

The 1985 Chemistry Articles Most Cited in 1985-1987: Quantum Mechanics, Superconductivity, and... Buckminster Fuller?!

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This study of the 1985 chemistry articles most cited in 1985-1987 shows several trends based on ISI® research-front activity. Among these are intense interest in the reaction chemistry of transition-metal molecules, in carbon-hydrogen activation, and in breaking organic bonds through transition-metal reagents. Also evident is continued strong interest in organic superconductors and nuclear magnetic resonance imaging techniques. New applications of quantum mechanics and thermodynamics and the discovery of a long-chain carbon molecule named after the late, distinguished inventor R. Buckminster Fuller are also discussed.

As longtime readers of *Current Contents*® know, we regularly identify and discuss papers in chemistry, the physical sciences, and the life sciences that become highly cited shortly after publication; indeed, our most recent examination of such papers concerned the 1984 chemistry articles most cited from 1984 to 1986.¹

This essay discusses the 1985 chemistry articles most cited from 1985 through 1987. Chemistry, like the life and physical sciences, partakes of other, more-or-less related fields; thus, the selection process for each involves more than simply determining a suitable citation threshold for establishing which papers to include. For chemistry, however, the selection process is more extensive and complicated.

As in previous essays on highly cited chemistry articles, we used an in-house, unpublished subset of the *Science Citation Index*® (SCI®) known as the "Chemistry Citation Index" to try to limit the papers we included in the study to pure chemistry, but this is an exercise in futility, since modern chemistry is so multidisciplinary. Once a rough list was compiled, we made an effort to remove papers that might just as easily be placed among the highly cited papers in the "physical" or "life" sciences. Nevertheless, the multidisciplinary nature of

chemistry is still evident in the Bibliography; for example, the list includes 10 papers from the *Journal of Chemical Physics*.

The 100 papers in the Bibliography received an average of about 44 citations each—4 in 1985, 18 in 1986, and 22 in 1987. The most-cited paper in the study is an analysis of four major organic reactions that led to a method of predicting the outcome of certain types of reactions; published by Satoru Masamune and colleagues, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, the paper received 112 citations—21 in 1985, 45 in 1986, and 46 in 1987. Using the CD-ROM version of the SCI,² we determined that this article has been cited an additional 28 times from January through June 1988. The 15 least-cited papers in the Bibliography received 32 citations each over the three-year study period—the threshold for inclusion in the essay. The median number of citations to papers in this study, however, is about 40.

Once the Bibliography is established, we always examine it in order to spot trends or unusual papers. In the 1985 list, we observed continued interest in organic superconductors, a new application of quantum mechanics, and a surprise: a substance named after the late, distinguished inventor R. Buckminster Fuller!³

Research Fronts

While eponymy is by no means unusual in science, it generally involves an individual who has made landmark contributions to a field. (Although, according to a dictum offered by Stephen M. Stigler, Department of Statistics, University of Chicago, Illinois, "No scientific discovery is named after its original discoverer." Writing in *Transactions of the New York Academy of Sciences*, in a *festschrift* issue honoring sociologist Robert K. Merton, Columbia University, New York [I also had the pleasure of contributing to this issue], Stigler titled his own pronouncement, with a facetious lack of humility, "Stigler's law of eponymy."⁴ Stigler was mentioned in our 1983 essay on eponymy.⁵)

Since Fuller was not a chemist, we were intrigued by the circumstances under which his name would be lent to a chemical. As it turned out, in trying to understand how long-chain carbon molecules are formed in interstellar space, H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, and R. E. Smalley (who led the effort), Rice Quantum Institute and Departments of Chemistry and Electrical Engineering, Rice University, Houston, Texas, discovered a molecule of 60 carbon atoms. They dubbed the molecule "buckminsterfullerene," since the structure they proposed for it is remarkably similar to the pattern on the hide of a soccer ball and to Bucky's famous geodesic dome. The authors are "disturbed," however, at the unwieldiness of their "rather fanciful but highly appropriate name," and have suggested a number of alternatives, including "ballene," "spherene," "soccerene," and "carbosoccer." Discussing this molecule in their book *Organic Chemistry: The Name Game*, chemists Alex Nickon, Johns Hopkins University, Baltimore, Maryland, and Ernest F. Silversmith, Morgan State University, Baltimore, point out that the cluster has also been informally referred to as "buckyball" and "BF."⁶ Kroto and colleagues state that they are willing to leave the final choice up to the chemistry community as a whole.

The paper by Kroto and colleagues was published in November 1985 but was not cited during that year (not surprising, perhaps, considering how late in the year it appeared). However, it picked up 44 citations in 1986 and 53 in 1987 (making it the second most-cited paper in the Bibliography). Remarkably, it also was cited 37 times in the first half of 1988. It is among the 26 papers forming the core of the 1986 research front on "Small alkali metal clusters, metal cluster ion photofragmentation, Fourier transform ion cyclotron resonance mass spectrometry, and magic number" (#86-2748). A list of the 1986 and 1987 research fronts with at least three of the papers in the Bibliography as core documents can be found in Table 1.

Research fronts form when pairs of earlier papers (from any year) are cited together frequently by later papers from a specific year—in this essay, we are concentrating on published (citing) papers from the years 1986 and 1987. The fact that a number of 1985 chemistry articles so quickly became core to new research fronts is an indication that they are on the cutting edge of their fields. It also verifies the importance and currency of the papers included in this study.

The fifth most-cited paper, a review article by Robert H. Crabtree, Sterling Chemistry Laboratory, Yale University, New Haven, Connecticut, is core to a research front in Table 1 and is indicative of the continued interest in breaking extremely strong organic bonds through transition-metal reagents. Crabtree's discussion of the literature on activating the "notoriously unreactive" set of substrates called alkanes was cited 32 times in 1986, 52 times in 1987, and 31 times from January through June 1988. It is core to the 1986 front on "Arene C-H bond activation, molecular hydrogen complexes, catalytic intermolecular h/d exchange, and aliphatic C-H bonds" (#86-3302). A total of six papers in the Bibliography deal with the subject of carbon-hydrogen activation, including another paper by Crabtree that was coauthored with Yale colleague Maryellen Lavin. It concerns an

Table 1: The 1986 and 1987 ISI® research fronts that include at least three of the 1985 chemistry papers as core documents. A=number of Bibliography papers that are core to each research front. B=total number of core documents. C=total number of citing papers published for the year designated by the prefix.

Number	Name	A	B	C
86-2094	Organic conductors, superconducting BEDT-TTF salts, and band electronic structures	5	45	293
86-2748	Small alkali metal clusters, metal cluster ion photofragmentation, Fourier transform ion cyclotron resonance mass spectrometry, and magic number	3	26	336
86-3302	Arene C-H bond activation, molecular hydrogen complexes, catalytic intermolecular h/d exchange, and aliphatic C-H bonds	3	20	255
86-5002	Oxidative coupling of methane, partial oxidation, and selective catalysts	4	6	31
87-1356	NMR spectroscopy, two-dimensional NMR spectra, distance geometry, H-1 spin systems, and water suppression	4	52	723
87-1442	Inductively coupled plasma mass spectrometry, boron isotope ratios in geological materials, and easily ionizable concomitant elements	3	22	131
87-1603	Electronic states, allowed 3-3 transitions for ions, and <i>ab initio</i> relativistic effective potentials	3	14	224
87-2095	High- T_c superconducting state of β -(BEDT-TTF) $_2$ I $_3$, molecular conductors, BEDT-TTF charge-transfer salts, band electronic structures, and ambient pressure	4	41	260
87-3077	Oxidative coupling of methane, oxide catalysts, and highly selective ethane formation	4	20	122
87-3442	Two polaron bipolaron state in polyaniline, electrochemical polymerization, polyaniline electrode films, and oxidation of pyrrole	3	42	365

extension of their earlier work on the activation of alkanes.

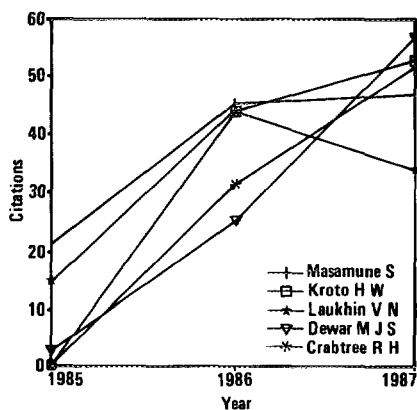
A related area concerns the study of the reaction chemistry of free clusters of transition-metal molecules in the gas phase. Two such papers were coauthored by M.D. Morse, M.E. Geusic, and colleagues, Rice University, and three by D.J. Trevor, R.L. Whetten, and colleagues, Exxon Research and Engineering Company, Annandale, New Jersey. Another paper, by J. Chandrasekhar and colleagues, Department of Chemistry, Purdue University, West Lafayette, Indiana, is a theoretical study of reactions in solution (as opposed to the gas phase).

An important catalytic reaction was discovered in 1985 by J.H. Lunsford and colleagues, Texas A&M University, College Station, and discussed in several papers in the Bibliography, including two by T. Ito, also of Texas A&M, Lunsford, and colleagues; one by D.J. Driscoll, also of Texas A&M, Lunsford, and colleagues; and another by K. Otsuka and colleagues, Department of Chemical Engineering, Tokyo Institute of Technology, Japan. The reaction, which involves the oxidative coupling of methane to higher hydrocarbons over oxide catalysts, is especially interesting because it is mediated by methyl radicals.

Quantum Mechanics and Thermodynamics

Other areas of interest discussed in articles among this year's top five most-cited papers include quantum mechanics and thermodynamics. A year-by-year comparison of the number of citations to each of these five papers is shown in Figure 1.

Figure 1: Most-cited 1985 chemistry papers. Year-by-year citations to the five 1985 chemistry papers most cited in the *SCF*®, 1985-1987. Papers shown are Masamune S. *Angew. Chem. Int. Ed.* 24:1-76, 1985; Kroto H W. *Nature* 318:162-3, 1985; Laukhin V N. *JETP Lett.—Engl. Tr.* 41:81-4, 1985; Dewar M J S. *J. Amer. Chem. Soc.* 107:3902-9, 1985; and Crabtree R H. *Chem. Rev.* 85:245-69, 1985.



Michael J.S. Dewar and colleagues, Department of Chemistry, University of Texas, Austin, report the latest results in their development of a quantum mechanical molecular model for use in the study of chemical reactions and reaction mechanisms. The paper, as the authors point out, represents the 76th part in their long series of articles, and was cited 3 times in 1985, 25 times in 1986, and 57 times in 1987, making it the fourth most-cited paper in the Bibliography; furthermore, it was cited an astounding 69 times through the first six months of this year, indicating intense and mounting interest in this topic. Dewar also had three papers⁷⁻⁹ in the 1984 study,¹ one coauthored by colleague Adriana B. Pierini.

A review by Reed M. Izatt, Department of Chemistry, Brigham Young University, Provo, Utah, and colleagues discusses the interrelationships between heat and other energy forms (such as kinetics, or motion) in reactions between anions and cations with macrocyclic polyethers and polyamines. Uncited in 1985, it received 34 citations in 1986 and 42 in 1987; it was also cited 29 times in the first half of 1988.

Nuclear Magnetic Resonance and Superconductivity

As noted in our 1984 study,¹ 1983's list was dominated by articles on nuclear magnetic resonance (NMR),¹⁰ an imaging technique that enables chemists to make use of the motion of atoms in the study of molecular structures. NMR techniques faded somewhat from the limelight in the 1984 study, but resurface in this year's study. In fact, by far the largest research front in Table 1 concerns NMR: "NMR spectroscopy, two-dimensional NMR spectra, distance geometry, H-1 spin systems, and water suppression" (#87-1356) consists of 723 current papers that cited 52 core documents.

Among the documents that are core to this front are two papers by Ad Bax and colleagues, Laboratory of Chemical Physics, National Institute of Arthritis, Diabetes, and Digestive and Kidney Diseases (NIADDKD), National Institutes of Health (NIH), Bethesda, Maryland; they

Table 2: The number of authors per paper for the 1985 chemistry articles most cited in the *SCF*[®], 1985-1987.

Number of Authors per Paper	Number of Papers
12	2
8	1
7	4
6	4
5	8
4	18
3	12
2	35
1	16

deal with the use of NMR in the study of peptides, small proteins, and other complex organic molecules. Bax is also a coauthor on two other papers in this year's list; his colleague Donald G. Davis, also of NIADDKD, NIH, is coauthor on three papers. As will be seen, other groups of authors also have several papers in the Bibliography, accounting for the fact that, although there are 265 unique authors in this year's list, there are 318 author occurrences. A full breakdown of the number of authors per paper is given in Table 2; there are 13 authors with three papers on the list, 24 with two, and 227 with one paper each.

Five papers in the study discuss superconductivity, an area that has become a "hot" topic (you should pardon the expression) recently in the field of the physical sciences as various laboratories have raced to see which would be the first to discover substances with virtually no resistance to electricity at temperatures substantially higher than near-absolute zero, the previous limit of the phenomenon. One of these, by V.N. Laukhin and colleagues, Institute of Chemical Physics, Academy of Sciences of the USSR, Moscow, is the third most-cited paper in the study. Cited a total of 92 times from 1985 through 1987, it was cited 14 times through the first six months of this year.

Keep in mind, however, that the application of superconductivity discussed by these authors is distinct from that being pursued by physicists. Chemists are concerned with a class of organic superconductors known as bis(ethylenedithio)tetrathiafulvalene, abbreviated BEDT-TTF; the breakthrough in

superconductivity, for which the 1987 Nobel in physics was awarded,¹¹ was published in 1986 by Karl Alex Müller and Johannes Georg Bednorz, IBM Zurich Research Laboratory, Rüschlikon, Switzerland,¹² and concerns superconductors that function at a much higher temperature than organic superconductors. Incidentally, the Bednorz and Müller paper is among the works included in the study of the 1986 physical-sciences papers most cited in 1986 and 1987, to be published early next year.

Another topic that appeared in our 1984 study and reappears in this one concerns complexes of molecular hydrogen. As noted by Roald Hoffmann, Department of Chemistry, Cornell University, Ithaca, New York, who won the Nobel Prize in chemistry in 1981,¹³ hydrogen can bind either as a molecule or by splitting into two hydrides.¹⁴ The first kind of binding was unknown until 1984, when G.J. Kubas and colleagues, Los Alamos National Laboratory, New Mexico, became the first to characterize examples of isolable molecular hydrogen complexes.¹⁵ Among the papers in this study that follow up on the Kubas group's work (which appeared in the 1984 study¹) are studies by S.P. Church and colleagues, Max Planck Institute for Radiation Chemistry, Mülheim/Ruhr, Federal Republic of Germany (FRG); R.H. Morris and colleagues, University of Toronto, Ontario, Canada; H.J. Robota and colleagues, Institute for Physical Chemistry, University of Munich, FRG; and R.K. Upmacis and colleagues, University of Nottingham, UK. This work is closely connected to the C-H activation work by Crabtree and others, mentioned earlier.

Incidentally, Hoffmann is one of two Nobelists whose work appears in this study's Bibliography. Continuing his recent work on transition metals, Hoffmann coauthored a paper with Shen-Shu Sung, also of Cornell, on the bonding of carbon monoxide to various metal surfaces, including chromium, cobalt, iron, nickel, and titanium. Hoffmann also appears as coauthor of another paper on transition metals, by Kazuyuki Tatsumi, Osaka University, Japan, and colleagues. Also in the Bibliography is a paper by 1987

Table 3: National locations of the institutional affiliations listed by authors in the Bibliography, according to total appearances (column A). B=number of papers coauthored with researchers affiliated with institutions in other countries. C=national locations of institutions listed by coauthors.

Country	A	B	C
US	75	8	Belgium, China, FRG, France, Italy, Japan, USSR, Yugoslavia
FRG	8	3	Austria, Czechoslovakia, Japan, US
UK	5	0	
France	4	2	Belgium, US
Japan	4	2	China, FRG, US
Australia	2	1	The Netherlands
Belgium	2	2	France, US
Canada	2	0	
The Netherlands	2	1	Australia
USSR	2	1	US
Yugoslavia	2	2	US
Austria	1	1	FRG
China	1	1	Japan, US
Czechoslovakia	1	1	FRG
Israel	1	0	
Italy	1	1	US

chemistry prizewinner Jean-Marie Lehn, Louis Pasteur University, Strasbourg, France, and College of France, Paris.¹⁶

It is also interesting to note that the Soviets are extremely active in organic superconductivity; indeed, both the Laukhin group, mentioned earlier, and R.P. Shibaeva and colleagues are affiliated with the USSR's Institute of Chemical Physics. The papers by these two groups are the only Soviet papers in this year's Bibliography. Table 3 gives a complete listing of the national affiliations of the institutions listed by the authors in the Bibliography.

The papers included in the Bibliography represent the work of 103 unique institutions (there are 141 institutional occurrences); the US accounted for 75 percent of the papers (or 66 percent of the affiliations) in this study. The leading institution, with nine occurrences, is the University of California; its Berkeley campus was listed six times, the Santa Barbara facilities twice, and the Riverside campus once. This is consistent with all our previous studies of highly cited chemistry papers: the University of California has never been ranked lower than third. Four institutions are listed four times each: Argonne National Laboratory, Illinois; NIH; Purdue; and Texas A&M.

Table 4: The 34 journals that published the papers listed in the Bibliography. The numbers in parentheses are the 1985 impact factors for the journals. (The 1985 impact factor equals the number of 1985 citations received by the 1983-1984 articles in a journal divided by the number of articles published by the journal during that same period.) Data were taken from the 1985 *JCR*[®]. The figures at the right indicate how many papers from each journal appear in the Bibliography.

Journal	Number of Papers
J. Amer. Chem. Soc. (4.32)	21
J. Chem. Phys. (3.10)	10
J. Phys. Chem. (3.05)	8
Account. Chem. Res. (7.67)	7
Anal. Chem. (3.41)	7
Chem. Phys. Lett. (2.29)	5
*Angew. Chem. Int. Ed. (5.35)	4
Chem. Rev. (5.42)	4
J. Chem. Soc. Chem. Commun. (2.42)	3
J. Magn. Resonance (3.20)	3
Mol. Cryst. Liquid Cryst. (1.24)	3
Inorg. Chem. (2.63)	2
Nature (12.86)	2
Can. J. Chem. (1.30)	1
Chem. Lett. (1.60)	1
Inorg. Chim. Acta (1.53)	1
Int. J. Mass Spectrom. Ion Proc. (1.44)	1
J. Appl. Cryst. (1.24)	1
J. Chem. Soc. Dalton Trans. (2.00)	1
J. Comput. Chem. (2.34)	1
J. Org. Chem. (2.16)	1
**Langmuir (N/A)	1
Mol. Phys. (2.29)	1
Org. Mass Spectrom. (1.65)	1
Organometallics (3.09)	1
***Pisma Zh. Eksp. Teor. Fiz. (1.52)	1
Phys. Rev. Lett. (6.91)	1
Polyhedron (1.33)	1
Prog. Anal. Atom. Spectrosc. (2.47)	1
Science (10.90)	1
Spectrochim. Acta Pt. B— At. Spec. (1.64)	1
Surface Sci. (4.01)	1
Tetrahedron (1.97)	1
Theochem—J. Mol. Struct. (0.81)	1

*also published in German as *Angew. Chem.*

**started publication in 1985

***translated in *JETP Lett.—Engl. Tr.* (1.52)

Conclusion

Some of the trends evident in this study have remained steady over the years. For instance, the *Journal of the American Chemical Society*, as it has in all five of our previous studies, published the most papers: it accounted for 21 percent of the works listed (see Table 4 for statistics on all 34 journals represented this year). Incidentally, *Langmuir* is a new American Chemical Society

journal that appears in our annual study for the first time.

All of the papers listed were published in English, although the Laukhin paper was originally published in Russian and translated into English; the number of citations to the Russian and English versions was virtually identical. In addition, four papers published in *Angewandte Chemie—International Edition in English* also appeared in the German edition. The *Angewandte Chemie* tendency to publish in English is marked throughout the scientific community, as our studies in chemistry and the life and physical sciences continue to show.

This study also shows that the interest in organic superconductors that we noted in our 1984 study continues unabated. However, a few differences from our last study are worth remarking on. Although two research fronts in the 1984 study dealt specifically with Diels-Alder reactions, none of this year's most active fronts seemingly addressed this topic. On the other hand, oxidation and oxidative coupling were prominent in this year's study but, strictly speaking, largely absent from last year's. In reality, of course, the absence of research fronts on a subject in one study or another does not mean that papers on the topic do not continue to be published. Indeed, were you to look at the counts for these papers for 1988, you would see that they received substantial citations—often in excess of this year's (1985) most-cited papers.

The flurry of activity in superconductivity and how molecules bind to one another that was evident in our 1984 study presaged the Nobel Prizes awarded in physics and chemistry in 1987. Although predictions are dangerous, it is possible that the kernel of a future Nobel Prize is to be found in this year's list. However, that generalization has been true ever since we started this exercise over a decade ago.

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A	B	C	D	Bibliographic Data
5	19	16	40	Ahrichs R, Bohm H-J, Ehrhardt C, Scharf P, Schiffer H, Lischka H & Schindler M. Implementation of an electronic structure program system on the CYBER 205. <i>J. Comput. Chem.</i> 6:200-8, 1985. 87-0342
3	16	13	32	Allara D L & Nuzzo R G. Spontaneously organized molecular assemblies. 2. Quantitative infrared spectroscopic determination of equilibrium structures of solution-adsorbed <i>n</i> -alkanoic acids on an oxidized aluminum surface. <i>Langmuir</i> 1:52-66, 1985. 86-0562
6	19	11	36	Armstrong D W, DeMond W, Alak A, Hinze W L, Riehl T E & Bui K H. Liquid chromatographic separation of diastereomers and structural isomers on cyclodextrin-bonded phases. <i>Anal. Chem.</i> 57:234-7, 1985. 86-1133
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5	7	23	35	Bax A & Davis D G. Practical aspects of two-dimensional transverse NOE spectroscopy. <i>J. Magn. Resonance</i> 63:207-13, 1985. 87-1356
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