	16	*Zh Vsesoy Khim Obshch Imen*	6
20	*J Chem Soc-Perkin*	16	*Science*	5
			Tetrahedron	5

[a] The boldface journals appear in both periods.

analysis of the trend in CICS research than found in the preceding section.

In Table 4, the statistics of CTs indexed to *JCICS* articles are summed up for the whole period since the *CA* 11th CI period and for each of three subperiods, which are adjusted so that the number of articles included in them may become roughly even.

This table shows the rapid growth in the vocabulary size of CTs (the number of different CTs) used for *JCICS* indexing. It suggests, again, the recent trend of diversification in subject areas covered by *JCICS*, although this may be partly due to the change in the *CA* indexing policy.

To confirm the trend of diffusion of interest in *JCICS* articles into new areas, I tried to categorize CTs frequently used for *JCICS* indexing and observe how the occurrences of the CTs in the individual categories change with time.

From Table 4 we can find that 224 CTs that occurred five or more times (i.e., indexed in five or more *JCICS* articles) account for 84% of all CT occurrences in *JCICS* articles through the whole period since 1981, though the 224 are only 21% of the total 1053 CTs used for indexing. Hence, we can expect use of the 224 CTs is enough for our purpose, i.e., to analyze subject topics dealt with by *JCICS* articles.

Table 7. Citing-Cited Relationship of *JCICS* with Other Journals (1997−1998)[a]

		x >= 15			7 <= *x* <= 14			*x* <= 6	
y >= 30	&	*Anal.Chem*	46,15	*	*Int J Quantum Chem*	45,11	*	*Angew Chem Int Edit*	33,6
	&	*Anal.Chim Acta*	47,16		*J Math Chem*	53,13		*Chem Graph Theory*	34,0
		Chemometr Intell Lab	33,17	#	*J Mol Biol*	30,7	*	*Chem Phys Lett*	49,2
		Comput Chem	33,16	*	*J Phys Chem A*	53,11	*	*Chem Rev*	30,4
	*	*Croat Chem Acta*	52,19				*	*J Chem Phys*	52,4
	*	*J Am Chem Soc*	171,29				*	*Nature*	35,0
		J Chem Inf Comput Sci	244,244				*	*Science*	52,1
		J Comput Aid Mol Des	46,28						
		J Comput Chem	91,23						
	#	*J Med Chem*	85,30						
	&	*Theochem-J Mol Struct*	49,30						
		Match-Commun Math Chem	30,15						
		Quant Struct-Act Rel	48,24						
	#	*Tetrahedron*	38,31						
15 <= *y* <= 29				#	*Biochemistry*	23,8	#	*Biopolymers*	16,2
				*	*J Chem Soc Farad T2*	18,7	*	*Bull Chem Soc Jpn*	27,5
				#	*J Chem Soc Perk T 2*	21,9	*	*Chem Soc Rev*	19,2
					J Mol Graphics	15,13		*Concepts Appl Mol Sim*	16,0
				#	*J Org Chem*	21,10	*	*Discrete Appl Math*	18,3
				#	*J Pharmaceut Sci*	22,8		*Graph Theory*	17,0
				*	*New J Chem*	16,9	*	*Indian J Chem A*	16,6
				*	*Pur Appl Chem*	22,10	#	*J Biol Chem*	18,2
					SAR QSAR Env Res	15,12	*	*J Chem Educ*	23,4
								Mol Connect Chem	25,0
								Neural Networks Chem	20,1
							*	*P Natl Acad Sci USA*	24,2
								Rev Comput Chem	18,0
								Tetrahedron Comput	17,0
							*	*Theor Chim Acta*	24,1
							*	*Top Curr Chem*	19,2
y <= 14	&	*Acta Cryst B*	5,22	*	*Chemistry Eur J*	0,10			
	&	*Acta Cryst C*	2,48	#	*Drug Discov Today*	10,9			
	#	*Inorg Chem*	5,21	#	*Environ Toxicol Chem*	11,9			
	#	*J Chem Soc Dalt*	1,22	#	*Eur J Med Chem*	5,7			
	#	*J Chem Soc Perk T 1*	6,16	#	*Inorg Chim Acta*	1,12			
	#	*J Organomet Chem*	0,17	*	*J Chem Soc Chem Comm*	10,14			
		Match-Commun Math Comp	2,15		*J Mol Model*	2,8			
	#	*Organometallics*	1,21	*	*J Phys Chem B*	0,7			
	#	*Perspect Drug Discov*	11,21	&	*J Struct Chem*	0,9			
				#	*Med Chem Res*	3,7			
				*	*Pol J Chem*	3,7			
					Polyhedron	0,11			
				*	*Rev Roum Chim*	13,10			
				#	*Tetrahedron Lett*	14,10			

[a] Each journal is classified by the number of articles (x) of the journal citing *JCICS* (columns) and the number of *JCICS* articles (y) citing the journal (rows). Each entry shows journal category (see footnote b), journal name, y and x, in this order. [b] Journal categories: *−broad areas; all chemistries; mathematics; physics; physical chemistry; #−inorganic, metal organic, organic and biological chemistries; &−analytical and structural chemistries, and no mark−CICS and mathematical chemistry fields.

One of the problems one encounters when analyzing subject keywords based on their occurrence frequency is that the expressions of the keywords are sometimes altered according to the indexing policy of the database producer. A list of all CTs used for indexing *JCICS* articles during the whole period concerned was checked to find the alterations of CT expression. The three types of alterations which are the simplest and the most common were as follows: (a) alteration from a singular to a plural form (e.g., PERIODICAL→PERIODICALS; STERIC EFFECT→STERIC EFFECTS), (b) alteration from an inverted to a normal form (e.g., KINETICS, REACTION→REACTION KINETICS), and (c) alteration from a nonabbreviated to an abbreviated form (e.g., DEOXYRIBONUCLEIC ACID→DNA). Unification of expression for these types reduced the total number of different CTs from 1072 to 1053.

The statistics in Table 4 and the subsequent discussions have been made after this unification. The resultant 224 CTs that occurred 5 or more times are classified into 15 subject categories as follows: A. chemical notations, B. molecular and material structure, C. molecular and material properties, D. structure−property relationships, E. chemical reactions and processes, F. analysis, spectroscopy, and structure elucidation, G. biological, pharmaceutical, and environmental sciences, H. quantum chemistry and molecular mechanics, I. modeling and simulations, J. topology and structural

Table 8. Contributions of Countries to Publications in, and Citations to, *JCICS* (1997–1998)

(a) contribution to publications			(b) contribution to citations		
country	publications	(%)	country	citing articles	(%)
USA	141	(40.6)	USA	490	(29.9)
England	36	(10.4)	England	258	(15.8)
France	20	(5.8)	Germany	155	(9.5)
Germany	20	(5.8)	France	109	(6.7)
Slovenia	19	(5.5)	Spain	82	(5.0)
Japan	15	(4.3)	Italy	79	(4.8)
Romania	15	(4.3)	Russia	66	(4.0)
Croatia	14	(4.0)	Japan	59	(3.6)
Russia	13	(3.7)	Switzerland	56	(3.4)
P R China	11	(3.2)	Poland	52	(3.2)
all articles	347	(100.0)	all citing articles	1638	(100.0)

Table 9. Regional Distribution of Publication in, and Citations to, *JCICS* (1997–1998)

region	publications	(%[a])	citing articles	(%[a])
USA and Canada	148	(42.7)	539	(32.9)
Latin America	13	(3.7)	46	(2.8)
Western Europe	120	(34.6)	907	(55.4)
Eastern Europe	95	(27.4)	358	(21.9)
Middle East and Africa	4	(1.2)	42	(2.6)
East Asia and Oceania	38	(11.0)	199	(12.1)

[a] The sum is over 100% since a publication (citation) may be contributed from more than one country.

Table 10. Contribution from U.S. Authors to ACS Journals (1997–1998)

	authorships				
journal name	U.S. (A)	all (B)	A/B (%)	articles (C)	A/C (%)
JCICS	141	418	33.7	347	40.6
J Phys Chem A	1246	3521	35.4	2825	44.1
J Org Chem	1573	3743	42.0	3416	46.0
Anal. Chem	982	1904	51.6	1785	55.0
J Am Chem Soc	2852	5366	53.1	4547	62.7
Biochemistry	2610	4838	53.9	3933	66.4
J Chem Educ	767	1093	70.2	1127	68.1

similarity, K. mathematics and statistics, L. information science, M. computer and telecommunication, N. class names of chemical substances, and O. miscellaneous.

These categories were determined by the author for the present purpose, by examining indexing use of those CTs for *JCICS* articles. All CTs under all subject categories are given in Table 11, together with their occurrences as index terms for *JCICS* articles.

Figure 2 shows how the usage rates of these CTs as index terms have changed for each category over the three subperiods into which the whole period of the last 20 years is divided.

According to the trend in usage rates, 15 categories can be classified into three groups: (1) growing subject categories—C. molecular and material properties, D. structure–property relationships, H. quantum chemistry and molecular mechanics, J. topology and structural similarity, G. biological, pharmaceutical, and environmental sciences, and I. modeling and simulations; (2) declining subject categories—A. chemical notations, E. chemical reactions and processes, L. information science, M. computer and telecommunication, and O. miscellaneous; and (3) stationary subject categories—B. molecular and material structure, F. analysis, spectroscopy, and structure elucidation, K. mathematics and statistics, and N. class names of chemical substances.

All of the growing categories relate to theoretical or calculational treatment of molecular structure and molecular properties. Again, we can observe that there is a growing concern in *JCICS* articles toward theoretical molecular chemistry and away from traditional information science and technology. In the growing categories, G and I are also growing in whole *CA* index term occurrences, but categories C, D, H, and J are roughly constant. This fact suggests increasing concern in the latter four categories seems to be characteristic of the CICS field.

3.4. Interdependency Relationships between *JCICS* and Other Journals. As another probe for investigating the relation between CICS and other subject fields, analysis of what articles cite, and are cited by, in the CICS field is of great interest. Unfortunately, *SCISEARCH*, the only database including citation data in the science and technology area, does not have the systematic subject indexing vocabulary or classification system of *CA*. Hence, the journals frequently cited by, and also frequently citing, articles published in *JCICS* are surveyed using *SCISEARCH* to gain some insight into the interdependency between the CICS field and other fields.

(1) Journals cited by the most of *JCICS* articles published in 1997–1998: In 347 articles published in the 1997–1998 issues of *JCICS*, there are 9286 citations, which reduce to 7143 unique articles. These cited articles are distributed among 2467 journals.

Now, which measure is the most adequate for evaluating the degree of impact of a journal X on a particular journal A (*JCICS* in the present case) based on citation data: (a) the number of citations to articles of X from articles of A, (b) the number of articles of X cited (at least once) by articles of A, or (c) the number of articles of A citing one or more article(s) of X?

Each of these measures has its own sense and features. The measure (a) is the most basic and is used in *Journal Citation Report* by the Institute for Scientific Information (ISI). However, it may be excessively influenced both by a few particular articles of X cited by many articles of A and by a few particular articles of A citing many articles of X. The measure (b) is not affected by the former but may be still affected by the latter. In the case of (c), the situation is opposite to this. For the subsequent discussion, the measure (c) is chosen because it might reflect most directly the range of *JCICS* articles on which journal X has an impact.

Table 5 lists the top 20 journals ranked by the decreasing order of the measure (c), namely, the number of *JCICS* articles of 1997–1998 which cite at least one article of the individual journal listed, with the measure (a), the number of citations to the journal from *JCICS* articles of 1997–1998. The journal list based on *JCICS* articles of 1981–1985 is also shown for comparison.

The journal cited by the most of *JCICS* articles of 1997–1998 is *JCICS* itself. Among the 347 articles, 244 cite at least one *JCICS* article. Seventeen journals other than *JCICS* are cited by more than 10% of the 347 and another 24 by more than 5%.

(2) Journals frequently citing *JCICS* in their articles published in 1997–1998: Of the articles which were published in 1997–1998 and indexed in *SCISEARCH*, 1638

refer to at least one *JCICS* article (including one published in *Journal of Chemical Documentation*, the precedent of *JCICS*). These 1638 articles are distributed among 374 journals and make 4288 citations to *JCICS*, which reduce to 1124 different *JCICS* articles.

By analogy to the discussion in (1) of this section, we can assume three measures for evaluating the degree of dependency of a journal Y on *JCICS*: (α) the number of citations to *JCICS* articles from articles of Y, (β) the number of *JCICS* articles cited by articles of Y, and (γ) the number of articles of Y citing one or more *JCICS* article(s).

In this case, however, the measure (β) makes little sense. The measure (γ) is preferred to the measure (α) for the following reasons: (i) it better matches the measure (c) chosen in the discussion in (1) and (ii) it cannot be known from conventional tools such as *Journal Citation Reports*.

Table 6 shows the top 20 journals ranked by the descending order of the measure (γ) for the 1997−1998 and 1981−1985 periods. Of the 374 journals, 14 contain 20 or more articles citing at least one *JCICS* article and 61 contain 5−19 articles. The top 14 journals and the next 61 account for 36% and 34% of the total 1124 citing articles, respectively. There are 244 *JCICS* articles in 1997−1998 having reference to other *JCICS* articles.

It should be noted that the statistics mentioned here, of course, do not include citations to *JCICS* by journals which are not the "source journals" of *SCISEARCH*.

To know how many citations are made to *JCICS* articles by journals in social sciences, *Social Science Citation Index* (*SSCISEARCH*) was searched in the same way as *SCISEARCH*. However, it was found that *JCICS* articles are much less cited by the source journals of *SSCISEARCH* than by the ones of *SCISEARCH*. Only 20 articles in 13 journals published in 1997−1998 and indexed in *SSCISEARCH* cite at least one *JCICS* articles, in contrast to 1638 articles in 374 journals in case of *SCISEARCH*. This indicates that *JCICS* much more influences natural scientists than social scientists.

(3) The temporal variation of frequently cited/citing journals: To examine to what extent the journal ranking on citations from/to *JCICS* is stable, journals frequently cited by *JCICS* are compared between the *JCICS* articles in 1997−1998 and 1981−1985 and also journals frequently citing *JCICS* between the journal publication years 1997−1998 and 1981−1985. The resulting journal listings are shown in Tables 5 and 6. In Table 5, showing the top 20 journals most frequently cited by *JCICS* articles in each of two periods, eight journals, including *JCICS* itself, appear in both the two different periods. In Table 6, showing the 20 journals most frequently citing *JCICS*, eight journals, including *JCICS* itself, appear in both periods.

In Table 5, which shows "affecting-on-*JCICS*" journals, journals appearing in the 1981−1985 period and disappearing in the 1997−1998 period include ones pertaining to the areas of chemical notation (*Comput. Representat.* and *Wiswesser Line Formu.*) and of information science (*J. Am. Soc. Inf. Sci.* and *Database*). In contrast, most of the newly appearing journals in the 1997−1998 period are in the areas of computer chemistry, molecular design, and physical chemistry/chemical physics. This shift is certainly consistent with the trend of research published in *JCICS*, which is described in the sections 3.2 and 3.3.

On the other hand, in Table 6, showing "depending-on-*JCICS*" journals, newly appearing journals in the 1997−1998 period pertain to crystallographic/organic/organometallic chemistry as well as the molecular design area, while no obvious feature is found in ones appearing in the 1981−1985 period which disappear in the 1997−1998 period.

(4) Categorization of journals by the frequencies of citations from/to *JCICS*: Based on the survey described in (1) and (2) in this section, the journals having a close relation (from the point of citation frequency) to *JCICS* can be categorized in a matrix form as shown in Table 7, which arranges the journals concerned along two axes, the numbers of *JCICS* articles in 1997−1998 citing those journals, and the number of articles of those journals in 1997−1998 which cite *JCICS* articles. In this table, the journals are roughly classified also by their main subject fields. For the upper-right side of the table, which contains the journals frequently cited by, but not so frequently citing, *JCICS* (they can be called "affecting-on-*JCICS*" journals), journals in the fields of broad areas of science, all chemistries, physics, and physical chemistry, are dominant. On the other hand, at the lower-left side of the table, occupied by the journals citing frequently, but not so frequently cited by, *JCICS* (they can be called "depending-on-*JCICS*" journals), quite a few journals are in the fields of inorganic, metal-organic, organic, or biological chemistry.

The correlation between the cited/citing ratio on *JCICS* and the subject field of journals seems, however, not to be strong. A detailed survey on subject keywords or classification items indexed to both *JCICS*-cited and *JCICS*-citing articles may give clearer insights, although this would require a considerable effort.

3.5. International Nature of *JCICS*. As described in section 3.1, *JCICS* has retained its outstanding position in terms of output of CICS articles. This suggests that *JCICS* has become a main medium of scholarly communication worldwide in the CICS field, although *JCICS* is a journal published by the American Chemical Society (ACS). For proving this supposition, the distribution among authors by country of affiliation was observed for two sets of articles stated in the preceding section, namely, (a) 347 *JCICS* articles of publication years 1997−1998 and (b) 1638 articles of publication years 1997−1998 which cite at least one *JCICS* article.

Tables 8 and 9 show the breakdown into countries of author affiliations and into broader regions, respectively. Both distributions, of publications and of citations, are very scattered among various countries. Contributions from authors affiliated in U.S. institutions are only 40% of publications in *JCICS* and 30% of citations to *JCICS*.

The international nature on authorships of *JCICS* is shown by comparing the proportions of U.S.A. authorships in the journal with those of some other journals also published by ACS. The proportions for the articles in these journals for publication years 1997−1998 are mentioned in Table 10. The reliance on U.S. authors of *JCICS* is the lowest among those ACS journals.

From the facts mentioned above, one can conclude that *JCICS* has a highly international nature. It may be a result of the lack of attractive international journals in the CICS field.

Table 11. Subject Categories and Controlled Terms (CTs) under Them[a]

A. Chemical Notations			
bond	(14)	ligands	(12)
chemical chains	(6)	nomenclature	(14)
chemical formula	(130)	nomenclature, general	(110)
code	(17)	protein sequences	(6)
functional groups	(18)	ring	(32)
B. Molecular and Material Structure			
aromaticity	(9)	crystal structure	(17)
bond angle	(5)	hydrogen bond	(13)
bond length	(9)	isomerism and isomers	(46)
bond order	(7)	isomers	(24)
chirality	(12)	molecular association	(6)
configuration	(8)	molecular structure	(413)
conformation	(33)	solvation	(6)
conforation (protein)	(5)	stereochemistry	(19)
conformation and conformers	(44)	stereoisomers	(7)
conformers	(6)		
C. Molecular and Material Properties			
boiling point	(42)	free energy	(15)
bond energy	(5)	heat of formation	(9)
dipole moment	(8)	molecular vibration	(5)
electron configuration	(6)	partition	(23)
electron configuration and electron density	(18)	physical properties	(14)
electron density	(7)	polarity	(7)
electronegativity	(7)	polarizability	(8)
electronic structure	(14)	potential energy and function	(10)
electrostatic potential	(8)	property	(8)
energy	(5)	solubility	(13)
energy level	(7)	total energy	(10)
entropy	(9)	vapor pressure	(7)
formation enthalpy	(6)		
D. Structure−Property Relationships			
additivity	(7)	QSAR (structure−activity relationship)	(165)
linear free energy relationship	(28)	steric effects	(8)
molecular structure-biological activivity relationship	(43)	structure-activity relationship	(34)
molecular structure-property relationship	(156)	substituent effects	(14)
E. Chemical Reactions and Processes			
process control and dynamics	(5)	rearrangement	(7)
reaction	(76)	ring closure and formation	(5)
reaction kinetics	(13)	synthesis	(50)
reaction mechanism	(22)	transition state structure	(16)
reactivity	(10)		
F. Analysis, Spectroscopy, and Structure Elucidation			
analysis	(22)	mass spectroscopy	(7)
chromatography, gas	(5)	molecular structure determination	(36)
crystal structure determination	(6)	molecular structure determination methods	(11)
crystallography	(6)	NMR (nuclear magnetic resonance)	(50)
IR spectra	(20)	NMR spectroscopy	(33)
IR spectroscopy	(10)	spectra	(11)
mass spectra	(14)	spectrochemical analysis	(8)
mass spectrometry	(5)	spectrometry	(6)
G. Biological, Pharmaceutical, and Environmental Sciences			
antitumor agents	(7)	health hazard	(5)
carcinogens	(7)	hydrophobicity	(10)
combinatorial chemistry	(23)	lipophilicity	(6)
combinatorial library	(36)	neoplasm inhibitors	(7)
drug design	(38)	pharmacophores	(38)
drug screening	(22)	receptors	(15)
environmental pollution	(6)	toxicity	(15)
estrogen receptors	(5)	transcortins	(5)
functional sites (enzyme)	(10)		
H. Quantum Chemistry and Molecular Mechanics			
AM1 MO (molecular orbital)	(8)	PM3 (molecular orbital)	(5)
LUMO (molecular orbital)	(5)	quantum chemistry	(16)
molecular mechanics	(8)	wave function	(6)
molecular orbital	(21)		
I. Modeling and Simulations			
biological simulation	(17)	neural network simulation (physicochemical)	(28)
genetic algorithm	(14)	physicochemical simulation	(19)
molecular dynamics simulation (physicochemical)	(5)	simulation and modeling, biological	(25)
molecular modeling	(64)	simulation and modeling, physicochemical	(96)
neural network simulation (biological)	(8)		

Table 11 (Continued)

	J. Topology and Structural Similarity		
clusters	(6)	molecular topology	(298)
graph theory	(73)	similarity theory	(17)
group theory	(6)	symmetry	(13)
	K. Mathematics and Statistics		
cluster analysis	(12)	pattern recognition	(7)
correlation analysis	(16)	principal component analysis	(13)
mathematical methods	(25)	regression analysis	(37)
mathematics	(133)	statistical analysis	(9)
matrix theory	(9)	statistical mechanics	(5)
optimization	(9)	statistics and statistical analysis	(41)
partial least squares	(6)		
	L. Information Science		
Chemical Abstracts Service	(57)	information science and technology	(304)
classification	(7)	libraries	(7)
databases	(71)	literature	(37)
indexes	(19)	nomographs	(90)
indexing	(23)	patents	(47)
information retrieval	(20)	periodicals	(19)
information science	(112)		
	M. Computer and Telecommunication		
algorithm	(304)	expert systems	(6)
communication	(5)	information systems	(58)
computer application	(319)	information theory	(9)
computer program	(333)	internet	(11)
computers	(18)	memory devices	(5)
	N. Class Names of Chemical Substances		
alcohols, properties	(12)	inorganic compounds	(8)
aldehydes, properties	(9)	ketones, properties	(9)
alkanes, properties	(62)	materials	(8)
alkanes, uses and miscellaneous	(7)	molecules	(31)
alkenes, properties	(15)	natural products	(5)
amines, properties	(9)	nitriles, properties	(5)
aromatic compounds	(16)	organic compounds, biological studies	(6)
aromatic hydrocarbons, biological studies	(5)	organic compounds, miscellaneous	(15)
aromatic hydrocarbons, miscellaneous	(10)	organic compounds, properties	(47)
aromatic hydrocarbons, properties	(40)	organic compounds, reactions	(8)
aromatic hydrocarbons, uses and miscellaneous	(5)	organometallic compounds	(5)
benzenoids	(16)	peptides, biological studies	(5)
carboxylic acids, properties	(6)	peptides, properties	(6)
chemical compounds	(27)	pesticides	(5)
chemicals	(24)	pharmaceuticals	(39)
cyclic compounds	(27)	phenols, properties	(5)
cycloalkanes	(16)	polycyclic aromatic hydrocarbons	(5)
drugs	(7)	polymers, miscellaneous	(16)
enzymes	(5)	polymers, properties	(8)
ethers, properties	(8)	polymers, uses, and miscellaneous	(9)
fullerenes	(31)	proteins (general), properties	(6)
fungicides	(5)	proteins, properties	(16)
heterocyclic compounds	(10)	proteins, specific or class	(7)
hydrocarbons, properties	(26)	solvents	(8)
hydrocarbons, uses, and miscellaneous	(6)	steroids, biological studies	(6)
	O. Miscellaneous		
automation	(5)	organic chemistry	(14)
chemical industry	(6)	risk assessment	(5)
chemistry	(94)	science	(16)
education	(26)	societies	(6)
history	(16)	technology	(5)
laboratories	(7)	thermodynamics	(12)

[a] Figures are the indexed occurrences to *JCICS* articles from 1981 to 2000.

4. CONCLUSIONS

(1) *JCICS* has been the outstanding journal in productivity in the *CA* subsection "Chemical information, documentation, and data processing" for the last 30 years. Research trends in the CICS field can be known by analyzing *JCICS* articles.

(2) Analysis of *CA* sections and subsections assigned to *JCICS* articles reveals that the main concern of the journal has extended from traditional chemical information science and computer applications to chemistry to the inclusion of theoretical (or calculational) molecular chemistry since the early 1990s.

(3) The above-mentioned trend is confirmed by examining variations in *CA* subject index terms (CTs) indexed to articles of the journal. While CTs in the subject categories of traditional information and computer sciences have continued

to decline, CTs in the categories on molecular chemistry have been rapidly growing.

(4) Journals frequently cited in *JCICS* are mainly ones covering physics, physical chemistry, mathematics, or a broad area of science or chemistry. On the other hand, within journals frequently citing *JCICS*, ones oriented to inorganic, metal organic, organic, or biological chemistry are rather dominant. However, these correlations are not very strong.

(5) *JCICS* has high internationality in the sense that the contribution from U.S. authors to both its publications and citations to it is only 30−40%, which is lower than that for any other ACS-published journal.

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