"Current Comments"

A List of 100 Most Cited 'Chemical' Articles

March 6, 1974 Number 10

We have published several lists of most cited articles and authors. Most have been drawn from the scientific literature as a whole, rather than from any single discipline. These lists have introduced an inevitable bias which is presumably due to the large size of the life-sciences literature. Recently we published a more 'specialized' list of mathematical and statistical papers.[1] Herewith is now provided another 'specialized' list of chemical articles highly cited in 1972.

Twenty of the articles selected have appeared on other lists we've published (see notes accompanying the list). The list was prepared by extracting from our ISI® data base bibliographic citations appearing in 1972 issues of chemistry journals. Chemistry was defined as any journal in the fields of general, analytical, organic, and physical chemistry covered in the *Science Citation Index* ® *(SCI* ®*)*.[2] Crystallography, electrochemistry, and chemical engineering were also included as chemical categories. Biochemistry was deliberately omitted. The articles cited in the 1972 issues of such journals were ranked by frequency of citation. The top 100 are listed below.

Only three journals, *J. Chem. Phys.*, *J. Amer. Chem. Soc.*, and *Acta Cryst.* account for 56% of the articles. Along with ten others, they account for fully 84%, as follows: *J. Chem. Phys.* 22, *JACS* 19, *Acta Cryst.* 15, *Chem. Rev.* 6, *Angew. Chem.* 4, *J. Chem. Soc.* 4, *Analyt. Chem.* 3, *Quart. Rev.* 3, *Accounts Chem. Res.* 2, *J. Biol. Chem.* 2, *Phys. Rev.* 2, *Rev. Mod. Phys.* 2. Sixteen other journals contributed the remaining 16% with 1 each. Twenty-eight percent of the articles were published in the 1950's, 54% in the 60's, and seven articles in 1970 and 1971.

Of these 100 papers, 15 are perennial classics. They appear among the 100 papers most cited by all *SCI* journals during the period 1961-1972.[3,4] In the list, their rank numbers are asterisked. Five others, also indicated in the list, appeared among 1970 papers most cited during the period 1970-1973 or among 1971 papers most cited in 1971 and 1972.[5,6]

The prominence of the *J. Chem. Phys.* brings out a point reported in an earlier study of *J. Chem. Phys.*[7] It is impossible to arbitrarily separate physics from chemistry--a fact that accounts for the large overlap between *Chemical Abstracts* and *Physics Abstracts.*

Unlike previous lists, where they are heavily represented because of life-sciences dominance, *Nature* provides only one paper, and *Science* none. One wonders about the role of the *Journal of Organic Chemistry*, which also contributed only one paper, and about a number of other well known chemical journals, such as *J. Phys. Chem.*, which contributed none at all.

The only non-English journal represented on the list appears to be *Angewandte Chemie*, which of course appears in English as well.

Since methodology seems to dominate other most-cited lists, it is worth noting that it does not appear to be so evident here. This would seem to indicate that once we have listed the super-cited methodology publications, most-cited papers will begin to include all sorts of "classics"--both theoretical and laboratory-oriented. Each reader will have to judge whether the list is a helpful guide to the selection of reading material for a "chemical" library or any other use.[8]

1. Garfield, E. Highly cited works in mathematics. I. "Pure" mathematics. *Current Contents® (CC®)* No. 47, 21 November 1973, p. 5-9; II. "Applied" mathematics. *CC* No. 48, 28 November 1973, p. 5-9.
2. *Science Citation Index 1972 Guide and Journal Lists.* Philadelphia: Institute for Scientific Information, Inc. 1973; "Source Journals Arranged by Category", p. 100-6; appears also as front matter in vol. 5 of *Science Citation Index 1972 Annual.*
3. Garfield, E. Selecting the all-time citation classics; here are the fifty most cited papers for 1961-1972. *CC* No. 2, 9 January 1974, p. 5-8.
4. ----------. The second fifty papers most cited from 1961-1972. *CC* No. 6, 6 February 1974, p. 5-9.
5. ----------. The 1970 papers most frequently cited from 1970-1973. *CC* No. 51, 19 December 1973, p. 5-8.
6. ----------. The 25 most cited 1971 papers reveal a great deal about research in 1971. *CC* No. 44, 31 October 1973, p. 5-8.
7. ----------. What is the "core" literature of chemical physics? *CC* No. 9, 1 March 1972, p. 5-8.
8. This article is based in part on data developed under NSF contract C-795.

List of the 100 'Chemical' Articles Most Cited in 1972

Rank	Times Cited	Bibliographical Data
1.	309	**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(9):3175, 1 May 1965.
2*	244	**Lowry, O.H., Rosebrough, N.J., Farr, A.L. & Randall, R.J.** Protein measurement with the Folin phenol reagent. *J. Biol. Chem.* 193:265, 1951.
3*	241	**Cromer, D.T. & Waber, J.T.** Scattering factors computed from relativistic Dirac-Slater wave functions, *Acta Cryst.* 18:104, 1965.
4.	199	**Woodward, R.B. & Hoffmann, R.** The conservation of orbital symmetry. *Angew. Chemie* 81:797, 1969; and *Angew. Chemie Internat. Ed.* 8: 781, 1969.

*These papers were among the 100 papers most cited during the period 1961-1972.
†These papers were among the 1970 papers most cited during the period 1970-1973.
!These papers were among the 1971 papers most cited in 1971-1972.

Rank	Times Cited	Bibliographical Data
5.	193	Cromer, D.T. Anomalous dispersion corrections computed from self-consistent field-relativistic Dirac-Slater wave functions. *Acta Cryst.* 18:17, 1965.
6.	166	Karle, J. & Karle, I.L. The symbolic addition procedure for phase determination for centrosymmetric and noncentrosymmetric crystals. *Acta Cryst.* 21:849, 1966.
7.	161	Pople, J.A. & Segal, G.A. Approximate self-consistent molecular orbital theory. III. CNDO results for AB_2 and AB_3 systems. *J. Chem. Phys.* 44:3289, 1966.
8.	149	Hanson, H.P., Herman, F., Lea, J.D. & Skillman, S. HFS atomic scattering factors. *Acta Cryst.* 17:1040, 1964.
9*	140	Hoffmann, R. An extended Hückel theory. I. Hydrocarbons. *J. Chem. Phys.* 39:1397, 1963.
10.	127	Hamilton, W.C. Significance tests on the crystallographic *R* factor. *Acta Cryst.* 18:502, 1965.
11.	114	Schomaker, V. & Trueblood, K.N. On the rigid-body motion of molecules in crystals. *Acta Cryst.* B24:63, 1968.
12!	114	Sanders, J.K.M. & Williams, D.H. Tris(dipivalomethanato) europium. A paramagnetic shift reagent for use in nuclear magnetic resonance spectroscopy. *J. Amer. Chem. Soc.* 93:641, 1971.
13*	108	Jaffe, H.H. A reëxamination of the Hammett equation. *Chem. Rev.* 53:191, 1953.
14.	107	Pople, J.A., Beveridge, D.L. & Dobosh, P.A. Approximate self-consistent molecular-orbital theory. V. Intermediate neglect of differential overlap. *J. Chem. Phys.* 47:2026, 1967.
15.	106	Hinckley, C.C. Paramagnetic shifts in solutions of cholesterol and the dipyridine adduct of trisdipivalomethanatoeuropium (III). A shift reagent. *J. Amer. Chem. Soc.* 91:5160, 1969.
16.	101	Mulliken, R.S. Electronic population analysis on LCAO-MO molecular wave functions. I. *J. Chem. Phys.* 23:1833, 1955.
17*	100	Karplus, M. Contact electron-spin coupling of nuclear magnetic moments. *J. Chem. Phys.* 30:11, 1959.
18.	96	Cromer, D.T. & Mann, J.B. X-ray scattering factors computed from numerical Hartree-Fock wave functions. *Acta Cryst.* A24:321, 1968.
19*	95	Pariser, R. & Parr, R.G. A semi-empirical theory of the electronic spectra and electronic structure of complex unsaturated molecules. II. *J. Chem. Phys.* 21:767, 1953.
20*	94	Roothaan, C.C.J. New developments in molecular orbital theory. *Rev. Mod. Phys.* 23:69, 1951.
21.	90	Pariser, R. & Parr, R.G. A semi-empirical theory of the electronic spectra and electronic structure of complex unsaturated molecules. I. *J. Chem. Phys.* 21:466, 1953.
22*	89	Spackman, D.H., Stein, W.H. & Moore, S. Automatic recording apparatus for use in the chromatography of amino acids. *Analyt. Chem.* 30:1190, 1958.

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23.	87	**Pople, J.A., Santry, D.P. & Segal, G.A.** Approximate self-consistent molecular orbital theory. I. Invariant Procedures. *J. Chem. Phys* 43:S129, 1965.
24.	80	**Hatchard, C.G. & Parker, C.A.** A new sensitive chemical actinometer. II. Potassium ferrioxalate as a standard chemical actinometer. *P. Roy. Soc.* A235:518, 1956.
25.	79	**Pople, J.A. & Setal, G.A.** Approximate self-consistent molecular orbital theory. II. Calculations with complete neglect of differential overlap. *J. Chem. Phys.* 43:S136, 1965.
26†	77	**Sanders, J.K.M. & Williams, D.H.** A shift reagent for use in nuclear magnetic resonance spectroscopy. A first-order spectrum of n-hexanol. *Chem. Comm.* pg. 422, 1970.
27.	75	**Nicholson, R.S. & Shain, I.** Theory of stationary electrode polarography single scan and cyclic methods applied to reversible, irreversible, and kinetic system. *Analyt. Chem.* 36:706, 1964.
28.	75	**Pople, J.A.** Electron interaction in unsaturated hydrocarbons. *T. Faraday Soc.* 49:1375, 1953.
29.	74	**Hammond, G.S.** A correlation of reaction rates. *J. Am. Chem. Soc.* 77:334, 1955.
30.	72	**Huzinaga, S.** Gaussian-type functions for polyatomic systems. I. *J. Chem. Phys.* 42:1293, 1965.
31.	71	**Busing, W.R. & Levy, H.A.** The effect of thermal motion on the estimation of bond lengths from diffraction measurements. *Acta Cryst.* 17:142, 1964.
32.	70	**Clementi, E.** *Ab initio* computations in atoms and molecules. *IBM J. Res. Develop.* 9:2, 1965.
33.	70	**Fessenden, R.W. & Schuler, R.H.** Electron spin resonance studies of transient alkyl radicals. *J. Chem. Phys.* 39:2147, 1963.
34*	69	**Bloembergen, N., Purcell, E.M. & Pound, R.V.** Relaxation effects in nuclear magnetic resonance absorption. *Phys. Rev.* 73:679, 1948.
35*	68	**Davis, B.J.** Disc electrophoresis. II. Method and application to human serum proteins. *Ann. N.Y. Acad. Sci.* 121:404, 1964.
36.	68	**Clementi, E. & Raimondi, D.L.** Atomic screening constants from SCF functions. *J. Chem. Phys.* 38:2686, 1963.
37†	66	**Demarco, P.V., Elzey, T.K., Lewis, R.B. & Wenkert, E.** Paramagnetic induced shifts in the proton magnetic resonance spectra of alcohols using tris(dipivalomethanato)europium (III). *J. Amer. Chem. Soc.* 92:5734, 1970.
38.	66	**Hinze, J. & Jaffe, H.H.** Electronegativity. I. Orbital electronegativity of neutral atoms. *J. Amer. Chem. Soc.* 84:540, 1962.
39.	66	**Wilson, A.J.C.** Determination of absolute from relative x-ray intensity data. *Nature* 150:151, 1942.

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40†	65	Kessler, H. Detection of hindered rotation and inversion by NMR spectroscopy. *Angew. Chem. Int. Ed.* 9:219, 1970; *Angew Chem.* 9:21, 1970.
41.	65	Job, P. Recherches sur la formation de complexes mineraux en solution, et sur leur stabilité. *Ann. Chim.* 9:113, 1928.
42!	65	Rondeau, R.E. & Sievers, R.E. New superior paramagnetic shift reagents for nuclear magnetic resonance spectral clarification. *J. Amer. Chem. Soc.* 93:1522, 1971.
43.	65	Frank, H.S. & Evans, M.W. Free volume and entropy in condensed systems. III. Entropy in binary liquid mixtures; partial molal entropy in dilute solutions; structure and thermodynamics in aqueous electrolytes. *J. Chem. Phys.* 13:507, 1945.
44.	65	Huisgen, R. 1,3-Dipolar cycloadditions; past and future. *Angew. Chem. Int. Ed.* 2:565, 1963; *Angew. Chem.* 75:604, 1963.
45.	63	Anbar, M. & Meta, P. A compilation of specific bimolecular rate constants for the reaction of hydrated electrons, hydrogen atoms and hydroxyl radicals with inorganic and organic compounds in aqueous solution. *Int. J. Appl. Radiat. Is.* 18:493, 1967.
46.	63	Karplus, M. Vicinal proton coupling in nuclear magnetic resonance. *J. Amer. Chem. Soc.* 85:2870, 1963.
47*	63	Bowden, K., Heilbron, I.M., Jones, E.R.H. & Weedon, B.C.L. Researches on acetylenic compounds. Part I. The preparation of acetylenic ketones by oxidation of acetylenic carbinols and glycols. *J. Chem. Soc. Lond.* pg. 39, 1946.
48.	62	Corfield, P.W.R., Doedens, R.J. & Ibers, J.A. Studies of metal--nitrogen multiple bonds. I. The crystal and molecular structure of nitridodichloro-tris(diethylphenylphosphine)rhenium (V), $ReNCl_2[P(C_2H_5)_2C_6H_5]_3$. *Inorg. Chem.* 6:197, 1967.
49.	62	Pople, J.A. & Gordon, M. Molecular orbital theory of the electronic structure of organic compounds. I. Substituent effects and dipole moments. *J. Amer. Chem. Soc.* 89:4253, 1967.
50.	61	Shannon, R.D. & Prewitt, C.T. Effective ionic radii in oxides and fluorides. *Acta Cryst.* B25:925, 1969.
51.	61	Brunauer, S., Emmett, P.H. & Teller, E. Absorption of gases in multimolecular layers. *J. Amer. Chem. Soc.* 60:309, 1938.
52.	60	Busing, W.R. & Levy, H.A. High Speed Computation of the absorption correction for single crystal diffraction measurements. *Acta Cryst.* 10:180, 1957.
53.	59	Osborn, J.A., Jardine, F.H., Young, J.F. & Wilkinson, G. The preparation and properties of tris(triphenylphosphine)halogenorhodium (I) and some reactions thereof including catalytic homogeneous hydrogenation of olefins and acetylenes and their derivatives. *J. Chem. Soc. Lond. A* pg. 1711, 1966.
54.	58	Pearson, R.G. Hard and soft acids and bases. *J. Amer. Chem. Soc.* 85:3533, 1963.
55.	58	Castellano, S. & Bothner-By, A.A. Analysis of NMR spectra by least squares. *J. Chem. Phys.* 41:3863, 1964.

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56.	57	**Hughes, E.W.** The crystal structure of melamine. *J. Amer. Chem. Soc.* 63:1737, 1941.
57.	57	**Pople, J.A., Beveridge, D.L. & Dobosh, P.A.** Molecular orbital theory of the electronic structure of organic compounds. II. Spin densities in paramagnetic species. *J. Amer. Chem. Soc.* 90:4201, 1968.
58.	57	**Sternhill, S.** Correlation of interproton spin-spin coupling constants with structure. *Quart. Rev. Chem. Soc.* 23:236, 1969.
59.	55	**McDaniel, D.H. & Brown, H.C.** An extended table of Hammett substituent constants based on the ionization of substituted benzoic acids. *J. Org. Chem.* 23:420, 1958.
60.	54	**Zachariasen, W.H.** The secondary extinction correction. *Acta Cryst.* 16:1139, 1963.
61.	54	**Brown, H.C. & Okamoto, Y.** Electrophilic substituent constants. *J. Amer. Chem. Soc.* 80:4979, 1958.
62*	54	**Folch, J., Lees, M. & Sloane Stanley, G.H.** A simple method for the isolation and purification of total lipides from animal tissues. *J. Biol. Chem.* 226:497, 1957.
63.	54	**Franks, F. & Ives, D.J.G.** The structural properties of alcohol--water mixtures. *Quart. Rev.* 20:1, 1966.
64.	53	**Hoffmann, R.** Trimethylene and the addition of methylene to ethylene. *J. Amer. Chem. Soc.* 90:1475, 1968.
65.	53	**Wolfsberg, M. & Helmholz, L.** Spectra and electronic structure of the tetrahedral ions M_nO_4–, CrO_4--, ClO_4. *J. Chem. Phys.* 20:837, 1952.
66.	51	**McConnell, H.R. & Robertson, R.E.** Isotropic nuclear resonance shifts. *J. Chem. Phys.* 29:1361, 1958.
67.	50	**Huisgen, R.** Kinetics and mechanism of 1,3-Dipolar cycloadditions; past & future. *Angew. Chem. Int. Ed.* 2:633; *Angew. Chem.* 75:742, 1963.
68.	50	**Kerr, J.A.** Bond dissociation energies by kinetic methods. *Chem. Rev.* 66:465, 1966.
69.	50	**Hehre, W.J., Stewart, R.F. & Pople, J.A.** Self consistent molecular-orbital methods. I. Use of Gaussian expansions of Slater-type atomic orbitals. *J. Chem. Phys.* 51:2657, 1969.
70.	49	**Hendrickson, J.B.** Molecular geometry. I. Machine computation of the common rings. *J. Amer. Chem. Soc.* 83:4537, 1961.
71.	49	**Santry, D.P. & Segal, G.A.** Approximate self-consistent molecular orbital theory. IV. Calculations on molecules including the elements sodium through chlorine. *J. Chem. Phys.* 47:158, 1967.
72.	49	**Mulliken, R.S., Rieke, C.A., Orloff, D. & Orloff, H.** Formulas and numerical tables for overlap integrals. *J. Chem. Phys.* 17:1248, 1949.
73.	48	**Westheimer, F.H.** Pseudo-rotation in the hydrolysis of phosphate esters. *Accounts Chem. Res.* 1:70, 1968.
74.	48	**Zachariasen, W.H.** A general theory of X-ray diffraction in crystals. *Acta Cryst.* 23:558, 1967.

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75.	48	**Frank, H.S. & Wen, W-Y.** Structural aspects of ion-solvent interaction in aqueous solutions: a suggested picture of water structure. *Discuss. Faraday Soc.* pg. 133, 1957.
76.	48	**Johnson, C.E., Jr. & Bovey, F.A.** Calculation of nuclear magnetic resonance spectra of aromatic hydrocarbons. *J. Chem. Phys.* 29:1012, 1958.
77.	48	**Irving, H.M. & Rossotti, H.S.** The calculation of formation curves of metal complexes from pH titration curves in mixed solvents. *J. Chem. Soc.* 2:2904, 1954.
78.	48	**Wiberg, K.B.** Application of the Pople-Santry-Segal CNDO method to the cyclopropylcarbinyl and cyclobutylcation and to bicyclobutane. *Tetrahedron* 24:1083, 1968.
79.	47	**Doyle, P.A. & Turner, P.S.** Relativistic Hartree-Fock X-ray and electron scattering factors. *Acta Cryst.* A24:390, 1968.
80.	47	**Parker, A.J.** Protic-dipolar aprotic solvent effects on rates of bimolecular reactions. *Chem. Rev.* 69:1, 1969.
81*	47	**Sweeley, C.C., Bentley, R., Makita, M. & Wells, W.W.** Gas-liquid chromatography of trimethylsilyl derivatives of sugars and related substances. *J. Amer. Chem. Soc.* 85:2497, 1963.
82.	46	**Hoffman, R.** Interaction of orbitals through space and through bonds. *Accounts Chem. Res.* 4:1, 1971.
83.	46	**Stewart, W.E. & Siddall, T.H., III.** Nuclear magnetic resonance studies of amides. *Chem. Rev.* 70:517, 1970.
84.	46	**Koopmans, T.** Über die Zuordnung von Wellenfunktionen und Eigenwerten zu den einzelnen Elektronen eines Atoms. *Physica* 1:104, 1933.
85.	46	**Parker, A.J.** Effects of solution on the properties of anions in dipolar aprotic solvent. *Quart. Rev.* 16:163, 1962.
86.	45	**Barfield, M. & Chakrabarti, B.** Long-range proton spin-spin coupling. *Chem. Rev.* 69:757, 1969.
87.	45	**Woodward, R.B. & Hoffman, R.** Stereochemistry of electrocyclic reactions. *J. Amer. Chem. Soc.* 87:395, 1965.
88.	45	**Carr, H.Y. & Purcell, E.M.** Effects of diffusion on free procession in nuclear magnetic resonance experiments. *Phys. Rev.* 94:630, 1954.
89.	45	**Roothan, C.C.J., Kolos, W. & Sack, R.A.** Ground state of systems of three particles with coulomb interaction. *Rev. Mod. Phys.* 32:179, 1960.
90.	43	**Karle, J. & Hauptman, H.** A theory of phase determination for the four types of non-centrosymmetric space group. *Acta Cryst.* 9:635, 1956.
91*	43	**Bray, G.A.** A simple efficient liquid scintillator for counting aqueous solutions in a liquid scintillation counter. *Analyt. Biochem.* 1:279, 1960.
92*	43	**Dubois, M., Gilles, K.A., Hamilton, J.K., Smith, F. & Rebers, P.A.** Colorimetric method for determination of sugars and related substances. *Analyt. Chem.* 28:350, 1956.
93.	42	**Sayre, D.** The squaring method: a new method for phase determination. *Acta Cryst.* 5:60, 1952.

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94.	42	**Paul, M.A. & Long, F.A.** Application of the H_0 acidity function to kinetics and mechanisms of acid catalysis. *Chem. Rev.* 57:935, 1957.
95.	42	**Onsager, L.** Electric moments of molecules in liquids. *J. Amer. Chem. Soc.* 58:1486, 1936.
96.	42	**Benesi, H.A. & Hildebrand, J.H.** A spectrophotometric investigation of the interaction of iodine with aromatic hydrocarbons. *J. Amer. Chem. Soc.* 71:2703, 1949.
97.	42	**Gutowski, H.S. & Holm, C.H.** Rate processes and nuclear magnetic resonance spectra II hindered internal rotation of amides. *J. Chem. Phys.* 25:1228, 1956.
98.	42	**Irving, H. & Rossotti, H.S.** Methods for computing successive stability constants from experimental formation curves. *J. Chem. Soc.* pg. 3397, 1953.
99.	42	**McLachlan, A.D.** Self-consistent field theory of the electron spin distribution in π-electron radicals. *Mol. Phys.* 3:233, 1960.
100.	42	**Ahrland, S., Chatt, J. & Davies, N.R.** The relative affinities of ligand atoms for acceptor molecules and ions. *Quart. Rev.* 12:265, 1958.

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