

Ian C Carmichael

List of Publications by Year in descending order

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143
papers

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101543

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144
times ranked

4616
citing authors

#	ARTICLE	IF	CITATIONS
1	Triplet-Triplet Absorption Spectra of Organic Molecules in Condensed Phases. <i>Journal of Physical and Chemical Reference Data</i> , 1986, 15, 1-250.	4.2	861
2	Role of Water in Electron-Initiated Processes and Radical Chemistry: Issues and Scientific Advances. <i>Chemical Reviews</i> , 2005, 105, 355-390.	47.7	560
3	Hydroxymethyl Group Conformation in Saccharides: Structural Dependencies of $^2J_{HH}$, $^3J_{HH}$, and $^1J_{CH}$ Spin-Spin Coupling Constants. <i>Journal of Organic Chemistry</i> , 2002, 67, 949-958.	3.2	185
4	Three-Bond $C^{\alpha}-O^{\alpha}-C^{\beta}$ Spin-Coupling Constants in Carbohydrates: Development of a Karplus Relationship. <i>Journal of the American Chemical Society</i> , 1998, 120, 11158-11173.	13.7	132
5	Extinction Coefficients of Triplet-Triplet Absorption Spectra of Organic Molecules in Condensed Phases: A Least-Squares Analysis. <i>Journal of Physical and Chemical Reference Data</i> , 1987, 16, 239-260.	4.2	130
6	Molecular Recognition of Trigonal Oxyanions Using a Ditopic Salt Receptor: Evidence for Anisotropic Shielding Surface around Nitrate Anion. <i>Journal of the American Chemical Society</i> , 2005, 127, 2922-2928.	13.7	128
7	Correlated $C^{\alpha}-C$ and $C^{\alpha}-O$ Bond Conformations in Saccharide Hydroxymethyl Groups: Parametrization and Application of Redundant $^1H-^1H$, $^{13}C-^1H$, and $^{13}C-^{13}C$ NMRJ-Couplings. <i>Journal of the American Chemical Society</i> , 2004, 126, 15668-15685.	13.7	124
8	Observation of Decreased Radiation Damage at Higher Dose Rates in Room Temperature Protein Crystallography. <i>Structure</i> , 2007, 15, 1531-1541.	3.3	121
9	Density Functional Calculations on Disaccharide Mimics: Studies of Molecular Geometries and Trans-O-glycosidic $^3J_{COCH}$ and $^3J_{COCC}$ Spin-Couplings. <i>Journal of the American Chemical Society</i> , 1999, 121, 9843-9851.	13.7	90
10	Molar absorption coefficients of transient species in solution. <i>Pure and Applied Chemistry</i> , 1991, 63, 289-300.	1.9	84
11	Radiation damage and dose limits in serial synchrotron crystallography at cryo- and room temperatures. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 4142-4151.	7.1	84
12	$^{13}C-^1H$ and $^{13}C-^{13}C$ Spin-Coupling Constants in Methyl 2 -d-Ribofuranoside and Methyl 2-Deoxy- 2 -d-erythro-pentofuranoside: Correlations with Molecular Structure and Conformation. <i>Journal of the American Chemical Society</i> , 1997, 119, 8946-8964.	13.7	81
13	DFT Investigation of Intermediate Steps in the Hydrolysis of γ -Al ₂ O ₃ (0001). <i>Journal of Physical Chemistry C</i> , 2009, 113, 2149-2158.	3.1	81
14	$^{13}C-^1H$ Spin-Coupling Constants in the 2 -d-Ribofuranosyl Ring: Effect of Ring Conformation on Coupling Magnitudes. <i>Journal of the American Chemical Society</i> , 1996, 118, 1413-1425.	13.7	79
15	One-bond $^{13}C-^1H$ spin-coupling constants in aldofuranosyl rings: effect of conformation on coupling magnitude. <i>Journal of the American Chemical Society</i> , 1995, 117, 8645-8650.	13.7	76
16	DFT characterization of coverage dependent molecular water adsorption modes on γ -Al ₂ O ₃ (0001). <i>Surface Science</i> , 2008, 602, 268-275.	1.9	73
17	Torsional effects on the one-bond $^{13}C-^{13}C$ spin coupling constant in ethylene glycol: insights into the behavior of $^1J_{CC}$ in carbohydrates. <i>Journal of the American Chemical Society</i> , 1993, 115, 10863-10870.	13.7	71
18	DFT and NMR Studies of $^2J_{COH}$, $^3J_{HCOH}$, and $^3J_{CCOH}$ Spin-Couplings in Saccharides: $C^{\alpha}-O$ Torsional Bias and H-Bonding in Aqueous Solution. <i>Journal of Organic Chemistry</i> , 2007, 72, 7071-7082.	3.2	68

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19	¹³ C- ¹ H and ¹³ C- ¹³ C Spin Coupling Behavior in Aldofuranosyl Rings from Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 1999, 103, 3783-3795.	2.5	63
20	[6-6]-Closed versus [6-5]-Open Isomers of Imino- and Methanofullerenes: A Comparison with Pristine C ₆₀ and (C ₅₉ N). <i>Journal of Physical Chemistry A</i> , 2000, 104, 8601-8608.	2.5	58
21	Two-bond ¹³ C- ¹³ C spin-coupling constants in carbohydrates: effect of structure on coupling magnitude and sign. <i>Carbohydrate Research</i> , 1996, 280, 177-186.	2.3	54
22	2-Deoxy- ¹² -d-erythro-pentofuranose: A Hydroxymethyl Group Conformation and Substituent Effects on Molecular Structure, Ring Geometry, and NMR Spin-Spin Coupling Constants from Quantum Chemical Calculations. <i>Journal of the American Chemical Society</i> , 2001, 123, 4781-4791.	13.7	52
23	¹ J _{CH} Correlates with Alcohol Hydrogen Bond Strength. <i>Journal of Organic Chemistry</i> , 2006, 71, 2878-2880.	3.2	51
24	Molecular orbital studies of hyperfine coupling constants in the H ₂ CN and H(HO)CN radicals. <i>The Journal of Physical Chemistry</i> , 1991, 95, 4702-4708.	2.9	50
25	Ab initio quadratic configuration interaction calculation of indirect NMR spin-spin coupling constants. <i>The Journal of Physical Chemistry</i> , 1993, 97, 1789-1792.	2.9	48
26	Atomic Spin Densities from Correlation-Consistent Basis Sets. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4633-4636.	2.5	46
27	¹³ C- ¹ H and ¹³ C- ¹³ C Spin Couplings in [2 ⁻ - ¹³ C] ₂ ⁻ -Deoxyribonucleosides: Correlations with Molecular Structure. <i>Journal of the American Chemical Society</i> , 1997, 119, 1737-1744.	13.7	44
28	2-Deoxy- ¹² -d-ribofuranosylamine: A Quantum Mechanical Calculations of Molecular Structure and NMR Spin-Spin Coupling Constants in Nitrogen-Containing Saccharides. <i>Journal of the American Chemical Society</i> , 2000, 122, 6435-6448.	13.7	44
29	Ab initio quadratic configuration interaction calculations of isotropic hyperfine coupling constants. <i>The Journal of Physical Chemistry</i> , 1991, 95, 108-111.	2.9	43
30	Ab initio calculation of the hyperfine coupling constants in B ₂ . <i>Journal of Chemical Physics</i> , 1989, 91, 1072-1078.	3.0	42
31	¹² -Fragmentation and Other Reactions Involving Aminyl Radicals from Amino Acids. <i>Journal of Physical Chemistry B</i> , 2000, 104, 643-649.	2.6	42
32	¹³ C-Labeled ¹⁵ N-Acetyl-neuraminic Acid in Aqueous Solution: Detection and Quantification of Acyclic Keto, Keto Hydrate, and Enol Forms by ¹³ C NMR Spectroscopy. <i>Journal of the American Chemical Society</i> , 2008, 130, 11892-11900.	13.7	41
33	Effective scavenging at cryotemperatures: further increasing the dose tolerance of protein crystals. <i>Journal of Synchrotron Radiation</i> , 2011, 18, 346-357.	2.4	39
34	Conformational Populations of ¹² -(1 ⁺ 4) ¹ O-Glycosidic Linkages Using Redundant NMR ¹ J _C -Couplings and Circular Statistics. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3042-3058.	2.6	39
35	Spectral, Kinetics, and Theoretical Studies of Radical Cations Derived from Thioanisole and Its Carboxylic Derivative. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9251-9260.	2.5	38
36	Amide ¹ Cis- ¹ Trans Isomerization in Aqueous Solutions of Methyl ¹⁵ N-Formyl- ¹³ C-glucosaminides and Methyl ¹⁵ N-Acetyl- ¹³ C-glucosaminides: Chemical Equilibria and Exchange Kinetics. <i>Journal of the American Chemical Society</i> , 2010, 132, 4641-4652.	13.7	38

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37	ESR measurement of the pKa of carboxyl radical and ab initio calculation of the carbon-13 hyperfine constant. <i>The Journal of Physical Chemistry</i> , 1990, 94, 1372-1376.	2.9	37
38	Homo- and Heterodimetallic Geminal Dianions Derived from the Bis(phosphinimine) $\{Ph_2P(NSiMe_3)_2\}_2CH_2$ and the Alkali Metals Li, Na, and K. <i>Chemistry - A European Journal</i> , 2008, 14, 3939-3953.	3.3	37
39	Geminal $^2J_{CCH}$ Spin-Spin Coupling Constants as Probes of the γ Glycosidic Torsion Angle in Oligosaccharides. <i>Journal of the American Chemical Society</i> , 2005, 127, 9781-9793.	13.7	36
40	Room-temperature scavengers for macromolecular crystallography: increased lifetimes and modified dose dependence of the intensity decay. <i>Journal of Synchrotron Radiation</i> , 2009, 16, 205-216.	2.4	36
41	$^2J_{CO}$ Spin-Spin Coupling Constants Across Glycosidic Linkages Exhibit a Valence Bond-Angle Dependence. <i>Journal of the American Chemical Society</i> , 2000, 122, 396-397.	13.7	34
42	^{13}C - ^{13}C NMR Spin-Spin Coupling Constants in Saccharides: Structural Correlations Involving All Carbons in Aldohexopyranosyl Rings. <i>Journal of Organic Chemistry</i> , 2007, 72, 7511-7522.	3.2	34
43	To scavenge or not to scavenge, that is STILL the question. <i>Journal of Synchrotron Radiation</i> , 2013, 20, 23-36.	2.4	33
44	Ab initio coupled-cluster calculations of isotropic hyperfine splitting in some diatomic hydrides. <i>The Journal of Physical Chemistry</i> , 1990, 94, 5734-5740.	2.9	30
45	Ab initio quadratic configuration interaction calculation of the isotropic hyperfine coupling constants in the ethyl radical. <i>The Journal of Physical Chemistry</i> , 1991, 95, 6198-6201.	2.9	30
46	On the Addition of $\cdot OH$ Radicals to the Ipso Positions of Alkyl-Substituted Aromatics: Production of 4-Hydroxy-4-methyl-2,5-cyclohexadien-1-one in the Radiolytic Oxidation of p-Cresol. <i>Journal of Physical Chemistry A</i> , 2002, 106, 12178-12183.	2.5	30
47	Use of Circular Statistics To Model $^1J_{Man-(1\rightarrow 2)-Man}$ and $^1J_{Man-(1\rightarrow 3)-Man}$ ^{13}C -Labeled Disaccharides and High-Mannose Oligosaccharides. <i>Biochemistry</i> , 2019, 58, 546-560.	2.5	29
48	Ab initio calculation of the structures and properties of some lithium-Lewis base complexes. <i>The Journal of Physical Chemistry</i> , 1981, 85, 3821-3826.	2.9	26
49	^{13}C - 1H and ^{13}C - ^{13}C NMR J -Couplings in ^{13}C -Labeled <i>N</i> -Acetyl-neuraminic Acid: Correlations with Molecular Structure. <i>Journal of Organic Chemistry</i> , 2008, 73, 4376-4387.	3.2	26
50	Theoretical Studies on Some S^1N Three-Electron Bonded Radical Cations. <i>Acta Chemica Scandinavica</i> , 1997, 51, 567-571.	0.7	26
51	A note on the total depletion method of measuring extinction coefficients of triplet-triplet transitions. <i>The Journal of Physical Chemistry</i> , 1985, 89, 4036-4039.	2.9	25
52	Ab initio configuration interaction study of the structure and magnetic properties of radicals and radical ions derived from group 13 trihydrides. <i>Chemical Physics</i> , 1987, 116, 351-367.	1.9	25
53	An NMR investigation of putative interresidue H-bonding in methyl β -D-cellobioside in solution. <i>Carbohydrate Research</i> , 2009, 344, 1582-1587.	2.3	25
54	<i>O</i> -Acetyl Side-Chains in Monosaccharides: Redundant NMR Spin-Couplings and Statistical Models for Acetate Ester Conformational Analysis. <i>Journal of Physical Chemistry B</i> , 2017, 121, 66-77.	2.6	25

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55	Characterization of Neutral Radicals from a Dissociative Electron Attachment Process. <i>Physical Review Letters</i> , 2017, 119, 053402.	7.8	24
56	Informing Saccharide Structural NMR Studies with Density Functional Theory Calculations. <i>Methods in Molecular Biology</i> , 2015, 1273, 289-331.	0.9	24
57	Density Functional Studies of Hydrogen Atom Addition to the CS Bond. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3641-3651.	2.5	23
58	Hydrogen and Deuterium Atoms in Octasilsesquioxanes: Experimental and Computational Studies. <i>Journal of the American Chemical Society</i> , 2006, 128, 6111-6125.	13.7	23
59	Oligosaccharide Trans-Glycoside ³ J_{COCC} Karplus Curves Are Not Equivalent: Effect of Internal Electronegative Substituents. <i>Journal of Organic Chemistry</i> , 2008, 73, 3255-3257.	3.2	23
60	Ab initio molecular orbital calculations on the tert-butyl radical, its isoelectronic neighboring radical ions and their third-row congeners. <i>The Journal of Physical Chemistry</i> , 1985, 89, 4727-4732.	2.9	22
61	Hyperfine Splitting in N ₄ ⁺ from ab Initio Calculation. <i>The Journal of Physical Chemistry</i> , 1994, 98, 5044-5048.	2.9	22
62	Evidence for ¹ I ² Scission in the Oxidation of Amino Acids. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4573-4580.	2.5	22
63	⁴ JCOCC and ⁴ JCCCC Has Probes of Exocyclic Hydroxymethyl Group Conformation in Saccharides. <i>Journal of Organic Chemistry</i> , 2005, 70, 7542-7549.	3.2	22
64	[¹³ C, ¹⁵ N]2-Acetamido-2-deoxy-d-aldohexoses and Their Methyl Glycosides: Synthesis and NMR Investigations of J-Couplings Involving ¹ H, ¹³ C, and ¹⁵ N. <i>Journal of Organic Chemistry</i> , 2006, 71, 466-479.	3.2	22
65	Isotropic coupling constants for the atoms boron-fluorine from correlated calculations based on spin-unrestricted wave functions. <i>The Journal of Physical Chemistry</i> , 1989, 93, 190-193.	2.9	21
66	Density Functional Investigation of High-Spin XY (X = Cr, Mo, W and Y = C, N, O) Molecules. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4846-4853.	2.5	21
67	¹ N-Acetyl Side-Chains in Saccharides: NMR J-Coupling Equations Sensitive to CH ¹ NH and NH ¹ CO Bond Conformations in 2-Acetamido-2-deoxy-aldohexopyranosyl Rings. <i>Journal of Organic Chemistry</i> , 2010, 75, 4899-4910.	3.2	21
68	Radiation damage to nucleoprotein complexes in macromolecular crystallography. <i>Journal of Synchrotron Radiation</i> , 2015, 22, 213-224.	2.4	21
69	The Rh ¹ ligand bond: RhX (X=C, N, O, F, P and Cl) molecules. <i>Chemical Physics Letters</i> , 2006, 421, 281-286.	2.6	20
70	NMR Spin-Couplings in Saccharides: Relationships Between Structure, Conformation and the Magnitudes of ¹ J_{HH}, ¹ J_{CH} and ¹ J_{CC} Values. <i>New Developments in NMR</i> , 2017, , 20-100.	0.1	20
71	Lifetimes and Modes of Decay of Sulfur-Centered Radical Zwitterions Containing Carboxylate and Phenyl Groups. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6503-6512.	2.5	19
72	Stripping off hydrogens in imidazole triggered by the attachment of a single electron. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6406-6415.	2.8	19

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73	OH cleavage from tyrosine: debunking a myth. <i>Journal of Synchrotron Radiation</i> , 2017, 24, 7-18.	2.4	19
74	RNA protects a nucleoprotein complex against radiation damage. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 648-657.	2.3	18
75	Radical Production in the Radiolysis of Liquid Pyridine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 461-465.	2.5	17
76	Dipole-Supported Electronic Resonances Mediate Electron-Induced Amide Bond Cleavage. <i>Physical Review Letters</i> , 2019, 122, 073002.	7.8	17
77	Hyperfine Splitting in HOCO from ab Initio Calculations. <i>The Journal of Physical Chemistry</i> , 1994, 98, 5896-5901.	2.9	16
78	Carbohydrate Reaction Intermediates: A Effect of Ring-Oxygen Protonation on the Structure and Conformation of Aldofuranosyl Rings. <i>Journal of the American Chemical Society</i> , 1997, 119, 8933-8945.	13.7	16
79	¹³ C-Labeled Idohexopyranosyl Rings: Effects of Methyl Glycosidation and C6 Oxidation on Ring Conformational Equilibria. <i>Journal of Organic Chemistry</i> , 2017, 82, 1356-1370.	3.2	16
80	B3LYP Investigation of HPO ₂ , trans-HOPO, cis-HOPO, and Their Radical Anions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 9390-9399.	2.5	15
81	On the Association and Structure of Radicals Derived from Dipyridil[3,2-a:2'-3'-c]phenazine. Contrast between the Electrochemical, Radiolytic, and Photochemical Reduction Processes. <i>Journal of Organic Chemistry</i> , 2006, 71, 2870-2873.	3.2	15
82	Synthesis and ¹³ C-Glycosidic Linkage Conformational Analysis of ¹³ C-Labeled Oligosaccharide Fragments of an Antifreeze Glycolipid. <i>Journal of Organic Chemistry</i> , 2019, 84, 1706-1724.	3.2	15
83	Correlation Effects on the Hyperfine Splitting in HNCN. <i>The Journal of Physical Chemistry</i> , 1995, 99, 6832-6835.	2.9	14
84	Isotropic coupling constant for the nitrogen atom from correlated calculations based on spin-unrestricted wave functions. <i>Journal of Chemical Physics</i> , 1990, 93, 863-864.	3.0	13
85	Direct EPR observation of the aminomethyl radical during the radiolysis of glycine. <i>Perkin Transactions II RSC</i> , 2000, , 907-908.	1.1	13
86	Generation of Thiyl Radicals by the Photolysis of 5-Iodo-4-thiouridine. <i>Journal of Organic Chemistry</i> , 2005, 70, 982-988.	3.2	13
87	Dissociative electron attachment to the gas-phase nucleobase hypoxanthine. <i>Journal of Chemical Physics</i> , 2015, 142, 215101.	3.0	13
88	Moment theory analysis of eROH- optical absorption spectra. <i>The Journal of Physical Chemistry</i> , 1980, 84, 1076-1082.	2.9	12
89	Dissociative electron attachment induced ring opening in five-membered heterocyclic compounds. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18271-18278.	2.8	12
90	Reconciling MATE and molecular dynamics models of linkage conformation in oligosaccharides. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14454-14457.	2.8	12

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91	Photon-induced electron transfer transitions of the solvated electrons. Journal of Chemical Physics, 1978, 69, 2652.	3.0	11
92	Deuterium Nuclear Spin- Lattice Relaxation Times and Quadrupolar Coupling Constants in Isotopically Labeled Saccharides. Journal of Magnetic Resonance, 2000, 144, 207-216.	2.1	11
93	Bimolecular Homolytic Substitution (SH2) Reactions with Hydrogen Atoms. Time-Resolved Electron Spin Resonance Detection in the Pulse Radiolysis of \pm -(Methylthio)acetamide. Journal of the American Chemical Society, 2004, 126, 14468-14474.	13.7	11
94	A critique of excitation models for partial saturation of transient absorbance. Journal of Photochemistry and Photobiology, 1985, 31, 179-192.	0.6	10
95	Ab initio configuration interaction study of the hyperfine coupling in fluorine molecular radical anion. The Journal of Physical Chemistry, 1987, 91, 6443-6445.	2.9	10
96	A Unified Analysis of Noncomparative Methods for Measuring the Molar Absorptivity of Triplet-Triplet Transitions. Applied Spectroscopy, 1987, 41, 1033-1038.	2.2	10
97	Density Functional Theory Study of Ultrashort and Overlong CC Single Bonds and the Lowest Nonbonding C- C Distance. Journal of Physical Chemistry A, 2000, 104, 6271-6276.	2.5	10
98	Transient Raman spectra, structure, and thermochemistry of the thiocyanate dimer radical anion in water. Journal of Chemical Physics, 2017, 146, 214305.	3.0	10
99	Numerical solution of semicontinuum models for excess electrons. Journal of Chemical Physics, 1978, 68, 4086-4092.	3.0	9
100	Rearrangement of 3-Deoxy- <i>erythro</i> -hexos-2-ulose in Aqueous Solution: NMR Evidence of Intramolecular 1,2-Hydrogen Transfer. Journal of Organic Chemistry, 2011, 76, 8151-8158.	3.2	9
101	Methyl [¹³ C]Glucopyranosiduronic Acids: Effect of COOH Ionization and Exocyclic Structure on NMR Spin-Couplings. Journal of Organic Chemistry, 2012, 77, 9521-9534.	3.2	9
102	¹³ C- ¹³ C spin-coupling constants in crystalline ¹³ C-labeled saccharides: conformational effects interrogated by solid-state ¹³ C NMR spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 23576-23588.	2.8	9
103	Pulse Radiolysis Investigation of Radicals Derived from Water-Soluble Cyanine Dyes: Implications for Super-resolution Microscopy. Journal of Physical Chemistry A, 2021, 125, 5779-5793.	2.5	9
104	Continuum model for solvated electrons. Journal of the Chemical Society, Faraday Transactions 2, 1974, 70, 1570.	1.1	8
105	Structure and magnetic properties of AH3 and AMe3 inorganic radicals and radical ions (A \rightarrow Al \cdot , Si, and Tl). J. Chem. Phys., 1974, 61, 1074-1081.	0.784314	8
106	Comparative theoretical study of Mu addition to the C=O and C=S bonds. Physica B: Condensed Matter, 2003, 326, 81-84.	2.7	8
107	Ab initio molecular orbital calculations on isolated vibrational frequencies in AMe3 radicals and radical ions (A = B-, C, N+, Al-, Si, P+). The Journal of Physical Chemistry, 1986, 90, 2057-2060.	2.9	7
108	EPR Detection of HNO2 \cdot - in the Radiolysis of Aqueous Nitrite and Quantum Chemical Calculation of Its Stability and Hyperfine Parameters. Journal of Physical Chemistry A, 2004, 108, 6599-6604.	2.5	7

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109	Radiation-damage investigation of a DNA 16-mer. <i>Journal of Synchrotron Radiation</i> , 2019, 26, 998-1009.	2.4	7
110	The inclusion of d-type Gaussian functions in the analytic method for the calculation of electrostatic molecular potentials. Interaction of a proton or a positive muon with carbon monoxide. <i>Journal of the Chemical Society, Faraday Transactions 2</i> , 1985, 81, 1761.	1.1	6
111	Hyperfine interactions in muonium-containing radicals. <i>Physica B: Condensed Matter</i> , 2006, 374-375, 290-294.	2.7	6
112	Chiral discrimination in the hydrogen-atom transfer between tyrosine and benzophenone in rigid peptides. <i>Chemical Physics Letters</i> , 2009, 473, 348-353.	2.6	6
113	<i>MA</i> Analysis of Aldofuranosyl Rings: Unbiased Modeling of Conformational Equilibria and Dynamics in Solution. <i>Biochemistry</i> , 2022, 61, 239-251.	2.5	6
114	<i>N</i> -Acetyl Side-Chain Conformation in Saccharides: Solution Models Obtained from <i>MA</i> Analysis. <i>Journal of Organic Chemistry</i> , 2022, 87, 8368-8379.	3.2	5
115	Comment on <i>Environmental effects on radiative rate constants with applications to linear polyenes</i> . <i>Journal of Chemical Physics</i> , 1979, 70, 5339-5340.	3.0	4
116	Bibliographies on radiation chemistry: VII. Triplet-triplet absorption spectra Part B (1976 – April, 1982). <i>Radiation Physics and Chemistry</i> (1977), 1982, 20, 179-197.	0.3	4
117	Bibliographies on radiation chemistry: VII. Triplet-triplet absorption spectra part A (1941–75). <i>Radiation Physics and Chemistry</i> (1977), 1982, 20, 119-134.	0.3	4
118	Development and use of numeric databases for properties of metastable chemical species in solution. <i>Journal of Chemical Information and Computer Sciences</i> , 1986, 26, 99-104.	2.8	4
119	Radiation damage within nucleoprotein complexes studied by macromolecular X-ray crystallography. <i>Radiation Physics and Chemistry</i> , 2016, 128, 118-125.	2.8	4
120	Electron-Induced Fragmentation of Methylated Formamides. <i>International Journal of Mass Spectrometry</i> , 2016, 410, 36-46.	1.5	4
121	Two-bond ¹³ C– ¹³ C spin-coupling constants in saccharides: dependencies on exocyclic hydroxyl group conformation. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 22912-22922.	2.8	4
122	Nonconventional NMR Spin-Coupling Constants in Oligosaccharide Conformational Modeling: Structural Dependencies Determined from Density Functional Theory Calculations. <i>ACS Omega</i> , 2022, 7, 23950-23966.	3.5	4
123	Spectral moments of solvated electrons. <i>Chemical Physics Letters</i> , 1978, 56, 339-342.	2.6	3
124	Bibliographies on radiation chemistry: VII. Triplet-triplet absorption spectra part C (April, 1982 – Dec., 1982). <i>TJ ETQq0 0,0,rgBT /Qverlock 10</i>	0.3	3
125	Reactions of hydrogen atoms with $\hat{\pm}$ -(alkylthio) carbonyl compounds. Time-resolved ESR detection and DFT calculations. <i>Research on Chemical Intermediates</i> , 2005, 31, 633-641.	2.7	3
126	Reactions of 1-Hydroxy-1-methylethyl Radicals with NO ₂ : $\hat{\pm}$ Time-Resolved Electron Spin Resonance. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11046-11052.	2.5	3

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127	Dissociative electron attachment to amide bond containing molecules: N-ethylformamide and N-ethylacetamide. <i>Journal of Chemical Physics</i> , 2020, 153, 224306.	3.0	3
128	Solvated electron wavefunctions. <i>Journal of Chemical Physics</i> , 1978, 68, 4644-4650.	3.0	2
129	Bibliographies on radiation chemistry: IV. Trapped electrons in glasses. <i>Radiation Physics and Chemistry</i> (1977), 1981, 17, 309-327.	0.3	2
130	Bibliographies on radiation chemistry: VIII. Radiation chemistry of crystalline ice. <i>Radiation Physics and Chemistry</i> (1977), 1983, 22, 981-987.	0.3	2
131	Application of the photoinduced electron transfer model to the hydrated-electron spectrum. <i>The Journal of Physical Chemistry</i> , 1982, 86, 3410-3415.	2.9	1
132	Electron paramagnetic resonance (EPR) study of \hat{I}^3 -radiation-induced radicals in 1,3,5-trithiane and its derivatives. <i>Research on Chemical Intermediates</i> , 2009, 35, 507-517.	2.7	1
133	Steric effects on intramolecular reactivity in cyclic dipeptides: Conformational analysis validated by a combined MD/DFT approach. <i>Chemical Physics Letters</i> , 2011, 512, 123-128.	2.6	1
134	OH radical reactions with the hydrophilic component of sphingolipids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1639-1648.	2.8	1
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137	Absorption spectra of dimer negative ions. <i>Journal of Chemical Physics</i> , 1983, 78, 23-26.	3.0	0
138	Bibliographies on radiation chemistry: VII. Triplet-triplet absorption spectra. <i>International Journal of Radiation Applications and Instrumentation Nuclear Tracks and Radiation Measurements</i> , 1987, 29, 315-324.	0.0	0
139	Numeric databases on the kinetics of transient species in solution. <i>International Journal of Radiation Applications and Instrumentation Nuclear Tracks and Radiation Measurements</i> , 1988, 32, 89-93.	0.0	0
140	Bibliographies on radiation chemistry. <i>International Journal of Radiation Applications and Instrumentation Nuclear Tracks and Radiation Measurements</i> , 1990, 36, 829-843.	0.0	0
141	Saccharide Structure and Reactivity Interrogated with Stable Isotopes. <i>ACS Symposium Series</i> , 2017, , 105-153.	0.5	0
142	Isopropyl 3-deoxy- \hat{I}^{\pm} -D-ribo-hexopyranoside (isopropyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 147 Td (3-deoxy- \hat{I}^{\pm} -D-ribo-hexopyranoside (isopropyl) Crystallographica Section C, <i>Structural Chemistry</i> , 2021, 77, 490-495.	0.5	0
143	Glycosidic linkage, N-acetyl side-chain, and other structural properties of methyl 2-acetamido-2-deoxy- \hat{I}^2 -D-glucopyranosyl-(1 $\hat{\alpha}$ '4)- \hat{I}^2 -D-mannopyranoside monohydrate and related compounds. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 287-297.	0.5	0