

Ian C Carmichael

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	<i>MAEAT</i> Analysis of Aldofuranosyl Rings: Unbiased Modeling of Conformational Equilibria and Dynamics in Solution. <i>Biochemistry</i> , 2022, 61, 239-251.	2.5	6
2	<i>N</i> -Acetyl Side-Chain Conformation in Saccharides: Solution Models Obtained from <i>MAEAT</i> Analysis. <i>Journal of Organic Chemistry</i> , 2022, 87, 8368-8379.	3.2	5
3	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
4	OH radical reactions with the hydrophilic component of sphingolipids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1639-1648.	2.8	1
5	Pulse Radiolysis Investigation of Radicals Derived from Water-Soluble Cyanine Dyes: Implications for Super-resolution Microscopy. <i>Journal of Physical Chemistry A</i> , 2021, 125, 5779-5793.	2.5	9
6	Isopropyl 3-deoxy- β -D-ribo-hexopyranoside (isopropyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 547 Td (3-deoxy- β -D-ribo-hexopyranoside) Crystallographica Section C, <i>Structural Chemistry</i> , 2021, 77, 490-495.	0.5	0
7	Two-bond ^{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
8	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
9	Reconciling <i>MAEAT</i> and molecular dynamics models of linkage conformation in oligosaccharides. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14454-14457.	2.8	12
10	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
11	Glycosidic linkage, <i>N</i> -acetyl side-chain, and other structural properties of methyl 2-acetamido-2-deoxy- β -D-glucopyranosyl-(1 \rightarrow 4)- β -D-mannopyranoside monohydrate and related compounds. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 287-297.	0.5	0
12	Dipole-Supported Electronic Resonances Mediate Electron-Induced Amide Bond Cleavage. <i>Physical Review Letters</i> , 2019, 122, 073002.	7.8	17
13	Radiation-damage investigation of a DNA 16-mer. <i>Journal of Synchrotron Radiation</i> , 2019, 26, 998-1009.	2.4	7
14	^{13}C spin-coupling constants in crystalline ^{13}C -labeled saccharides: conformational effects interrogated by solid-state ^{13}C NMR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 23576-23588.	2.8	9
15	Use of Circular Statistics To Model β -Man-(1 \rightarrow 2)- β -Man and β -Man-(1 \rightarrow 3)- β -Man <i>O</i> -Glycosidic Linkage Conformation in ^{13}C -Labeled Disaccharides and High-Mannose Oligosaccharides. <i>Biochemistry</i> , 2019, 58, 546-560.	2.5	29
16	Synthesis and <i>O</i> -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
17	Dissociative electron attachment induced ring opening in five-membered heterocyclic compounds. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18271-18278.	2.8	12
18	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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19	OH cleavage from tyrosine: debunking a myth. <i>Journal of Synchrotron Radiation</i> , 2017, 24, 7-18.	2.4	19
20	¹³ C-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
21	Transient Raman spectra, structure, and thermochemistry of the thiocyanate dimer radical anion in water. <i>Journal of Chemical Physics</i> , 2017, 146, 214305.	3.0	10
22	Conformational Populations of ¹³ C-Glycosidic Linkages Using Redundant NMR Spin-Couplings and Circular Statistics. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3042-3058.	2.6	39
23	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
24	Characterization of Neutral Radicals from a Dissociative Electron Attachment Process. <i>Physical Review Letters</i> , 2017, 119, 053402.	7.8	24
25	Saccharide Structure and Reactivity Interrogated with Stable Isotopes. <i>ACS Symposium Series</i> , 2017, , 105-153.	0.5	0
26	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
27	Radiation damage within nucleoprotein complexes studied by macromolecular X-ray crystallography. <i>Radiation Physics and Chemistry</i> , 2016, 128, 118-125.	2.8	4
28	Electron-Induced Fragmentation of Methylated Formamides. <i>International Journal of Mass Spectrometry</i> , 2016, 410, 36-46.	1.5	4
29	RNA protects a nucleoprotein complex against radiation damage. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 648-657.	2.3	18
30	Radiation damage to nucleoprotein complexes in macromolecular crystallography. <i>Journal of Synchrotron Radiation</i> , 2015, 22, 213-224.	2.4	21
31	Dissociative electron attachment to the gas-phase nucleobase hypoxanthine. <i>Journal of Chemical Physics</i> , 2015, 142, 215101.	3.0	13
32	Informing Saccharide Structural NMR Studies with Density Functional Theory Calculations. <i>Methods in Molecular Biology</i> , 2015, 1273, 289-331.	0.9	24
33	To scavenge or not to scavenge, that is STILL the question. <i>Journal of Synchrotron Radiation</i> , 2013, 20, 23-36.	2.4	33
34	Methyl [¹³ C]Glucopyranosiduronic Acids: Effect of COOH Ionization and Exocyclic Structure on NMR Spin-Couplings. <i>Journal of Organic Chemistry</i> , 2012, 77, 9521-9534.	3.2	9
35	Rearrangement of 3-Deoxy- ¹³ C-erythro-hexos-2-ulose in Aqueous Solution: NMR Evidence of Intramolecular 1,2-Hydrogen Transfer. <i>Journal of Organic Chemistry</i> , 2011, 76, 8151-8158.	3.2	9
36	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

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37	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
38	Amide <i>Cis</i> ~ <i>Trans</i> Isomerization in Aqueous Solutions of Methyl <i>N</i> -Formyl- <i>D</i> -glucosaminides and Methyl <i>N</i> -Acetyl- <i>D</i> -glucosaminides: Chemical Equilibria and Exchange Kinetics. <i>Journal of the American Chemical Society</i> , 2010, 132, 4641-4652.	13.7	38
39	<i>N</i> -Acetyl Side-Chains in Saccharides: NMR <i>J</i> -Coupling Equations Sensitive to CH~NH and NH~CO Bond Conformations in 2-Acetamido-2-deoxy-aldohexopyranosyl Rings. <i>Journal of Organic Chemistry</i> , 2010, 75, 4899-4910.	3.2	21
40	An NMR investigation of putative interresidue H-bonding in methyl β -cellobioside in solution. <i>Carbohydrate Research</i> , 2009, 344, 1582-1587.	2.3	25
41	Electron paramagnetic resonance (EPR) study of β -radiation-induced radicals in 1,3,5-trithiane and its derivatives. <i>Research on Chemical Intermediates</i> , 2009, 35, 507-517.	2.7	1
42	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
43	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
44	DFT Investigation of Intermediate Steps in the Hydrolysis of β -Al ₂ O ₃ (0001). <i>Journal of Physical Chemistry C</i> , 2009, 113, 2149-2158.	3.1	81
45	DFT characterization of coverage dependent molecular water adsorption modes on β -Al ₂ O ₃ (0001). <i>Surface Science</i> , 2008, 602, 268-275.	1.9	73
46	Homo- and Heterodimetallic Geminal Dianions Derived from the Bis(phosphinimine) {Ph ₂ P(NSiMe ₃) ₂ CH ₂ } ₂ and the Alkali Metals Li, Na, and K. <i>Chemistry - A European Journal</i> , 2008, 14, 3939-3953.	3.3	37
47	Oligosaccharide Trans-Glycoside ³ <i>J</i> COCC Karplus Curves Are Not Equivalent: Effect of Internal Electronegative Substituents. <i>Journal of Organic Chemistry</i> , 2008, 73, 3255-3257.	3.2	23
48	¹³ C-Labeled <i>N</i> -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
49	¹³ C~ ¹ H and ¹³ C~ ¹³ C NMR <i>J</i> -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	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
51	DFT and NMR Studies of 2JCOH, 3JHCOH, and 3JCCOH Spin-Couplings in Saccharides: C~O Torsional Bias and H-Bonding in Aqueous Solution. <i>Journal of Organic Chemistry</i> , 2007, 72, 7071-7082.	3.2	68
52	Observation of Decreased Radiation Damage at Higher Dose Rates in Room Temperature Protein Crystallography. <i>Structure</i> , 2007, 15, 1531-1541.	3.3	121
53	¹ JCH Correlates with Alcohol Hydrogen Bond Strength. <i>Journal of Organic Chemistry</i> , 2006, 71, 2878-2880.	3.2	51
54	[¹³ C, ¹⁵ N]2-Acetamido-2-deoxy- <i>D</i> -aldohexoses and Their Methyl Glycosides: Synthesis and NMR Investigations of <i>J</i> -Couplings Involving ¹ H, ¹³ C, and ¹⁵ N. <i>Journal of Organic Chemistry</i> , 2006, 71, 466-479.	3.2	22

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55	On the Association and Structure of Radicals Derived from Dipyrindil[3,2-a:2â€™3â€™-c]phenazine. Contrast between the Electrochemical, Radiolytic, and Photochemical Reduction Processes. <i>Journal of Organic Chemistry</i> , 2006, 71, 2870-2873.	3.2	15
56	Reactions of 1-Hydroxy-1-methylethyl Radicals with NO ₂ :Â Time-Resolved Electron Spin Resonance. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11046-11052.	2.5	3
57	Hydrogen and Deuterium Atoms in Octasilsesquioxanes:Â Experimental and Computational Studies. <i>Journal of the American Chemical Society</i> , 2006, 128, 6111-6125.	13.7	23
58	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
59	The Rhâ€™ligand bond: RhX (X=C, N, O, F, P and Cl) molecules. <i>Chemical Physics Letters</i> , 2006, 421, 281-286.	2.6	20
60	Hyperfine interactions in muonium-containing radicals. <i>Physica B: Condensed Matter</i> , 2006, 374-375, 290-294.	2.7	6
61	Reactions of hydrogen atoms with Î±-(alkylthio) carbonyl compounds. Time-resolved ESR detection and DFT calculations. <i>Research on Chemical Intermediates</i> , 2005, 31, 633-641.	2.7	3
62	4JCOCCHand4JCCCCHas Probes of Exocyclic Hydroxymethyl Group Conformation in Saccharides. <i>Journal of Organic Chemistry</i> , 2005, 70, 7542-7549.	3.2	22
63	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
64	Radical Production in the Radiolysis of Liquid Pyridine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 461-465.	2.5	17
65	Geminal 2JCCH Spinâ€™Spin Coupling Constants as Probes of the Î± Glycosidic Torsion Angle in Oligosaccharides. <i>Journal of the American Chemical Society</i> , 2005, 127, 9781-9793.	13.7	36
66	Molecular Recognition of Trigonal Oxyanions Using a Ditopic Salt Receptor:Â Evidence for Anisotropic Shielding Surface around Nitrate Anion. <i>Journal of the American Chemical Society</i> , 2005, 127, 2922-2928.	13.7	128
67	Role of Water in Electron-Initiated Processes and Radical Chemistry:â€™ Issues and Scientific Advances. <i>Chemical Reviews</i> , 2005, 105, 355-390.	47.7	560
68	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
69	Bimolecular Homolytic Substitution (SH ₂) Reactions with Hydrogen Atoms. Time-Resolved Electron Spin Resonance Detection in the Pulse Radiolysis of Î±-(Methylthio)acetamide. <i>Journal of the American Chemical Society</i> , 2004, 126, 14468-14474.	13.7	11
70	EPR Detection of HNO ₂ â€™ in the Radiolysis of Aqueous Nitrite and Quantum Chemical Calculation of Its Stability and Hyperfine Parameters. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6599-6604.	2.5	7
71	Correlated Câ€™C and Câ€™O Bond Conformations in Saccharide Hydroxymethyl Groups:Â Parametrization and Application of Redundant 1Hâ€™1H, 13Câ€™1H, and 13Câ€™13C NMRJ-Couplings. <i>Journal of the American Chemical Society</i> , 2004, 126, 15668-15685.	13.7	124
72	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

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73	Comparative theoretical study of Mu addition to the C=O and C=S bonds. <i>Physica B: Condensed Matter</i> , 2003, 326, 81-84.	2.7	8
74	On the Addition of $\dot{\text{C}}\text{OH}$ 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
75	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
76	Hydroxymethyl Group Conformation in Saccharides: Structural Dependencies of $^2\text{J}_{\text{HH}}$, $^3\text{J}_{\text{HH}}$, and $^1\text{J}_{\text{CH}}$ Spin-Spin Coupling Constants. <i>Journal of Organic Chemistry</i> , 2002, 67, 949-958.	3.2	185
77	Evidence for $\dot{\text{I}}^2$ Scission in the Oxidation of Amino Acids. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4573-4580.	2.5	22
78	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
79	2-Deoxy- $\dot{\text{I}}^2$ -d-erythro-pentofuranose: 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
80	Deuterium Nuclear Spin-Lattice Relaxation Times and Quadrupolar Coupling Constants in Isotopically Labeled Saccharides. <i>Journal of Magnetic Resonance</i> , 2000, 144, 207-216.	2.1	11
81	Direct EPR observation of the aminomethyl radical during the radiolysis of glycine. <i>Perkin Transactions II RSC</i> , 2000, , 907-908.	1.1	13
82	$\dot{\text{I}}^2$ -Fragmentation and Other Reactions Involving Aminyl Radicals from Amino Acids. <i>Journal of Physical Chemistry B</i> , 2000, 104, 643-649.	2.6	42
83	[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
84	$^2\text{J}_{\text{CO}}$ 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
85	Density Functional Theory Study of Ultrashort and Overlong CC Single Bonds and the Lowest Nonbonding C \cdots C Distance. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6271-6276.	2.5	10
86	2-Deoxy- $\dot{\text{I}}^2$ -d-ribofuranosylamine: 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
87	^{13}C - ^1H 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
88	Density Functional Calculations on Disaccharide Mimics: Studies of Molecular Geometries and Trans-O-glycosidic $^3\text{J}_{\text{COCH}}$ and $^3\text{J}_{\text{COCC}}$ Spin-Couplings. <i>Journal of the American Chemical Society</i> , 1999, 121, 9843-9851.	13.7	90
89	Three-Bond C \cdots O \cdots C \cdots C 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
90	Atomic Spin Densities from Correlation-Consistent Basis Sets. <i>Journal of Physical Chemistry A</i> , 1997, 101, 4633-4636.	2.5	46

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91	^{13}C - ^1H and ^{13}C - ^{13}C Spin-Coupling Constants in Methyl β -D-Ribofuranoside and Methyl 2-Deoxy- β -D-erythro-pentofuranoside: A Correlations with Molecular Structure and Conformation. Journal of the American Chemical Society, 1997, 119, 8946-8964.	13.7	81
92	^{13}C - ^1H and ^{13}C - ^{13}C Spin Couplings in [$^{2\text{-}^{13}\text{C}}$]-Deoxyribonucleosides: Correlations with Molecular Structure. Journal of the American Chemical Society, 1997, 119, 1737-1744.	13.7	44
93	Carbohydrate Reaction Intermediates: Effect of Ring-Oxygen Protonation on the Structure and Conformation of Aldofuranosyl Rings. Journal of the American Chemical Society, 1997, 119, 8933-8945.	13.7	16
94	Theoretical Studies on Some Sulfur Three-Electron Bonded Radical Cations. Acta Chemica Scandinavica, 1997, 51, 567-571.	0.7	26
95	^{13}C - ^1H Spin-Coupling Constants in the β -D-Ribofuranosyl Ring: Effect of Ring Conformation on Coupling Magnitudes. Journal of the American Chemical Society, 1996, 118, 1413-1425.	13.7	79
96	Two-bond ^{13}C - ^{13}C spin-coupling constants in carbohydrates: effect of structure on coupling magnitude and sign. Carbohydrate Research, 1996, 280, 177-186.	2.3	54
97	Correlation Effects on the Hyperfine Splitting in HNCN. The Journal of Physical Chemistry, 1995, 99, 6832-6835.	2.9	14
98	One-bond ^{13}C - ^1H spin-coupling constants in aldofuranosyl rings: effect of conformation on coupling magnitude. Journal of the American Chemical Society, 1995, 117, 8645-8650.	13.7	76
99	Hyperfine Splitting in HOCO from ab Initio Calculations. The Journal of Physical Chemistry, 1994, 98, 5896-5901.	2.9	16
100	Hyperfine Splitting in N_4^+ from ab Initio Calculation. The Journal of Physical Chemistry, 1994, 98, 5044-5048.	2.9	22
101	Torsional effects on the one-bond ^{13}C - ^{13}C spin coupling constant in ethylene glycol: insights into the behavior of $^1\text{J}_{\text{CC}}$ in carbohydrates. Journal of the American Chemical Society, 1993, 115, 10863-10870.	13.7	71
102	Ab initio quadratic configuration interaction calculation of indirect NMR spin-spin coupling constants. The Journal of Physical Chemistry, 1993, 97, 1789-1792.	2.9	48
103	Molar absorption coefficients of transient species in solution. Pure and Applied Chemistry, 1991, 63, 289-300.	1.9	84
104	Ab initio quadratic configuration interaction calculation of the isotropic hyperfine coupling constants in the ethyl radical. The Journal of Physical Chemistry, 1991, 95, 6198-6201.	2.9	30
105	Ab initio quadratic configuration interaction calculations of isotropic hyperfine coupling constants. The Journal of Physical Chemistry, 1991, 95, 108-111.	2.9	43
106	Molecular orbital studies of hyperfine coupling constants in the H_2CN and $\text{H}(\text{HO})\text{CN}$ radicals. The Journal of Physical Chemistry, 1991, 95, 4702-4708.	2.9	50
107	Ab initio coupled-cluster calculations of isotropic hyperfine splitting in some diatomic hydrides. The Journal of Physical Chemistry, 1990, 94, 5734-5740.	2.9	30
108	Bibliographies on radiation chemistry. International Journal of Radiation Applications and Instrumentation Nuclear Tracks and Radiation Measurements, 1990, 36, 829-843.	0.0	0

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109	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
110	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
111	Ab initio calculation of the hyperfine coupling constants in B2. <i>Journal of Chemical Physics</i> , 1989, 91, 1072-1078.	3.0	42
112	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
113	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
114	Ab initio configuration interaction study of the hyperfine coupling in fluorine molecular radical anion. <i>The Journal of Physical Chemistry</i> , 1987, 91, 6443-6445.	2.9	10
115	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
116	A Unified Analysis of Noncomparative Methods for Measuring the Molar Absorptivity of Triplet-Triplet Transitions. <i>Applied Spectroscopy</i> , 1987, 41, 1033-1038.	2.2	10
117	Ab initio configuration interaction study of the structure and magnetic properties of radicals and radical ions derived from group 13-15 trihydrides. <i>Chemical Physics</i> , 1987, 116, 351-367.	1.9	25
118	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
119	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
120	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
121	Structure and magnetic properties of AH3 and AMe3 inorganic radicals and radical ions (A = B, C, N+, Al-, Si, P+). <i>The Journal of Physical Chemistry</i> , 1986, 90, 2057-2060.	2.9	7
122	Ab initio molecular orbital calculations on isolated vibrational frequencies in AMe3 radicals and radical ions (A = B-, C, N+, Al-, Si, P+). <i>The Journal of Physical Chemistry</i> , 1986, 90, 2057-2060.	2.9	7
123	A critique of excitation models for partial saturation of transient absorbance. <i>Journal of Photochemistry and Photobiology</i> , 1985, 31, 179-192.	0.6	10
124	Bibliographies on radiation chemistry: VII. Triplet-triplet absorption spectra part C (April, 1982 - Dec., 1983). <i>International Journal of Radiation Applications and Instrumentation Nuclear Tracks and Radiation Measurements</i> , 1983, 35, 103-108.	0.0	0
125	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
126	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

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127	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. Journal of the Chemical Society, Faraday Transactions 2, 1985, 81, 1761.	1.1	6
128	Bibliographies on radiation chemistry: VIII. Radiation chemistry of crystalline ice. Radiation Physics and Chemistry (1977), 1983, 22, 981-987.	0.3	2
129	Absorption spectra of dimer negative ions. Journal of Chemical Physics, 1983, 78, 23-26.	3.0	0
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