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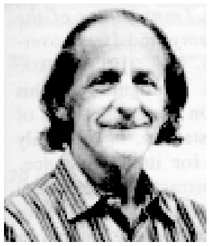

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Journal Citation Studies. 46. Physical Chemistry and Chemical Physics Journals. Part 3. The Evolution of Physical Chemistry to Chemical Physics

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In Part 2 of this study[1] we discussed the difficulties that we encountered in defining a "core" list of physical chemistry journals. Modern chemists will appreciate the futility of trying to separate that field from chemical physics. Consequently, we chose a core list of 31 journals that encompassed the high-impact periodicals from both disciplines. That list is reprinted in Table 1 for convenience. However, I will not repeat the explanation of the process used to select these journals. In this third part of the study, we examine the field of physical chemistry/chemical physics by treating all 31 core journals as one "macrojournal."

"Macrojournal" of Physical Chemistry/Chemical Physics

By using the categorical (or "macrojournal") approach, we can often obtain a clearer picture of a discipline than if we examined one journal at a time. This type of analysis also allows us to measure the contribution of the total annual output of one area of science. For example, in 1983 the "macrojournal" of physical chemistry/chemical physics published over 10,000 papers, or 2 percent of the 450,000 papers covered in the 1983 *Journal Citation Reports®* (*JCR®*) section of the *Science Citation Index®* (*SCI®*). These 10,000 papers cited 250,000 references in 1983, or 3 percent of all the references included in the *JCR*. This is an average of about 25 references per source article, 7 more than the average for all journal articles indexed in the *JCR*.

These 10,000 articles received about 215,000 citations, or about 3 percent of the 7,955,000 citations given to all journal articles covered in the 1983 *JCR*. **Just three journals accounted for over 50 percent of these citations**—the *Journal of Chemical Physics* (74,000), the *Journal of Physical Chemistry* (23,100), and *Chemical Physics Letters* (18,500). The preeminence of the *Journal of Chemical Physics* is due to the large number of papers it has published, but equally important is its high impact.

However, as with any citation analysis, it is important to remember that while one journal may dominate in citations, other less cited journals in the same field may be equally important. As David A. Young, editor of the *Journal of the Chemical Society—Faraday Transactions I* and *II*, recently reminded us, "There is strength in diversity: the conclusions which [some] thinkers will draw from...[this] survey will undoubtedly serve to weaken such publications as the *Berichte der Bunsen-Gesellschaft für Physikalische Chemie*, the three sections of *Nuovo Cimento della Societã Italiana di Fisica*, *Journal de Chimie Physique et de Physico-Chimie Biologique*, *Zeitschrift für Physikalische Chemie—Leipzig*, and the *Faraday Transactions I* and *II*, even *Molecular Physics*, to the benefit of the two giants [*Journal of Chemical Physics* and *Journal of Physical Chemistry*]. Were this to happen...the damage done to the international scientific community would be serious and irreparable. A monopoly of effective publications would be created...."[2] Note that several of the journals mentioned by Young are *not* listed in this study, either because they did not meet our "core journal" requirements (described in Part 2), or they do not specifically cover physical chemistry or chemical physics. *Journal de Chimie Physique et de Physico-Chimie Biologique*, for example, covers a more general range of physical-chemical subject matter, including biological physical chemistry. In 1983 it cited the *Journal of the American Chemical Society* (*JACS*), a general chemistry journal, more than it cited specific physical chemistry and chemical physics journals. Had we extended our tables further and expanded our definition of a core journal, we could have included data for dozens of smaller or less subject-specific journals. One example of the latter is the multidisciplinary Soviet journal *Doklady Akademii Nauk SSSR*. It ranked 80th in the list of journals that cited the core in 1983. However, the *JCR* shows that it is cited quite often by the *Zhurnal Fizicheskoi Khimii*.

In Table 2 we list the 50 journals that most frequently cited the physical-chemical core group in 1983. This table and Table 3, discussed later, helped us to identify the 31 core journals. The 50 journals listed in Table 2 represent 3 percent of the over 1,500 journals that cited articles published in the macrojournal in 1983. But they account for 34 percent of the citations that the macrojournal received. Twenty-six of these 50 journals are themselves core journals. Forty percent of the references that they cited in 1983 were to the macrojournal of physical chemistry/chemical physics. The 24 non-core journals included in the table gave out only 9 percent of their total references to the macrojournal.

It is interesting that the 50 journals listed in Table 2 do not include any biochemistry journals. Crystallography, an important part of physical chemistry, is closely tied to both physical biochemistry and molecular biology. This is not apparent in our listing, however, because the core of physical chemistry and chemical physics is rather self-contained. The dominance of chemical physics journals pushes molecular biology and physical biochemistry journals below the threshold for Table 2. In addition, biochemistry articles are fragmented among the many different journals in which they are published. Most biochemistry journals rank below those listed in Table 2. When their citation

Table 1: Core physical chemistry/chemical physics journals indexed by the *SCI*® in 1983.

Annual Review of Physical Chemistry
Berichte der Bunsen-Gesellschaft fur Physikalische Chemie
Chemical Physics
Chemical Physics Letters
Faraday Discussions of the Chemical Society
International Journal of Chemical Kinetics
International Journal of Quantum Chemistry
Journal of Catalysis
Journal of Chemical and Engineering Data
Journal of Chemical Physics
Journal of Chemical Thermodynamics
Journal of Colloid and Interface Science
Journal of Computational Chemistry
Journal of Magnetic Resonance
Journal of Molecular Spectroscopy
Journal of Molecular Structure
Journal of Photochemistry
Journal of Physical Chemistry
Journal of Solution Chemistry
Journal of the Chemical Society—Faraday Transactions I
Journal of the Chemical Society—Faraday Transactions II
Journal of the Chemical Society—Perkin Transactions II
Kinetics and Catalysis—English Translation
Molecular Physics
Photochemistry and Photobiology
Radiation Physics and Chemistry
Surface Science
THEOCHEM—Journal of Molecular Structure
Theoretica Chimica Acta
Zeitschrift fur Physikalische Chemie—Leipzig
Zhurnal Fizicheskoi Khimii

Table 2: The 50 journals that most frequently cited core physical chemistry/chemical physics journals in the 1983 *SCI*®. An asterisk (*) indicates a core journal. A = citations to core journals. B = citations to all journals. C = self-citations. D = percent of total citations that are core-journal citations (A/B). E = percent of total citations that are self-citations (self-*citing* rate, C/B). F = percent of core-journal citations that are self-citations (C/A). G = 1983 impact factor. H = 1983 immediacy index. I = 1983 source items.

	A	B	C	D	E	F	G	H	I
*J. Chem. Phys.	25,398	53,542	15,263	47.4	28.5	60.1	2.96	.77	1847
*J. Phys. Chem.	11,838	28,645	2729	41.3	9.5	23.1	2.65	.59	887
*Chem. Phys. Lett.	10,177	21,631	2382	47.1	11.0	23.4	2.23	.50	1176
J. Amer. Chem. Soc.	6548	58,661	---	11.2	---	---	4.47	.83	1777
*Chem. Phys.	6284	12,029	932	52.2	7.8	14.8	2.31	.48	371
*Surface Sci.	5376	15,695	3752	34.3	23.9	69.8	3.99	.71	535
*Mol. Phys.	4019	7857	1018	51.2	13.0	25.3	2.03	.51	302
*Int. J. Quantum Chem.	3213	8666	653	37.1	7.5	20.3	1.15	.35	309
*J. Catal.	3125	7309	2035	42.8	27.8	65.1	2.37	.49	316
Phys. Rev. B—Condensed Matter	2936	49,717	---	5.9	---	---	3.27	.71	1961
*J. Colloid Interface Sci.	2536	8122	1420	31.2	17.5	56.0	1.48	.30	386
*THEOCHEM—J. Mol. Struct.	2514	6524	98	38.5	1.5	3.9	.69	.19	246
*J. Mol. Spectrosc.	2435	4388	1136	55.5	25.9	46.7	1.97	.41	226
*J. Magn. Resonance	2286	5200	1173	44.0	22.6	51.3	2.78	.73	310
*J. Chem. Soc. Faraday Trans. I	2169	6449	566	33.6	8.8	26.1	1.38	.46	271
*J. Mol. Struct.	2151	5808	473	37.0	8.1	22.0	1.06	.26	292
Phys. Rev. A—Gen. Phys.	2053	21,413	---	9.6	---	---	2.64	.61	913
Can. J. Chem.	1939	12,410	---	15.6	---	---	1.24	.29	483
*Zh. Fiz. Khim. SSSR	1931	8381	1049	23.0	12.5	54.3	.30	.09	794
Inorg. Chem.	1776	25,473	---	7.0	---	---	2.68	.46	848
Bull. Chem. Soc. Jpn.	1712	16,069	---	10.7	---	---	.96	.32	882
*J. Chem. Soc. Faraday Trans. II	1543	3743	195	41.2	5.2	12.6	1.59	.46	143
*J. Chem. Soc. Perkin Trans. II	1398	8511	612	16.4	7.2	43.8	1.38	.35	324
*Annu. Rev. Phys. Chem.	1391	2907	27	47.9	.9	1.9	8.08	.43	21
*Ber. Bunsen Ges. Phys. Chem.	1376	5074	314	27.1	6.2	22.8	1.39	.27	209
*Photochem. Photobiol.	1248	6390	914	19.5	14.3	73.2	2.21	.65	230
J. Electron. Spectrosc. Relat. Ph.	1225	4181	---	29.3	---	---	2.00	.54	164
Macromolecules	1194	9367	---	12.8	---	---	2.39	.58	344
J. Electroanal. Chem. Interfac.	1114	10,519	---	10.6	---	---	1.88	.42	489
J. Phys.—B—At. Mol. Phys.	1083	10,656	---	10.2	---	---	2.57	.72	387
Anal. Chem.	1043	22,172	---	4.7	---	---	3.36	.50	630
*Theor. Chim. Acta	1043	2541	231	41.1	9.1	22.2	2.19	.54	87
Phys. Rev. Lett.	1007	19,867	---	5.1	---	---	6.46	1.50	1165
Z. Naturforsch. Sect. A	1005	4377	---	23.0	---	---	1.07	.32	219
*Radiat. Phys. Chem.	958	3173	257	30.2	8.1	26.8	.83	.09	189
Usp. Khim. SSSR	915	11,167	---	8.2	---	---	1.26	.01	80
Compr. Chem. Kinet.	910	2055	---	44.3	---	---	---	---	---
J. Phys.—C—Solid State Phys.	893	15,447	---	5.8	---	---	2.71	.70	600
*J. Comput. Chem.	836	2247	40	37.2	1.8	4.8	1.98	.60	70
J. Org. Chem.	817	33,602	---	2.4	---	---	2.03	.40	1227
*J. Photochem.	811	2344	140	34.6	6.0	17.3	1.30	.24	114
ACS Symp. Ser.	803	18,104	---	4.4	---	---	.62	.19	611
Thermochim. Acta	801	7183	---	11.2	---	---	.80	.32	471
Int. J. Mass Spectrom. Ion Proc.	800	5989	---	13.4	---	---	1.79	.41	544
*Int. J. Chem. Kinet.	785	2309	255	34.0	11.0	32.5	1.41	.43	98
Mol. Cryst. Liquid Cryst.	772	6007	---	12.9	---	---	2.11	.19	352
*J. Chem. Thermodyn.	764	2603	390	29.4	15.0	51.1	1.18	.50	146
Appl. Catal.	738	2632	---	28.0	---	---	1.22	.32	113
Fluid Phase Equilibria	734	3006	---	24.4	---	---	1.84	.26	146
Solid State Commun.	727	13,783	---	5.3	---	---	1.92	.37	947

counts are combined, however, the total indicates a greater impact than is otherwise evident in Table 2. For example, the number of citations given to the macrojournal by all the *biochemistry* journals in the 1983 *SCI* is over 5,000, which would rank this hypothetical "citing macrojournal of biochemistry" seventh in Table 2.

The *Journal of Chemical Physics* ranks first among the 50 journals in Table 2; in 1983 it gave out 25,400 citations to the macrojournal, nearly 50 percent of all the references it cited that year. The *Journal of Physical Chemistry* is ranked second, with 11,800 citations to the macrojournal, followed by *Chemical Physics Letters* (10,200), and *JACS* (6,500). The fifth most-citing journal is *Chemical Physics* (6,300). Only 2 of the top 10 journals in Table 2 are non-core journals—*JACS* and *Physical Review B—Condensed Matter* (2,900). When we combine the figures for the *Journal of the Chemical Society—Faraday Transactions I* and *II*, it moves up into this top 10 grouping, with 3,700 citations. In Part 2 of this study we commented that this journal was split into its two parts "only for ease of production." According to Young, it really should be considered as one journal.[3]

When we look at Table 3, the top 50 journals most cited *by* the macrojournal of physical chemistry/chemical physics in 1983, we find that chemical physics journals continue to rank at the top. The 50 journals in Table 3 account for 58 percent of all the citations given out by the macrojournal in 1983; 22 of these journals are themselves core journals. Of the citations that they received in 1983, 47 percent were from other core journals. The 28 non-core journals accounted for just 5 percent of the 1983 citations given out by the macrojournal. One of these "journals" is *Advances in Chemical Physics*, a book series published annually. The 1983 volume contained 13 articles. However, the series received over 1,750 citations in 1983, of which about 1,020 were from the macrojournal of physical chemistry/chemical physics. *Advances in Chemical Physics* does not appear in Table 2, however, because it cited the macrojournal only 620 times, ranking it 58th in that listing.

The *Journal of Chemical Physics* is ranked first in Table 3, as it was in Table 2. It was cited by the macrojournal 37,700 times in 1983. That is, it received one-fourth of all the citations that the macrojournal of physical chemistry/chemical physics gave to the 50 journals in 1983. *JACS* is the second most-cited journal (12,200), followed by *Chemical Physics Letters* (10,700). The *Journal of Physical Chemistry* ranked fourth, receiving 8,900, or 6 percent, of the core citations. If we again combine the citation counts for the two parts of the *Faraday Transactions* and add this number to that for its precursor, the *Transactions of the Faraday Society*, which also appears in Table 3, the number of citations that the combined journal received from the macrojournal is over 4,500. This overall figure again raises the ranking of the journal to the top 10.

Impact Factor

The 1983 impact factor for a journal is the average number of citations received in 1983 by the articles published in that journal in 1981 and 1982. When we first began calculating impact over 10 years ago, we chose to use a 2-year period for articles to equalize the difference between those articles that are cited in the first year and those that are not cited until the next year. Our data indicate that the average amount of time for a journal article to peak in citations is two years. In addition, by taking two years of data together we obtain a larger sample—about 20 percent—of the total number of citations to that journal.

Calculating impact factors permits us to compare large journals with small ones. For all core journals in this study, the median 1983 impact is 1.5, while for all 4,250 *JCR* journals it is 0.2. The *Annual Review of Physical Chemistry* and *Surface Science* are relatively small, but their 1983 impact factors are 8.1 and 4.0, respectively. In contrast, the *Journal of Chemical Physics* is a "large" journal, but its 1983 impact is "only" 3.0. Column

Table 3: The 50 journals most cited by core physical chemistry/chemical physics journals in the 1983 *SCI*®. An asterisk (*) indicates a core journal. A = citations from core journals. B = citations from all journals. C = self-citations. D = percent of total citations that are core-journal citations (A/B). E = percent of total citations that are self-citations (self-cit*ed* rate, C/B). F = percent of core-journal citations that are self-citations (C/A). G = 1983 impact factor. H = 1983 immediacy index. I = 1983 source items.

	A	B	C	D	E	F	G	H	I
*J. Chem. Phys.	37,682	73,961	15,263	51.0	20.6	40.5	2.96	.77	1847
J. Amer. Chem. Soc.	12,229	113,183	---	10.8	---	---	4.47	.83	1777
*Chem. Phys. Lett.	10,677	18,485	2382	57.8	12.9	22.3	2.23	.50	1176
*J. Phys. Chem.	8859	23,067	2729	38.4	11.8	30.8	2.65	.59	887
*Surface Sci.	5407	14,436	3752	37.5	26.0	69.4	3.99	.71	535
*Mol. Phys.	4662	7554	1018	61.7	13.5	21.8	2.03	.51	302
*Chem. Phys.	4152	6135	932	67.7	15.2	22.5	2.31	.48	371
*J. Mol. Spectrosc.	3381	5513	1136	61.3	20.6	33.6	1.97	.41	226
*J. Catal.	3231	7647	2035	42.3	26.6	63.0	2.37	.49	316
Phys. Rev. B—Condensed Matter	3221	41,410	---	7.8	---	---	3.27	.71	1961
Phys. Rev. Lett.	3060	48,031	---	6.4	---	---	6.46	1.50	1165
Phys. Rev.	2783	29,909	---	9.3	---	---	---	---	0
Phys. Rev. A—Gen. Phys.	2502	18,190	---	13.8	---	---	2.64	.61	913
*J. Colloid Interface Sci.	2204	6851	1420	32.2	20.7	64.4	1.48	.30	386
*J. Magn. Resonance	1986	4984	1173	39.9	23.5	59.1	2.78	.73	310
*Int. J. Quantum Chem.	1905	3280	653	58.1	19.9	34.3	1.15	.35	309
Proc. Roy. Soc. London Ser. A	1814	11,429	---	15.9	---	---	1.49	.39	132
*Theor. Chim. Acta	1709	3206	231	53.3	7.2	13.5	2.19	.54	87
+Trans. Faraday Soc.	1649	5950	---	27.7	---	---	---	---	0
*J. Chem. Soc. Faraday Trans. I	1522	3724	566	40.9	15.2	37.2	1.38	.46	271
Can. J. Chem.	1364	9980	---	13.7	---	---	1.24	.29	483
*J. Chem. Soc. Faraday Trans. II	1337	3069	195	43.6	6.4	14.6	1.59	.46	143
*Zh. Fiz. Khim. SSSR	1317	3576	1049	36.8	29.3	79.7	.30	.09	794
Bull. Chem. Soc. Jpn.	1304	10,851	---	12.0	---	---	.96	.32	882
*J. Mol. Struct.	1291	2865	473	45.1	16.5	36.6	1.06	.26	292
*Ber. Bunsen Ges. Phys. Chem.	1246	3524	314	35.4	8.9	25.2	1.39	.27	209
*Photochem. Photobiol.	1238	5011	914	24.7	18.2	73.8	2.21	.65	230
J. Phys.—B—At. Mol. Phys.	1179	8430	---	14.0	---	---	2.57	.72	387
Inorg. Chem.	1127	22,646	---	5.0	---	---	2.68	.46	848
Advan. Chem. Phys.	1022	1752	---	58.3	---	---	7.65	1.31	13
J. Chem. Soc.	1016	13,084	---	7.8	---	---	---	---	0
J. Chem. Soc. Chem. Commun.	1000	18,038	---	5.5	---	---	2.62	.42	1003
*J. Chem. Soc. Perkin Trans. II	953	4350	612	21.9	14.1	64.2	1.38	.35	324
Can. J. Phys.	949	4118	---	23.1	---	---	.97	.32	214
Nature	948	117,732	---	.8	---	---	9.26	2.16	1268
Solid State Commun.	919	13,892	---	6.6	---	---	1.92	.37	947
Z. Naturforsch. Sect. A	899	3735	---	24.1	---	---	1.07	.32	219
J. Vac. Sci. Technol.	885	7430	---	11.9	---	---	3.14	---	0
J. Org. Chem.	840	31,227	---	2.7	---	---	2.03	.40	1227
J. Phys.—C—Solid State Phys.	840	11,449	---	7.3	---	---	2.71	.70	600
Proc. Nat. Acad. Sci. US—Phys. Sci.	835	117,000	---	.7	---	---	8.72	1.80	1616
Rev. Mod. Phys.	801	6426	---	12.5	---	---	19.85	2.33	21
Biochim. Biophys. Acta	799	69,240	---	1.2	---	---	2.41	.49	2080
Account. Chem. Res.	765	5764	---	13.3	---	---	8.23	1.08	66
Appl. Phys. Lett.	765	17,444	---	4.4	---	---	3.31	.71	803
J. Appl. Phys.	755	26,878	---	2.8	---	---	1.65	.39	1162
Acta Crystallogr. B—Struct. Sci.	752	8767	---	8.6	---	---	.91	.47	119
*Annu. Rev. Phys. Chem.	738	1507	27	49.0	1.8	3.7	8.08	.43	21
*Int. J. Chem. Kinet.	714	1336	255	52.3	18.7	35.7	1.41	.43	98
*J. Chem. Thermodyn.	686	1846	390	37.2	21.1	56.9	1.18	.50	146

+precursor to *J. Chem. Soc. Faraday Trans. I* and *II* (1972).

G in Tables 2 and 3, and the first column in Table 4, list 1983 impacts.

In some fields it takes much longer for articles to be cited. We have discovered from past studies that if we change the two-year base period used to calculate impact, some types of journals are found to have higher impacts. In this study, the highest impact period for physical chemistry and chemical physics journals is

1980-1981 rather than 1981-1982, the two-year period we would normally use to calculate 1983 impact. That is, the average 1980-1981 article from the physical chemistry/chemical physics core journals was cited more often in 1983 than articles published in other years. Table 4 shows the 1983 impact factors for 10 journals using the following two-year ranges: 1981-1982, 1980-1981, 1979-1980, 1978-1979, and 1977-1978.

Characteristically, a review journal, such as the *Annual Review of Physical Chemistry*, has high impact in comparison to primary research journals. In general, review articles are cited more heavily than original research papers, although there are exceptions. **Reviews often become surrogates for dozens of papers in a research front that would otherwise be cited separately.**

Half-Life

The cit*ed* and cit*ing* half-lives, or median ages of the literature that cites and is cited by other articles, provide another perspective on the temporal aspects of citation. For the 31 core journals in this study, these data for 1983 are listed in Table 5. *THEOCHEM—Journal of Molecular Structure* and the *Journal of Computational Chemistry*, the two youngest journals in the study, have the shortest cit*ed* half-lives in Table 5, at 1.7 and 2.2 years, respectively. That is, the median age of all *THEOCHEM* papers cited in 1983 is only 1.7 years. The longest cit*ed* half-life in Table 5 is greater than 10 years (*Journal of Chemical and Engineering Data*), followed by 9.7 years (*Zhurnal Fizicheskoi Khimii*), 9.6 years (*Journal of Physical Chemistry*), and 9.4 years (*Journal of Chemical Physics*). For all 31 journals combined, the average cit*ed* half-life in 1983 is 5.8 years. For surgery journals[4] this figure is 7.3 and for analytical chemistry,[5] 5.5 years.

Cit*ing* half-life is the median age of the papers cited *by* a journal. In Table 5 the shortest cit*ing* half-lives are 4.1 years (*Faraday Discussions of the Chemical Society*) and 4.8 years (*Annual Review of Physical Chemistry*). Four journals have a cit*ing* half-life that is greater than 10 years: the *Journal of Chemical and Engineering Data*, the *Journal of Chemical Thermodynamics*, the *Journal of Solution Chemistry*, and *Zeitschrift für Physikalische Chemie—Leipzig*. *THEOCHEM*, which had the shortest cit*ed* half-life above, has a cit*ing* half-life of 8.4. The average cit*ing* half-life for all core journals is 7.6 years.

Immediacy

Yet another way to measure a journal's current influence is by looking at its 1983 immediacy index; that is, how often its 1983 articles were cited in 1983. These indexes appear in column H in Tables 2 and 3. For the core journals in this study, the median immediacy is 0.5, compared with 0.2 for all *JCR* journals in 1983. *Faraday Discussions of the Chemical Society*, which does not have a letters section, has the highest individual 1983 immediacy, at 2.2, while the *Journal of Chemical Physics* follows at 0.8; the *Journal of Magnetic Resonance*, *Surface Science*, and *Photochemistry*

Table 4: The 1983 impact factors of selected core journals using different two-year bases. Journals are listed in alphabetic order.

	1981-1982	**1980-1981**	**1979-1980**	**1978-1979**	**1977-1978**
Annu. Rev. Phys. Chem.	8.08	10.40	8.76	6.17	6.95
Chem. Phys.	2.31	2.33	2.03	1.89	1.78
Chem. Phys. Lett.	2.23	2.24	1.87	1.56	1.33
Faraday Discuss. Chem. Soc.	2.78	2.64	3.05	3.23	2.12
J. Catal.	2.37	2.79	3.01	2.92	2.36
J. Chem. Phys.	2.96	3.05	2.95	2.65	2.24
J. Magn. Resonance	2.78	2.68	1.94	1.93	1.91
J. Phys. Chem.	2.65	2.66	2.22	1.84	1.60
Photochem. Photobiol.	2.21	2.27	2.27	2.32	2.17
Surface Sci.	3.99	3.98	3.34	2.88	2.78

Table 5: The 1983 *SCI*® *cited* and *citing* half-lives of core physical chemistry/chemical physics journals. Journals with no listing either received or gave less than 100 citations in 1983. A half-life of ≥ 10.0 indicates that more than 50% of the citations received by or given from the journal were to articles over 10 years old.

Cited Half-Life	Citing Half-Life	
5.6	4.8	Annu. Rev. Phys. Chem.
6.7	8.1	Ber. Bunsen Ges. Phys. Chem.
4.2	6.9	Chem. Phys.
4.7	6.2	Chem. Phys. Lett.
4.9	4.1	Faraday Discuss. Chem. Soc.
5.1	8.8	Int. J. Chem. Kinet.
5.2	7.6	Int. J. Quantum Chem.
5.7	6.2	J. Catal.
≥10.0	≥10.0	J. Chem. Eng. Data
9.4	7.2	J. Chem. Phys.
5.0	9.3	J. Chem. Soc. Faraday Trans. I
5.6	8.4	J. Chem. Soc. Faraday Trans. II
6.4	9.8	J. Chem. Soc. Perkin Trans. II
6.2	≥10.0	J. Chem. Thermodyn.
7.2	9.2	J. Colloid Interface Sci.
2.2	8.0	J. Comput. Chem.
4.4	6.1	J. Magn. Resonance
7.6	8.3	J. Mol. Spectrosc.
5.1	9.5	J. Mol. Struct.
4.0	7.9	J. Photochem.
9.6	6.9	J. Phys. Chem.
6.0	≥10.0	J. Solut. Chem.
6.8	7.3	Mol. Phys.
4.9	5.4	Photochem. Photobiol.
3.1	8.0	Radiat. Phys. Chem.
4.4	5.1	Surface Sci.
1.7	8.4	THEOCHEM—J. Mol. Struct.
8.9	8.7	Theor. Chim. Acta
9.2	≥10.0	Z. Phys. Chem.—Leipzig
9.7	9.5	Zh. Fiz. Khim. SSSR

Kinetics and Catalysis does not appear on this table because we did not receive all of its 1983 issues in time to meet the *JCR*® publication deadline.

and Photobiology at 0.7; and the *Journal of Computational Chemistry* and the *Journal of Physical Chemistry* at 0.6. Of course, an article published early in the year will have a better chance of being cited than one published later. And as a result, journals published weekly or monthly will theoretically have some advantage in immediacy over journals published quarterly or twice a year.[6] This depends, however, on the precise date of publication. The *Faraday Discussions of the Chemical Society* has the highest immediacy but, as mentioned earlier, is published twice a year, after the April and September meetings of the Faraday Division of the Chemical Society. Of the other 30 journals in Table 1, 3 are published twice a month. Sixteen journals are published monthly, three are quarterlies, and one is an annual. Seven journals have an irregular publishing schedule, producing 10, 15, 18, 27, 30, or 44 issues a year.

Overall Rankings

If we take a composite look at the data presented so far in this study, the following core journals rank in the top 10 core journals according to impact, immediacy, number of citations received in 1983, and number of references given out in 1983 (they are listed alphabetically): *Chemical Physics Letters*, the *Journal of Chemical Physics*, the *Journal of Physical Chemistry*, and *Surface Science*, which is "a journal devoted to the physics and chemistry of interfaces."

Most-Cited Articles Published in Non-Core Journals

As a final analysis of the core physical chemistry/chemical physics journals, we also looked at the physical chemistry and chemical physics articles published in *non*-core journals that the core journals cited in 1983. We identified these papers by examining the references that the core journals gave out in 1983. We then looked to see which of these references were to articles published in non-core journals. By focusing only on those non-core articles that were cited 30 or more times by the core, we arrived at the list of 16 papers in Table 6. The citations that they received in 1983 from the core (column A) and their total citations from 1955 to 1984 (column B) in all *SCI* indexed journals are also listed, as are the papers' ISI research-front numbers. The names of many of these fronts were published in Part 1 of this study.[7]

The list in Table 6 includes several papers that have appeared previously in *Current Contents*® essays. For example, the article by J. Stephen Binkley, John A. Pople, and Warren J. Hehre, Department of Chemistry, Carnegie-Mellon University, Pittsburgh, and Department of Chemistry, University of California, Irvine, also appeared in the study of 1980 chemistry articles most cited from 1980 to 1982.[8] Binkley's paper is core to research front #83-0092, which involves molecular orbital calculations of force fields and electronic structure of polyacetylene and polyatomic molecules, discussed in depth in Part 1.

The most-cited paper in Table 6, written by Enrico Clementi and Carla Roetti, IBM Research Laboratory, San Jose, California, is core to "Theoretical analysis of electron impact ionization of rare gases and other atoms" (#83-0089).

Terry J. Balle and Willis H. Flygare's 1981 article on the Fabry-Perot cavity pulsed Fourier transform microwave spectrometer is also core to #83-0092 mentioned earlier. This paper appeared in our recent two-part study of 1981

Table 6: Highly cited articles published in non-core journals cited at least 30 times by core physical chemistry/chemical physics journals in the 1983 *SCI*®. A = 1983 citations from core journals. B = total 1955-1984 *SCI* citations. C = bibliographic data. An asterisk (*) indicates that the paper was the subject of a *Citation Classic*® commentary. The issue, year, and edition of *Current Contents*® in which the commentary appeared follow the bibliographic reference. *SCI* research-front numbers also follow the reference.

A	B	C
32	78	**Balle T J & Flygare W H.** Fabry-Perot cavity pulsed Fourier transform microwave spectrometer with a pulsed nozzle particle source. *Rev. Sci. Instr.* 52:33-45, 1981. 83-0092
34	461	**Barker J A & Henderson D.** What is "liquid"? Understanding the states of matter. *Rev. Mod. Phys.* 48:587-671, 1976. 83-0023
40	993	**Bingham R C, Dewar M J S & Lo D H.** Ground states of molecules. XXV. MINDO/3. An improved version of the MINDO semiempirical SCF-MO method. *J. Amer. Chem. Soc.* 97:1285-301, 1975. 83-0092
51	366	**Binkley J S, Pople J A & Hehre W J.** Self-consistent molecular orbital methods. 21. Small split-valence basis sets for first-row elements. *J. Amer. Chem. Soc.* 102:939-50, 1980. 83-0092
44	2201	**Chandrasekhar S.** Stochastic problems in physics and astronomy. *Rev. Mod. Phys.* 15:1-89, 1943. 83-0992
52	1018	**Clementi E & Roetti C.** Roothaan-Hartree-Fock atomic wavefunctions. *At. Data Nucl. Data Tables* 14:177-82, 1974. 83-0089
31	417	**Cooley J W.** An improved eigenvalue corrector formula for solving the Schrodinger equation for central fields. *Math. Computation* 15:363-74, 1961.
47	695	***Dewar M J S & Thiel W.** Ground states of molecules. 38. The MNDO method. Approximations and parameters. *J. Amer. Chem. Soc.* 99:4899-907, 1977. (14/85/ET&AS and PC&ES) 83-0092
30	579	**Hohenberg P & Kohn W.** Inhomogeneous electron gas. *Phys. Rev. B* 136:864-71, 1964. 83-0291
37	775	**Kramers H A.** Brownian motion in a field of force and the diffusion model of chemical reactions. *Physica* 7:284-304, 1940. 83-0992
38	394	**Moller C & Plesset M S.** Note on an approximation treatment for many-electron systems. *Phys. Rev.* 46:618-22, 1934.
30	237	**Morris G A & Freeman R.** Letter to editor. (Enhancement of nuclear magnetic resonance signals by polarization transfer.) *J. Amer. Chem. Soc.* 101:760-2, 1979. 83-0547
32	204	**Pulay P, Fogarasi G, Pang F & Boggs J E.** Systematic *ab initio* gradient calculation of molecular geometries, force constants, and dipole moment derivatives. *J. Amer. Chem. Soc.* 101:2550-60, 1979. 83-0092
41	2149	**Roothaan C C J.** New developments in molecular orbital theory. *Rev. Mod. Phys.* 23:69-89, 1951. 83-0092
31	177	**Tardy D C & Rabinovitch B S.** Intermolecular vibrational energy transfer in thermal unimolecular systems. *Chem. Rev.* 77:369-408, 1977. 83-0185
30	227	**Tauster S J, Fung S C & Garten R L.** Strong metal-support interactions. Group 8 noble metals supported on TiO_2. *J. Amer. Chem. Soc.* 100:170-5,1978. 83-0282

chemistry articles most cited from 1981 to 1983.[9] The papers by Michael J.S. Dewar and Walter Thiel, Department of Chemistry, University of Texas, Austin, and Clemens C.J. Roothaan, Departments of Chemistry and Physics, University of Chicago, Illinois, are also core to #83-0092 and were discussed previously.[10,11]

"Stochastic problems in physics and astronomy," by 1983 Nobel Prize winner Subrahmanyan Chandrasekhar, University of Chicago, was published in *Reviews of Modern Physics*. In fact, several non-core physics journals are represented in Table 6 by papers from *Reviews in Modern Physics*, *Physical Review*, *Physical Review B*, and *Physica*, while *JACS* and the only other general chemistry journal in the group, *Chemical Reviews*, account for 6 and 1, respectively, of the 16 articles in Table 6. One mathematics journal—*Mathematics of Computation*—and one nuclear data journal—*Atomic Data & Nuclear Data Tables*—also published papers heavily cited by our core group of journals.

Five of the journals in Table 6 (*Atomic Data & Nuclear Data Tables*, *Chemical Reviews*, *Mathematics of Computation*, *Physica*, and *Review of Scientific Instruments*) did not appear in Tables 2 and 3, where we list the journals that most often cited and were most often cited by the core group in 1983. Obviously, some articles from these journals are of relevance to physical chemistry and chemical physics, as indicated by their presence in Table 6. But the *journals* in which they were published are not regularly cited by chemists or physicists.

Conclusion

This then concludes our study of the "core" journals of physical chemistry and chemical physics for 1983. Although physical chemistry and chemical physics are both represented by journals in our core list, **it would appear that some journals are physical chemistry in name only. Chemical physics is the dominant force in both fields.** But, according to Mostafa A. El-Sayed, editor of the *Journal of Physical Chemistry*, "Since most of so-called chemical physics is carried out in chemistry departments (at least in the US), [the researchers] are called physical chemists." He concludes, "Thus it is my belief that physical chemistry is alive and well, because it has evolved with time."[12] Originally we had planned to subtitle this third part of the study, "Is physical chemistry dead? Long live chemical physics!" But El-Sayed's comment caused us to change that subtitle.

I'd like to thank all the other editors and researchers who also reviewed this extensive and difficult study. The subject boundaries of scientific fields are often as complex and confused as those of the political parties in the US. The differences between physical chemists and chemical physicists often become rather obscure. In a recent article, John Maddox, editor of *Nature*, stated that "the essence of a chemist is that he should be able to recite the Periodic Table and know which parts of it have which properties. This knowledge, the privileged possession of university teachers and their students as recently as half a century ago, is now more widely shared. People who build lasers have been forced to learn the language; so too have those who would design novel semiconductors or ternary alloys that are both magnetic and superconducting. Even the chemists' special knowledge of reactions, the feeling for the difference between a first-order and a second-order reaction, for example, has been partly hijacked by astrophysicists eager to know what happens to elements of the

Periodic Table in the spaces between stars."[13]

Malcolm W. Browne of the *New York Times* agrees with Maddox, noting that "the Nobel committee awarded its 1985 chemistry prize to a pair of mathematicians." And, he said, "Today's chemical discoveries are being rooted out in non-traditional ways. Both analysis and synthesis, the yin and yang of chemistry, are increasingly based on physics and mathematics, with help from a welter of computer-controlled instruments.... Physics and mathematics are...enabling chemists to understand the complex nature and effects of catalysts, and to predict the rates and results of chemical reactions."[14]

This three-part study of physical chemistry and chemical physics should therefore be useful to scientists and librarians in institutes of chemical physics or physical chemistry, as well as administrators who might use it to examine their reasons for keeping the two fields separate.

* * * * *

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