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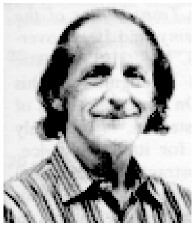

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# Journal Citation Studies. 46. Physical Chemistry and Chemical Physics Journals. Part 2. Core Journals and Most-Cited Papers

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In Part 1 of this analysis[1] we introduced the 31 core journals that are the focus of this three-part study. The list is reprinted in Table 1. Selecting these journals was a complex and difficult task, and I can say with complete candor that the use of the *Journal Citation Reports*® (*JCR*®) data to analyze the field of "physical chemistry" proved to be one of the most challenging assignments we ever undertook. Abigail Grissom and I, and several others at ISI®, struggled with the complexities of this problem for over two years. Indeed, our analysis is the result of numerous iterations of data primarily used in defining the "core" journals of physical chemistry by an algorithmic procedure. This task was difficult because we had to deal with the inherent problem of outmoded terminologies that scientists cling to in spite of vast changes in nomenclature. Perhaps the classic example that explains what I mean is the continued use of the title *Philosophical Magazine* by a modern journal of theoretical, experimental, and applied physics.

I began this exercise assuming naively that a publication such as the *Journal of Physical Chemistry* could reasonably be assumed to be the "core" journal of "physical chemistry." But that journal and the *Annual Review of Physical Chemistry* have titles that today are misleading. Although, according to B.S. Rabinovitch, editor of the *Annual Review of Physical Chemistry*, "It is not that the names have become inappropriate, it is that the subject matter of physical chemistry has altered in its refinement, methods, and technique although always concerned with 'chemistry.' The use of the term chemical physics to describe some research work undertaken in Chemistry Departments by chemists is a custom governed by politics and other social factors, but does not alter the fact that the subject matter—investigated by chemists and carried on in Chemistry Departments—is part of the domain of chemistry and constitutes physical chemistry. That some people prefer to call this chemical physics, or that some of it is published in the *Journal of Chemical Physics* is irrelevant. Such matter as appears in the *Journal of Physical Chemistry* and the *Annual Review of Physical Chemistry* is properly physical chemistry."[2] It is apparent that tradition, politics, and other social factors influence our choice of journal names as much as the "logic" of linguistic change.

As can be seen instantly in any issue of the *JCR* for the past decade, citation patterns reveal what activity has been occurring in the evolution of the century-old field of physical chemistry on its way to modern chemical physics. In short it is the transition of physical chemistry from the macro- and micro- substance level to the molecular and atomic level. If the lay observer asks why distinctions such as physical chemistry versus chemical physics persist, it is in part because the practice of chemistry and physics involves the application of physical-chemical knowledge accumulated long before the advent of modern chemical physics.

To return to our main theme then, our original problem in this study was to

**Table 1:** Core physical chemistry/chemical physics journals indexed by the *SCI*® in 1983, with the year each began publication*, the publisher country, and the language of publication.

| | | | |
|---|---|---|---|
| Annual Review of Physical Chemistry | 1950 | USA | Eng |
| Berichte der Bunsen-Gesellschaft fur Physikalische Chemie | 1894 | FRG | Eng/Fr/Ger |
| Chemical Physics | 1973 | Neth | Eng |
| Chemical Physics Letters | 1967 | Neth | Eng |
| Faraday Discussions of the Chemical Society | 1907 | UK | Eng |
| International Journal of Chemical Kinetics | 1969 | USA | Eng/Fr/Ger |
| International Journal of Quantum Chemistry | 1967 | USA | Eng/Fr/Ger |
| Journal of Catalysis | 1962 | USA | Eng |
| Journal of Chemical and Engineering Data | 1956 | USA | Eng |
| Journal of Chemical Physics | 1933 | USA | Eng |
| Journal of Chemical Thermodynamics | 1969 | UK | Eng |
| Journal of Colloid and Interface Science | 1946 | USA | Eng |
| Journal of Computational Chemistry | 1980 | USA | Eng |
| Journal of Magnetic Resonance | 1969 | USA | Eng |
| Journal of Molecular Spectroscopy | 1957 | USA | Eng |
| Journal of Molecular Structure | 1967 | Neth | Eng/Fr/Ger |
| Journal of Photochemistry | 1972 | Switz | Eng/Fr/Ger |
| Journal of Physical Chemistry | 1896 | USA | Eng |
| Journal of Solution Chemistry | 1972 | USA | Eng |
| Journal of the Chemical Society—Faraday Transactions I | 1905 | UK | Eng |
| Journal of the Chemical Society—Faraday Transactions II | 1905 | UK | Eng |
| Journal of the Chemical Society—Perkin Transactions II | 1966 | UK | Eng |
| Kinetics and Catalysis—English Translation | 1960 | USA/USSR | Eng |
| Molecular Physics | 1958 | UK | Eng |
| Photochemistry and Photobiology | 1962 | USA | Eng/Fr/Ger |
| Radiation Physics and Chemistry | 1969 | UK | Eng |
| Surface Science | 1964 | Neth | Eng/Fr/Ger |
| THEOCHEM—Journal of Molecular Structure | 1981 | Neth | Eng/Fr/Ger |
| Theoretica Chimica Acta | 1962 | USA | Eng/Fr/Ger |
| Zeitschrift fur Physikalische Chemie—Leipzig | 1887 | GDR | Eng/Fr/Ger |
| Zhurnal Fizicheskoi Khimii | 1930 | USSR | Russ |

*includes all superseded titles

identify the group of core journals listed in Table 1. We examined a vast amount of data and other literature to perform this task. In fact we gathered together so much information that we had to divide this essay into three parts so that we could present it all. Part 1 has already covered the historic aspects of the two fields; in this second installment we will discuss the 31 core journals that comprise the "macrojournal" of physical chemistry/chemical physics. We will also explain how we selected these periodicals.

## Core Journals

As any modern chemist knows, it is impossible to discuss physical chemistry without simultaneously reviewing chemical physics. As you can see from the list of journals we included in Table 1, these two disciplines encompass catalysis, chemical engineering, colloid science, computational chemistry, interfacial science, kinetics, magnetic resonance, molecular physics, molecular spectroscopy and structure, photochemistry and photobiology, quantum theory, radiation physics and chemistry, solution chemistry, surface science, thermodynamics, and theoretical chemistry. In a study reported in *Current Contents*® (*CC*®) over 13 years ago, I showed how little biochemistry is cited in this field.[3] That has not changed much today.

We chose the 31 core journals by looking at what each physical chemistry and chemical physics journal cited in 1983 and what journals cited them. We started with the *Journal of Physical Chemistry* only to find in the *JCR* that **it was more closely connected to journals in chemical physics than to itself**. We've included a subset of these data for 1983 in Table 2. It shows the 10 journals that were most cited in 1983 by the *Journal of Physical Chemistry* and the 10 journals

**Table 2:** Citations given to and received by the *Journal of Physical Chemistry* in 1983.

The 10 journals most cited by *J. Phys. Chem.* in 1983. A = citations from *J. Phys. Chem.* B = citations from all journals. C = percent of total citations from *J. Phys. Chem.* D = 1983 impact factor. E = 1983 immediacy index. F = 1983 source items.

| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| J. Chem. Phys. | 4180 | 73,961 | 5.7 | 2.96 | .77 | 1847 |
| J. Phys. Chem. | 2729 | 23,067 | 11.8 | 2.65 | .59 | 887 |
| J. Amer. Chem. Soc. | 2377 | 113,183 | 2.1 | 4.47 | .83 | 1777 |
| Chem. Phys. Lett. | 1240 | 18,485 | 6.7 | 2.23 | .50 | 1176 |
| Chem. Phys. | 401 | 6135 | 6.5 | 2.31 | .48 | 371 |
| Mol. Phys. | 398 | 7554 | 5.3 | 2.03 | .51 | 302 |
| J. Catal. | 336 | 7647 | 4.4 | 2.37 | .49 | 316 |
| J. Colloid Interface Sci. | 318 | 6851 | 4.6 | 1.48 | .30 | 386 |
| Surface Sci. | 254 | 14,436 | 1.8 | 3.99 | .71 | 535 |
| *Trans. Faraday Soc. | 249 | 5950 | 4.2 | — | — | 0 |

The 10 journals that most frequently cited *J. Phys. Chem.* in 1983. A = citations to *J. Phys. Chem.* B = citations to all journals. C = percent of total citations to *J. Phys. Chem.* D = 1983 impact factor. E = 1983 immediacy index. F = 1983 source items.

| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| J. Phys. Chem. | 2729 | 28,645 | 9.5 | 2.65 | .59 | 887 |
| J. Chem. Phys. | 1283 | 53,542 | 2.4 | 2.96 | .77 | 1847 |
| J. Amer. Chem. Soc. | 1098 | 58,661 | 1.9 | 4.47 | .83 | 1777 |
| Chem. Phys. Lett. | 680 | 21,631 | 3.1 | 2.23 | .50 | 1176 |
| J. Colloid Interface Sci. | 496 | 8122 | 6.1 | 1.48 | .30 | 386 |
| Inorg. Chem. | 393 | 25,473 | 1.5 | 2.68 | .46 | 848 |
| J. Chem. Soc. Faraday Trans. I | 389 | 6449 | 6.0 | 1.38 | .46 | 271 |
| Bull. Chem. Soc. Jpn. | 377 | 16,069 | 2.4 | .96 | .32 | 882 |
| J. Catal. | 320 | 7309 | 4.4 | 2.37 | .49 | 316 |
| Can. J. Chem. | 309 | 12,410 | 2.5 | 1.24 | .29 | 483 |

*precursor to *Journal of the Chemical Society—Faraday Transactions I* and *II* (1972).

that most often cited it that year. (It is interesting that the general chemical journal, *Bulletin of the Chemical Society of Japan*, appears in Table 2. Japanese physical chemists and chemical physicists may publish in that journal because Japanese publishers do not publish many periodicals devoted specifically to physical chemistry and chemical physics.) We conducted the same exercise for the *Journal of Chemical Physics* (see Table 3, the top 10 journals that it cited in 1983 and vice versa) and continued the process for each journal in the two fields.

We then put together two separate lists of journals based on this information. (One list had only physical chemistry journals; the other included chemical physics journals.) The next step was to look at what each of these groups cited. In both lists chemical physics journals were highly cited. We then combined the lists, including only those journals that significantly cited the other core journals. We looked at what these journals cited, and, with the help of Henry Small, ISI's director of research, as well as the journal-evaluation group at ISI, we determined which journals from fields such as catalysis, colloid science, interfacial science, and so on, should also be included in the core. This exhaustive process eventually resulted in the core list of 31 journals in Table 1, although the *Journal of the Chemical Society—Faraday Transactions I* and *II*, each listed separately, should really be considered as one journal. It is published in two parts only for ease of production, according to its editor, David Young.[4] We'll have more to say about this journal later. And when we discuss

**Table 3:** Citations given to and received by the *Journal of Chemical Physics* in 1983.

The 10 journals most cited by *J. Chem. Phys.* in 1983. A = citations from *J. Chem. Phys.* B = citations from all journals. C = percent of total citations from *J. Chem. Phys.* D = 1983 impact factor. E = 1983 immediacy index. F = 1983 source items.

| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| J. Chem. Phys. | 15,263 | 73,961 | 20.6 | 2.96 | .77 | 1847 |
| Chem. Phys. Lett. | 2887 | 18,485 | 15.6 | 2.23 | .50 | 1176 |
| J. Phys. Chem. | 1283 | 23,067 | 5.6 | 2.65 | .59 | 887 |
| J. Amer. Chem. Soc. | 1244 | 113,183 | 1.1 | 4.47 | .83 | 1777 |
| Chem. Phys. | 1215 | 6135 | 19.8 | 2.31 | .48 | 371 |
| Mol. Phys. | 1171 | 7554 | 15.5 | 2.03 | .51 | 302 |
| Phys. Rev. A—Gen. Phys. | 1079 | 18,190 | 5.9 | 2.64 | .61 | 913 |
| Phys. Rev. | 1024 | 29,909 | 3.4 | — | — | 0 |
| Phys. Rev. Lett. | 921 | 48,031 | 1.9 | 6.46 | 1.50 | 1165 |
| Phys. Rev. B—Condensed Matter | 894 | 41,410 | 2.2 | 3.27 | .71 | 1961 |

The 10 journals that most frequently cited *J. Chem. Phys.* in 1983. A = citations to *J. Chem. Phys.* B = citations to all journals. C = percent of total citations to *J. Chem. Phys.* D = 1983 impact factor. E = 1983 immediacy index. F = 1983 source items.

| | A | B | C | D | E | F |
|---|---|---|---|---|---|---|
| J. Chem. Phys. | 15,263 | 53,542 | 28.5 | 2.96 | .77 | 1847 |
| J. Phys. Chem. | 4180 | 28,645 | 14.6 | 2.65 | .59 | 887 |
| Chem. Phys. Lett. | 4130 | 21,631 | 19.1 | 2.23 | .50 | 1176 |
| Chem. Phys. | 2856 | 12,029 | 23.7 | 2.31 | .48 | 371 |
| J. Amer. Chem. Soc. | 2100 | 58,661 | 3.6 | 4.47 | .83 | 1777 |
| Mol. Phys. | 1681 | 7857 | 21.4 | 2.03 | .51 | 302 |
| Int. J. Quantum Chem. | 1266 | 8666 | 14.6 | 1.15 | .35 | 309 |
| Phys. Rev. A—Gen. Phys. | 1251 | 21,413 | 5.8 | 2.64 | .61 | 913 |
| Phys. Rev. B—Condensed Matter | 1223 | 49,717 | 2.5 | 3.27 | .71 | 1961 |
| THEOCHEM—J. Mol. Struct. | 893 | 6524 | 13.7 | .69 | .19 | 246 |

its rankings by citation in Part 3 of this study, we will examine each part as a separate entity and then combine these two parts and examine them as one journal. The reader should also note that only the second part of the *Journal of the Chemical Society—Perkin Transactions* is included here. Part I covers organic and bio-organic chemistry.

It is unfortunate that we could not include the newest physical chemistry/chemical physics journal, *Langmuir*, in this study. The American Chemical Society's new journal of surfaces and colloids is named after the noted physical chemist and Nobel laureate, Irving Langmuir.[5] This journal, which is published every two months, began in January 1985. To date just six issues have appeared. A cursory look at the references listed in it seems to confirm that it cites the core journals in this study quite heavily. We also did not include *Advances in Chemical Physics* in the core list primarily because, until recently, we treated it in the *Science Citation Index®* (*SCI®*) as a book series rather than a journal. However, it does show up in the *JCR* and in our analysis in Part 3 of this study.

Of the journals selected for our analysis, 19 publish exclusively in English, while 10 are multilingual, publishing articles in English, French, and German. Two are published in separate English and Russian editions. (See Table 1.) *Zhurnal Fizicheskoi Khimii* contains only Russian-language articles, although an English translation is published in London under the title *Russian Journal of Physical Chemistry*. *Kinetics and Catalysis*, the English translation of the Soviet *Kinetika i Kataliz*, is also included here. The reason that we process the original version of one and the translation of the other is simply that we added a few key journals to the original *SCI* database and later on included new journals in their translated form. Citation counts for both versions of translated journals are unified in the *JCR*. So the impact calculation for these journals is approximately correct except for delay in citations caused by the lag in publishing translations.

The countries in which the 31 core journals are published are also listed in Table 1. As you can see, almost half of the journals are from the US. Seven journals are published in the UK, five in The Netherlands, and one journal each is published in the German Democratic Republic (GDR), the Federal Republic of Germany, Switzerland, and the USSR.

The oldest continuously published *core* journal is the *Journal of Physical Chemistry*, established in 1896. It is published by the American Chemical Society, as is the *Journal of Chemical and Engineering Data*, also in Table 1. *Zeitschrift für Physikalische Chemie—Leipzig*, which started publishing earlier, in 1887, changed its title several times and suspended publication for six years in the 1940s. It was founded in Leipzig, now in the GDR, as *Zeitschrift für Physikalische Chemie, Stöchiometrie und Verwandtschaftslehre* (*Journal for Physical Chemistry, Stoichiometry and Chemical Affinity*). In 1928 it split into two parts—*Section A: Chemical Thermodynamics, Kinetics, Electrochemistry, and Theory of Properties*, and *Section B: Chemistry of Simple Reactions and Structure of Matter*. But in 1943, during World War II, these two sections were rejoined to form *Zeitschrift für Physikalische Chemie—Leipzig*. The journal ceased publication in October 1944 and did not resume again until 1950. It continues to be published in Leipzig.[6-8]

Another journal, now published in Munich, was also called *Zeitschrift für Physikalische Chemie* until 1983. It is not included in this study. This journal, which was first published in 1954 in Frankfurt and then in Wiesbaden, is now published by Oldenbourg Verlag, Munich, and is called *Zeitschrift für Physikalische Chemie Neue Folge, International Journal of Research in Physical Chemistry and Chemical Physics*. Because the journal's original title is identical to that of the Leipzig journal, citations to it may be attributed to the Leipzig journal, especially since researchers do not always provide complete journal titles in their references. Now that the Munich journal has modified its title, there will be less possibility of confusion in the future. Note that it has added an English "second" title that substantiates the point of this essay.

There are, of course, additional journals in Table 1, such as *Berichte der Bunsen-Gesellschaft für Physikalische Chemie*, that over the years have changed their titles or not published continuously. Some have even changed their focus. Tracking these often complicated journal histories is interesting. But we are unable to explain each journal's history in detail in this study.

The two most recent journals in Table 1 are the *Journal of Computational Chemistry*, started in 1980, and *THEOCHEM—Journal of Molecular Structure*, established in 1981. *THEOCHEM* is published by Elsevier in conjunction with the *Journal of Molecular Structure*, established in 1967. The *Journal of Chemical Physics* did not begin publishing until 1933; the 40-year gap between its founding and that of the *Journal of Physical Chemistry* symbolizes the revolution in chemistry that occurred in that period. *Chemical Physics Letters* and *Chemical Physics* were not established by North Holland until 1967 and 1973, respectively. These dates should not be surprising since we know from Part 1 of this study that physical chemistry developed before chemical physics. And Subbiah Arunachalam, editor of the *Indian Journal of Technology*, reminds us that the development of physical chemistry and chemical physics is analogous to the development of classical biology and modern molecular and cell biology. Classical biology and microbiology had to mature before specialization in cell or molecular biology could occur. The levels of perception move from the gross to the fine. In short, physical chemistry symbolizes an earlier stage of a vast area of research that is now more often called chemical physics because modern chemistry and physics seek and provide molecular- and submolecular-level explanations for what physical chemistry sought at the compound or substance level. Chemical physics can deal with the two major concerns of physical chemistry: thermodynamic situations, where time does not play a factor; and time-dependent processes such as kinetics, catalysis, and photochemistry.[9]

## Most-Cited Papers

Another way that we examine core journals in these types of studies is by looking at their most-cited papers. In Table 4 we have listed these articles for each core journal, based on citation data from the 1955-1983 *SCI*. The numbers are also given for the 1983 research fronts in which these papers appear. Since these fronts were discussed in detail in Part 1 of this study, we won't repeat that information here. Four journals—*Journal of the Chemical Society—Perkin Transactions II*, *Radiation Physics and Chemistry*, *THEOCHEM—Journal of Molecular Structure*, and *Journal of Computational Chemistry*—are not represented in Table 4 for several reasons. The last two journals only recently began publishing. The complex history of the various sections of the *Journal of the Chemical Society* makes it difficult to identify all papers for a particular section without an article-by-article analysis. The time and effort for such a project could not be justified for this study.

For example, *Faraday Transactions I* and *II* and *Perkin Transactions II*, the sections of the *Journal of the Chemical Society* included here, all began publishing under their current titles in 1972. However, the former two began in 1905 as one journal, *Transactions of the Faraday Society*, as mentioned in Part 1. And beginning in January 1986 these two journals will again undergo a title modification. Young explains this change: "A marked imbalance has developed between *Faraday I* and *II*, since their inception in 1972.... It can be [partially] attributed to a longer-term trend, whereby the development of a new instrumental technique is often best regarded as a contribution to 'chemical physics' but when the technique matures and is widely applied to practical problems, it is seen as contributing to 'physical chemistry.' This happens regularly, and it results in a net flow of papers from *Faraday II* to *I*. In order to redress the balance it has been decided to designate *Faraday I* as a *Journal of Physical Chemistry in Condensed Phases* and *Faraday II* as a *Journal of Molecular and Chemical Physics*.... The coverage of *Faraday II* will thus be keyed to the growth points in chemical physics, while *Faraday I* will cover all major areas of physical chemistry, including those which exploit modern experimental techniques."[4]

Another problem created by journals that change titles is illustrated in Table 4 where the most-cited paper from the *Faraday Discussions of the Chemical Society* was actually published in *Discussions of the Faraday Society*, the journal's title from 1947 to 1972. And an additional difficulty in identifying most-cited papers has to do with tracking citations to articles published in Soviet journals as well as their translations.

The most-cited paper in Table 4, by Robert F. Stewart, Ernest R. Davidson, and William T. Simpson, Department of Chemistry, University of Washington, Seattle, was published in the *Journal of Chemical Physics*. Entitled "Coherent x-ray scattering for the hydrogen atom in the hydrogen molecule," it has been cited over 6,500 times. In 1977 Davidson published a *Citation Classic*® commen-

**Table 4:** The most-cited article from each core physical chemistry/chemical physics journal cited at least 50 times in the *SCI*®, 1955-1983, in alphabetic order by first author. A = 1955-1983 citations. The 1984 citations appear in parentheses. B = bibliographic data. C = total number of papers from that journal cited at least 50 times. An asterisk (*) before a paper indicates that it 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 for 1983 also follow the reference.

| A | | B | C |
|---|---|---|---|
| 189 | (20) | **Baerends E J, Ellis D E & Ros P.** Self-consistent molecular Hartree-Fock-Slater calculations. I. The computational procedure. *Chem. Phys.* 2:41-51, 1973. | 56 |
| 1187 | (146) | **Bondi A.** van der Waals volumes and radii. *J. Phys. Chem.* 68:441-51, 1964. | 1383 |
| 82 | (2) | **Boreskov G K.** Mechanism of catalytic oxidation reactions on solid oxide catalysts. *Kinet. Catal.—Engl. Tr.* 14:7-24, 1973. | 7 |
| 303 | (24) | **Campbell I D, Dobson C M, Williams R J P & Xavier A V.** Resolution enhancement of protein PMR spectra using the difference between a broadened and a normal spectrum. *J. Magn. Resonance* 11:172-81, 1973. | 84 |
| 191 | (57) | **Doi M & Edwards S F.** Dynamics of concentrated polymer systems. Part 1.—Brownian motion in the equilibrium state. *J. Chem. Soc. Faraday Trans. II* 74:1789-801, 1978. 83-0495 | 40 |
| 254 | (4) | **Fox H W & Zisman W A.** The spreading of liquids on low-energy surfaces. I. Polytetrafluoroethylene. *J. Colloid Sci.* 5:514-31, 1950. 83-0806 | 203 |
| 614 | (39) | **Frank H S & Wen W-Y.** III. Ion-solvent interaction. Structural aspects of ion-solvent interaction in aqueous solutions: a suggested picture of water structure. *Discuss. Faraday Soc.* 24:133-40, 1957. 83-0948 | 94 |
| 307 | (21) | **Gouterman M.** Spectra of porphyrins. *J. Mol. Spectrosc.* 6:138-63, 1961. | 249 |
| 181 | (33) | **Israelachvili J N, Mitchell D J & Ninham B W.** Theory of self-assembly of hydrocarbon amphiphiles into micelles and bilayers. *J. Chem. Soc. Faraday Trans. I* 72:1525-68, 1976. 83-0075 | 26 |
| 254 | (13) | ***Kell G S.** Precise representation of volume properties of water at one atmosphere. *J. Chem. Eng. Data* 12:66-9, 1967. (31/79/ET&AS) | 21 |
| 317 | (33) | **Kok B, Forbush B & McGloin M.** Cooperation of charges in photosynthetic $O_2$ evolution—I. A linear four step mechanism. *Photochem. Photobiol.* 11:457-75, 1970. | 150 |
| 194 | (14) | **Kuchitsu K, Fukuyama T & Morino Y.** Average structures of butadiene, acrolein, and glyoxal determined by gas electron diffraction and spectroscopy. *J. Mol. Struct.* 1:463-79, 1968. | 32 |
| 663 | (70) | **Marcus R A.** Chemical and electrochemical electron-transfer theory. *Annu. Rev. Phys. Chem.* 13:155-95, 1964. 83-0075 | 89 |
| 885 | (29) | **Mataga N & Nishimoto K.** Electronic structure and spectra of nitrogen heterocycles. *Z. Phys. Chem.—Leipzig* 13:140-57, 1957. 83-0092 | 70 |
| 220 | (20) | **McIver J W & Komornicki A.** Rapid geometry optimization for semi-empirical molecular orbital methods. *Chem. Phys. Lett.* 10:303-6, 1971. 83-0211 | 348 |
| 807 | (20) | ***McLachlan A D.** Self-consistent field theory of the electron spin distribution in π-electron radicals. *Mol. Phys.* 3:233-52, 1960. (24/81/PC&ES) | 342 |
| 111 | (5) | **O'Neal H E & Benson S W.** Entropies and heat capacities of free radicals. *Int. J. Chem. Kinet.* 1:221-43, 1969. | 19 |
| 323 | (11) | **Parry E P.** An infrared study of pyridine adsorbed on acidic solids. Characterization of surface acidity. *J. Catal.* 2:371-9, 1963. | 207 |
| 147 | (18) | **Picker P, Leduc P-A, Philip P R & Desnoyers J E.** Heat capacity of solutions by flow microcalorimetry. *J. Chem. Thermodyn.* 3:631-42, 1971. | 18 |
| 175 | (25) | **Picker P, Tremblay E & Jolicoeur C.** A high-precision digital readout flow densimeter for liquids. *J. Solut. Chem.* 3:377-84, 1974. 83-0506 | 18 |
| 253 | (56) | **Pople J A, Binkley J S & Seeger R.** Theoretical models incorporating electron correlation. *Int. J. Quantum Chem. Symp.* 10:1-19, 1976. 83-0092 | 44 |
| 415 | (20) | **Powell C J.** Attenuation lengths of low-energy electrons in solids. *Surface Sci.* 44:29-46, 1974. 83-0058 | 399 |
| 294 | (43) | **Rehm D & Weller A.** Kinetik und Mechanismus der Elektronubertragung bei der Fluoreszenzloschung in Acetonitril (Kinetics and mechanism of electron transfer by fluorescence quenching in acetonitril). *Ber. Bunsen Ges. Phys. Chem.* 73:834-9, 1969. 83-0075 | 107 |
| 416 | (25) | **Roos B & Siegbahn P.** Gaussian basis sets for the first and second row atoms. *Theor. Chim. Acta* 17:209-15, 1970. 83-0092 | 145 |
| 6072 | (435) | ***Stewart R F, Davidson E R & Simpson W T.** Coherent x-ray scattering for the hydrogen atom in the hydrogen molecule. *J. Chem. Phys.* 42:3175-87, 1965. (48/77) 83-0344 | 6314 |
| 125 | (24) | **Sutin N.** Light-induced electron transfer reactions. *J. Photochem.* 10:19-40, 1979. | 4 |
| 205 | (8) | **Temkin M I.** Adsorption equilibrium and the kinetics of processes on nonhomogeneous surfaces and in the interaction between adsorbed molecules. *Zh. Fiz. Khim. SSSR* 15:296-332, 1941. | 41 |

tary that gave a straightforward explanation for the prolific number of citations to the paper: "[It] was written in response to a recognized need. It contains a table of X-ray scattering factors appropriate for a bonded hydrogen atom. This table has been incorporated in most standard X-ray crystallography computer packages and generates an 'automatic' citation each time a new crystal structure containing a hydrogen atom is solved."[10] This paper also appeared in a study on the most-cited physical-sciences papers from the 1960s.[11]

Incidentally, to give adequate justice to the many articles published by the *Journal of Chemical Physics*, we would have to do a separate study. The journal has published over 20,000 articles since 1974. And more than 200 papers from it have been cited over 300 times, almost 1 percent of the articles it published in the last decade. The second most-cited article from that journal received about 2,600 citations since its publication in 1970. Interestingly, it too discusses scattering factors for X rays. Don T. Cromer and David Liberman, Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico, authored "Relativistic calculation of anomalous scattering factors for X rays."[12]

Two additional papers in Table 4 have been the subject of *Citation Classic* commentaries. George S. Kell, Division of Applied Chemistry, National Research Council, Ottawa, Canada, discussed "Precise representation of volume properties of water at one atmosphere," which has been cited over 267 times.[13] The classic work by Andrew D. McLachlan, Department of Theoretical Chemistry, University Chemical Laboratory, University of Cambridge, UK, has received about 830 citations. It describes the self-consistent field theory of electron spin distribution in π-electron radicals.[14]

Van der Waals volumes and radii are the subject of the second most-cited paper in the list. Published in the *Journal of Physical Chemistry* in 1964, it has been cited over 1,300 times. The author, Arnold Bondi, Shell Development Company, Emeryville, California, died in 1979. Perhaps one of his colleagues will one day comment on this classic paper for *CC* readers.

## Conclusion

In Part 3, our next and final installment of this study, we will continue our analysis of the 31 core journals. There we will present in tabular form the results of our detailed citation study of the "macrojournal" of physical chemistry/chemical physics. At that time we will summarize our findings.

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