

Ian C Carmichael

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4622409/publications.pdf>

Version: 2024-02-01

143
papers

5,318
citations

101384

36
h-index

95083

68
g-index

144
all docs

144
docs citations

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. | 1.9 | 861 |
| 2 | Role of Water in Electron-Initiated Processes and Radical Chemistry: Issues and Scientific Advances. <i>Chemical Reviews</i> , 2005, 105, 355-390. | 23.0 | 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. | 1.7 | 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. | 6.6 | 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. | 1.9 | 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. | 6.6 | 128 |
| 7 | Correlated $C^{\alpha}-C$ and $C^{\alpha}-O$ Bond Conformations in Saccharide Hydroxymethyl Groups: Parametrization and Application of Redundant $^1H^{\alpha}-^1H$, $^{13}C^{\alpha}-^1H$, and $^{13}C^{\alpha}-^{13}C$ NMR J-Couplings. <i>Journal of the American Chemical Society</i> , 2004, 126, 15668-15685. | 6.6 | 124 |
| 8 | Observation of Decreased Radiation Damage at Higher Dose Rates in Room Temperature Protein Crystallography. <i>Structure</i> , 2007, 15, 1531-1541. | 1.6 | 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. | 6.6 | 90 |
| 10 | Molar absorption coefficients of transient species in solution. <i>Pure and Applied Chemistry</i> , 1991, 63, 289-300. | 0.9 | 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. | 3.3 | 84 |
| 12 | $^{13}C^{\alpha}-^1H$ and $^{13}C^{\alpha}-^{13}C$ 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. | 6.6 | 81 |
| 13 | DFT Investigation of Intermediate Steps in the Hydrolysis of $\hat{\pm}\text{-Al}_{2}\text{O}_{3}$ (0001). <i>Journal of Physical Chemistry C</i> , 2009, 113, 2149-2158. | 1.5 | 81 |
| 14 | $^{13}C^{\alpha}-^1H$ 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. | 6.6 | 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. | 6.6 | 76 |
| 16 | DFT characterization of coverage dependent molecular water adsorption modes on $\hat{\pm}\text{-Al}_{2}\text{O}_{3}$ (0001). <i>Surface Science</i> , 2008, 602, 268-275. | 0.8 | 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. | 6.6 | 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. | 1.7 | 68 |

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 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. | 1.1 | 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. | 1.1 | 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. | 1.1 | 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. | 6.6 | 52 |
| 23 | ¹ J _{CH} Correlates with Alcohol Hydrogen Bond Strength. <i>Journal of Organic Chemistry</i> , 2006, 71, 2878-2880. | 1.7 | 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. | 1.1 | 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. | 6.6 | 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. | 6.6 | 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. | 1.2 | 42 |
| 31 | ¹² -Fragmentation and Other Reactions Involving Aminyl Radicals from Amino Acids. <i>Journal of Physical Chemistry B</i> , 2000, 104, 643-649. | 1.2 | 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. | 6.6 | 41 |
| 33 | Effective scavenging at cryotemperatures: further increasing the dose tolerance of protein crystals. <i>Journal of Synchrotron Radiation</i> , 2011, 18, 346-357. | 1.0 | 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. | 1.2 | 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. | 1.1 | 38 |
| 36 | Amide ¹ Cis- ¹ Trans Isomerization in Aqueous Solutions of Methyl ¹⁵ N-Formyl- ¹ -glucosaminides and Methyl ¹⁵ N-Acetyl- ¹ -glucosaminides: Chemical Equilibria and Exchange Kinetics. <i>Journal of the American Chemical Society</i> , 2010, 132, 4641-4652. | 6.6 | 38 |

| # | ARTICLE | IF | CITATIONS |
|----|---|-----|-----------|
| 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. | 1.7 | 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. | 6.6 | 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. | 1.0 | 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. | 6.6 | 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. | 1.7 | 34 |
| 43 | To scavenge or not to scavenge, that is STILL the question. <i>Journal of Synchrotron Radiation</i> , 2013, 20, 23-36. | 1.0 | 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. | 1.1 | 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. | 1.2 | 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. | 1.7 | 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. | 0.9 | 25 |
| 53 | An NMR investigation of putative interresidue H-bonding in methyl β -cellobioside in solution. <i>Carbohydrate Research</i> , 2009, 344, 1582-1587. | 1.1 | 25 |
| 54 | O -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. | 1.2 | 25 |

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 55 | Characterization of Neutral Radicals from a Dissociative Electron Attachment Process. <i>Physical Review Letters</i> , 2017, 119, 053402. | 2.9 | 24 |
| 56 | Informing Saccharide Structural NMR Studies with Density Functional Theory Calculations. <i>Methods in Molecular Biology</i> , 2015, 1273, 289-331. | 0.4 | 24 |
| 57 | Density Functional Studies of Hydrogen Atom Addition to the CS Bond. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3641-3651. | 1.1 | 23 |
| 58 | Hydrogen and Deuterium Atoms in Octasilsesquioxanes: Experimental and Computational Studies. <i>Journal of the American Chemical Society</i> , 2006, 128, 6111-6125. | 6.6 | 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. | 1.7 | 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 Scission in the Oxidation of Amino Acids. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4573-4580. | 1.1 | 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. | 1.7 | 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. | 1.7 | 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. | 1.1 | 21 |
| 67 | ¹ N-Acetyl Side-Chains in Saccharides: NMR ¹ 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. | 1.7 | 21 |
| 68 | Radiation damage to nucleoprotein complexes in macromolecular crystallography. <i>Journal of Synchrotron Radiation</i> , 2015, 22, 213-224. | 1.0 | 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. | 1.2 | 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. | 1.1 | 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. | 1.3 | 19 |

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 73 | OH cleavage from tyrosine: debunking a myth. <i>Journal of Synchrotron Radiation</i> , 2017, 24, 7-18. | 1.0 | 19 |
| 74 | RNA protects a nucleoprotein complex against radiation damage. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 648-657. | 1.1 | 18 |
| 75 | Radical Production in the Radiolysis of Liquid Pyridine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 461-465. | 1.1 | 17 |
| 76 | Dipole-Supported Electronic Resonances Mediate Electron-Induced Amide Bond Cleavage. <i>Physical Review Letters</i> , 2019, 122, 073002. | 2.9 | 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. | 6.6 | 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. | 1.7 | 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. | 1.1 | 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. | 1.7 | 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. | 1.7 | 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. | 1.2 | 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. | 1.7 | 13 |
| 87 | Dissociative electron attachment to the gas-phase nucleobase hypoxanthine. <i>Journal of Chemical Physics</i> , 2015, 142, 215101. | 1.2 | 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. | 1.3 | 12 |
| 90 | Reconciling MATE and molecular dynamics models of linkage conformation in oligosaccharides. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14454-14457. | 1.3 | 12 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-------|-----------|
| 91 | Photon-induced electron transfer transitions of the solvated electrons. Journal of Chemical Physics, 1978, 69, 2652. | 1.2 | 11 |
| 92 | Deuterium Nuclear Spin Lattice Relaxation Times and Quadrupolar Coupling Constants in Isotopically Labeled Saccharides. Journal of Magnetic Resonance, 2000, 144, 207-216. | 1.2 | 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. | 6.6 | 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. | 1.2 | 10 |
| 97 | Density Functional Theory Study of Ultrashort and Overlong CC Single Bonds and the Lowest Nonbonding C \cdots C Distance. Journal of Physical Chemistry A, 2000, 104, 6271-6276. | 1.1 | 10 |
| 98 | Transient Raman spectra, structure, and thermochemistry of the thiocyanate dimer radical anion in water. Journal of Chemical Physics, 2017, 146, 214305. | 1.2 | 10 |
| 99 | Numerical solution of semicontinuum models for excess electrons. Journal of Chemical Physics, 1978, 68, 4086-4092. | 1.2 | 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. | 1.7 | 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. | 1.7 | 9 |
| 102 | ¹³ C \cdots 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. | 1.3 | 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. | 1.1 | 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 AH ₃ and AMe ₃ inorganic radicals and radical ions (A \rightarrow A $\dot{}$, Si, and Tl). <i>J. Chem. Phys.</i> 1974, 61, 1074-1081. | 0.784 | 14 |
| 106 | Comparative theoretical study of μ addition to the C=O and C=S bonds. Physica B: Condensed Matter, 2003, 326, 81-84. | 1.3 | 8 |
| 107 | Ab initio molecular orbital calculations on isolated vibrational frequencies in AMe ₃ 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 HNO ₂ \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. | 1.1 | 7 |

| # | ARTICLE | IF | CITATIONS |
|-----|--|-----|-----------|
| 109 | Radiation-damage investigation of a DNA 16-mer. <i>Journal of Synchrotron Radiation</i> , 2019, 26, 998-1009. | 1.0 | 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. | 1.3 | 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. | 1.2 | 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. | 1.2 | 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. | 1.7 | 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. | 1.2 | 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. | 0.4 | 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. | 0.4 | 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. | 1.4 | 4 |
| 120 | Electron-Induced Fragmentation of Methylated Formamides. <i>International Journal of Mass Spectrometry</i> , 2016, 410, 36-46. | 0.7 | 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. | 1.3 | 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. | 1.6 | 4 |
| 123 | Spectral moments of solvated electrons. <i>Chemical Physics Letters</i> , 1978, 56, 339-342. | 1.2 | 3 |
| 124 | Bibliographies on radiation chemistry: VII. Triplet-triplet absorption spectra part C (April, 1982 – Dec., 1982). <i>Radiation Physics and Chemistry</i> (1977), 1982, 20, 199-204. | 0.4 | 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. | 1.3 | 3 |
| 126 | Reactions of 1-Hydroxy-1-methylethyl Radicals with NO ₂ : Time-Resolved Electron Spin Resonance. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11046-11052. | 1.1 | 3 |

| # | ARTICLE | IF | CITATIONS |
|-----|---|-----|-----------|
| 127 | Dissociative electron attachment to amide bond containing molecules: N-ethylformamide and N-ethylacetamide. <i>Journal of Chemical Physics</i> , 2020, 153, 224306. | 1.2 | 3 |
| 128 | Solvated electron wavefunctions. <i>Journal of Chemical Physics</i> , 1978, 68, 4644-4650. | 1.2 | 2 |
| 129 | Bibliographies on radiation chemistry: IV. Trapped electrons in glasses. <i>Radiation Physics and Chemistry</i> (1977), 1981, 17, 309-327. | 0.4 | 2 |
| 130 | Bibliographies on radiation chemistry: VIII. Radiation chemistry of crystalline ice. <i>Radiation Physics and Chemistry</i> (1977), 1983, 22, 981-987. | 0.4 | 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. | 1.3 | 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. | 1.2 | 1 |
| 134 | OH radical reactions with the hydrophilic component of sphingolipids. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 1639-1648. | 1.3 | 1 |
| 135 | Response to $\hat{\epsilon}^{\text{TM}}\hat{\epsilon}^{\text{TM}}$ Parity and differentiability restrictions on the electric field dependence of the mobility of charged particles in gases and liquids $\hat{\epsilon}^{\text{TM}}\hat{\epsilon}^{\text{TM}}$. <i>Journal of Chemical Physics</i> , 1979, 70, 1576-1576. | 1.2 | 0 |
| 136 | Compton profiles of solvated electrons. <i>Chemical Physics Letters</i> , 1979, 61, 96-99. | 1.2 | 0 |
| 137 | Absorption spectra of dimer negative ions. <i>Journal of Chemical Physics</i> , 1983, 78, 23-26. | 1.2 | 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} - $\langle \text{sc} \rangle \text{D} \langle / \text{sc} \rangle$ - $\langle i \rangle$ ribo $\langle / i \rangle$ -hexopyranoside (isopropyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 147 Td (3-deoxy- \hat{I}^{\pm} - $\langle \text{sc} \rangle \text{D} \langle / \text{sc} \rangle$ - $\langle i \rangle$ ribo $\langle / i \rangle$ -hexopyranoside (isopropyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 147 Td Crystallographica Section C, <i>Structural Chemistry</i> , 2021, 77, 490-495. | 0.2 | 0 |
| 143 | Glycosidic linkage, $\langle i \rangle \text{N} \langle / i \rangle$ -acetyl side-chain, and other structural properties of methyl 2-acetamido-2-deoxy- \hat{I}^2 - $\langle \text{sc} \rangle \text{D} \langle / \text{sc} \rangle$ -glucopyranosyl-(1 $\hat{\text{a}}$ '4)- \hat{I}^2 - $\langle \text{sc} \rangle \text{D} \langle / \text{sc} \rangle$ -mannopyranoside monohydrate and related compounds. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2020, 76, 287-297. | 0.2 | 0 |