

J Raul Alvarez-Idaboy

List of Publications by Year in descending order

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134
papers

6,092
citations

61857

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73
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138
all docs

138
docs citations

138
times ranked

3996
citing authors

#	ARTICLE	IF	CITATIONS
1	Food Antioxidants: Chemical Insights at the Molecular Level. Annual Review of Food Science and Technology, 2016, 7, 335-352.	5.1	294
2	A computational methodology for accurate predictions of rate constants in solution: Application to the assessment of primary antioxidant activity. Journal of Computational Chemistry, 2013, 34, 2430-2445.	1.5	289
3	On the Importance of Prereactive Complexes in Moleculeâ€™ Radical Reactions:â€™ Hydrogen Abstraction from Aldehydes by OH. Journal of the American Chemical Society, 2001, 123, 2018-2024.	6.6	244
4	Antioxidant Activity of <i>trans</i> -Resveratrol toward Hydroxyl and Hydroperoxyl Radicals: A Quantum Chemical and Computational Kinetics Study. Journal of Organic Chemistry, 2012, 77, 3868-3877.	1.7	226
5	A Quantum Chemical and Classical Transition State Theory Explanation of Negative Activation Energies in OH Addition To Substituted Ethenes. Journal of the American Chemical Society, 2000, 122, 3715-3720.	6.6	218
6	Kinetics of radicalâ€™molecule reactions in aqueous solution: A benchmark study of the performance of density functional methods. Journal of Computational Chemistry, 2014, 35, 2019-2026.	1.5	211
7	Computational strategies for predicting free radical scavengers' protection against oxidative stress: Where are we and what might follow?. International Journal of Quantum Chemistry, 2019, 119, e25665.	1.0	178
8	Glutathione: mechanism and kinetics of its non-enzymatic defense action against free radicals. RSC Advances, 2011, 1, 1763.	1.7	136
9	Counterpoise corrected interaction energies are not systematically better than uncorrected ones: comparison with CCSD(T) CBS extrapolated values. Theoretical Chemistry Accounts, 2010, 126, 75-85.	0.5	130
10	ROS Initiated Oxidation of Dopamine under Oxidative Stress Conditions in Aqueous and Lipidic Environments. Journal of Physical Chemistry B, 2011, 115, 12234-12246.	1.2	119
11	Gas phase reactions of C1â€™C4alcohols with the OH radical: A quantum mechanical approach. Physical Chemistry Chemical Physics, 2002, 4, 4648-4662.	1.3	108
12	Can a Single Water Molecule Really Catalyze the Acetaldehyde + OH Reaction in Tropospheric Conditions?. Journal of Physical Chemistry Letters, 2010, 1, 3112-3115.	2.1	108
13	The mechanism of the Baeyerâ€™Villiger rearrangement: quantum chemistry and TST study supported by experimental kinetic data. Organic and Biomolecular Chemistry, 2007, 5, 3682.	1.5	106
14	A new approach to counterpoise correction to BSSE. Journal of Computational Chemistry, 2006, 27, 1203-1210.	1.5	105
15	OH Radical Gas Phase Reactions with Aliphatic Ethers: A Variational Transition State Theory Study. Journal of Physical Chemistry A, 2009, 113, 13913-13920.	1.1	103
16	Guanosine + OH Radical Reaction in Aqueous Solution: A Reinterpretation of the UVâ€™vis Data Based on Thermodynamic and Kinetic Calculations. Organic Letters, 2009, 11, 5114-5117.	2.4	100
17	Empirically Fitted Parameters for Calculating pK_a Values with Small Deviations from Experiments Using a Simple Computational Strategy. Journal of Chemical Information and Modeling, 2016, 56, 1714-1724.	2.5	97
18	A New Specific Mechanism for the Acid Catalysis of the Addition Step in the Baeyerâ€™Villiger Rearrangement. Organic Letters, 2006, 8, 1763-1765.	2.4	92

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19	Quantum chemistry and TST study of the mechanisms and branching ratios for the reactions of OH with unsaturated aldehydes. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 7649.	1.3	88
20	On the Chemical Repair of DNA Radicals by Glutathione: Hydrogen vs Electron Transfer. <i>Journal of Physical Chemistry B</i> , 2012, 116, 9316-9325.	1.2	85
21	Piceatannol, a better peroxy radical scavenger than resveratrol. <i>RSC Advances</i> , 2013, 3, 20209.	1.7	85
22	Mechanism and kinetics studies on the antioxidant activity of sinapinic acid. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 11199.	1.3	80
23	Canolol: A Promising Chemical Agent against Oxidative Stress. <i>Journal of Physical Chemistry B</i> , 2011, 115, 8590-8596.	1.2	77
24	Rate Constant Dependence on the Size of Aldehydes in the NO ₃ + Aldehydes Reaction. An Explanation via Quantum Chemical Calculations and CTST. <i>Journal of the American Chemical Society</i> , 2001, 123, 8387-8395.	6.6	71
25	Rate Coefficient and Mechanism of the Gas Phase OH Hydrogen Abstraction Reaction from Formic Acid: A Quantum Mechanical Approach. <i>Journal of Physical Chemistry A</i> , 2002, 106, 9520-9528.	1.1	71
26	Comprehensive Investigation of the Antioxidant and Pro-oxidant Effects of Phenolic Compounds: A Double-Edged Sword in the Context of Oxidative Stress?. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6198-6214.	1.2	71
27	The Baeyer-Villiger reaction: solvent effects on reaction mechanisms. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 3682.	1.5	70
28	Theoretical Determination of the Rate Constant for OH Hydrogen Abstraction from Toluene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10155-10162.	1.1	69
29	On the peroxy scavenging activity of hydroxycinnamic acid derivatives: mechanisms, kinetics, and importance of the acid-base equilibrium. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12534.	1.3	68
30	Glycolaldehyde + OH Gas Phase Reaction: A Quantum Chemistry + CVT/SCT Approach. <i>Journal of Physical Chemistry A</i> , 2005, 109, 169-180.	1.1	65
31	Physicochemical Insights on the Free Radical Scavenging Activity of Sesamol: Importance of the Acid/Base Equilibrium. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13101-13109.	1.2	64
32	On the possible catalytic role of a single water molecule in the acetone+OH gas phase reaction: a theoretical pseudo-second-order kinetics study. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 209-217.	0.5	64
33	OH hydrogen abstraction reactions from alanine and glycine: A quantum mechanical approach. <i>Journal of Computational Chemistry</i> , 2001, 22, 1138-1153.	1.5	57
34	Theoretical Explanation of Nonexponential OH Decay in Reactions with Benzene and Toluene under Pseudo-First-Order Conditions. <i>Journal of Physical Chemistry A</i> , 2008, 112, 7608-7615.	1.1	57
35	Mechanism and Kinetics of the Water-Assisted Formic Acid + OH Reaction under Tropospheric Conditions. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5138-5146.	1.1	57
36	Antioxidant activity of propyl gallate in aqueous and lipid media: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13137.	1.3	56

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37	Hydrogen Abstraction Reactions from Phenolic Compounds by Peroxyl Radicals: Multireference Character and Density Functional Theory Rate Constants. <i>Journal of Physical Chemistry A</i> , 2016, 120, 4634-4642.	1.1	55
38	Structure-Reactivity Relationship in Ketones + OH Reactions: A Quantum Mechanical and TST Approach. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2740-2749.	1.1	52
39	Theoretical study of the initial reaction between OH and isoprene in tropospheric conditions. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 1392-1399.	1.3	51
40	Computational and experimental study of the interactions between ionic liquids and volatile organic compounds. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9830.	1.3	51
41	Mechanism of the OH-propene-O ₂ reaction: An ab initio study. <i>International Journal of Chemical Kinetics</i> , 1999, 31, 29-36.	1.0	49
42	Mechanism and Kinetics of the Reaction of OH Radicals with Glyoxal and Methylglyoxal: A Quantum Chemistry+CVT/SCT Approach. <i>ChemPhysChem</i> , 2004, 5, 1379-1388.	1.0	49
43	Quantum Chemical and Conventional Transition-State Theory Calculations of Rate Constants for the NO ₃ + Alkane Reaction. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4645-4650.	1.1	48
44	Free-radical scavenging by tryptophan and its metabolites through electron transfer based processes. <i>Journal of Molecular Modeling</i> , 2015, 21, 213.	0.8	47
45	A Quantum Chemical and TST Study of the OH Hydrogen-Abstraction Reaction from Substituted Aldehydes: FCHO and ClCHO. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9034-9039.	1.1	43
46	Branching Ratios of Aliphatic Amines + OH Gas-Phase Reactions: A Variational Transition-State Theory Study. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 322-327.	2.3	43
47	Thiophenols, Promising Scavengers of Peroxyl Radicals: Mechanisms and kinetics. <i>Journal of Computational Chemistry</i> , 2019, 40, 2103-2110.	1.5	43
48	Single water-molecule catalysis in the glyoxal + OH reaction under tropospheric conditions: Fact or fiction? A quantum chemistry and pseudo-second order computational kinetic study. <i>Chemical Physics Letters</i> , 2010, 501, 11-15.	1.2	41
49	Coumarin-Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 662-670.	2.5	41
50	On the evolution of one-electron-oxidized deoxyguanosine in damaged DNA under physiological conditions: a DFT and ONIOM study on proton transfer and equilibrium. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12476.	1.3	39
51	A quantum chemical study on the free radical scavenging activity of tyrosol and hydroxytyrosol. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	38
52	Dihydroxybenzoic acids as free radical scavengers: mechanisms, kinetics, and trends in activity. <i>New Journal of Chemistry</i> , 2014, 38, 2639.	1.4	37
53	Lipoic Acid and Dihydrolipoic Acid. A Comprehensive Theoretical Study of Their Antioxidant Activity Supported by Available Experimental Kinetic Data. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1642-1652.	2.5	37
54	Melatonin and its metabolites as chemical agents capable of directly repairing oxidized DNA. <i>Journal of Pineal Research</i> , 2019, 66, e12539.	3.4	37

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55	Influence of the Environment on the Protective Effects of Guaiacol Derivatives against Oxidative Stress: Mechanisms, Kinetics, and Relative Antioxidant Activity. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7129-7137.	1.2	33
56	Antioxidant activity of fraxetin and its regeneration in aqueous media. A density functional theory study. <i>RSC Advances</i> , 2014, 4, 52920-52932.	1.7	33
57	Dual antioxidant/pro-oxidant behavior of the tryptophan metabolite 3-hydroxyanthranilic acid: a theoretical investigation of reaction mechanisms and kinetics. <i>New Journal of Chemistry</i> , 2017, 41, 3829-3845.	1.4	33
58	Mechanism and rate coefficients of the gas phase OH hydrogen abstraction reaction from asparagine: a quantum mechanical approach. <i>Computational and Theoretical Chemistry</i> , 2002, 617, 77-86.	1.5	32
59	Role of Allyl Group in the Hydroxyl and Peroxyl Radical Scavenging Activity of <i>S</i> -Allylcysteine. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13408-13417.	1.2	32
60	Quantum chemical and conventional TST calculations of rate constants for the OH+alkane reaction. <i>Chemical Physics</i> , 2005, 310, 213-223.	0.9	31
61	Theoretical study on the peroxyl radicals scavenging activity of esculetin and its regeneration in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 1197-1207.	1.3	31
62	Antioxidant activity of selected natural polyphenolic compounds from soybean via peroxyl radical scavenging. <i>RSC Advances</i> , 2014, 4, 38918-38930.	1.7	30
63	Reinvestigating the Role of Multiple Hydrogen Transfers in Baeyer-Villiger Reactions. <i>Journal of Organic Chemistry</i> , 2007, 72, 6580-6583.	1.7	28
64	A proton-coupled electron sequential transfer mechanism: theoretical evidence about its biological relevance. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28525-28528.	1.3	26
65	Non-alkane behavior of cyclopropane and its derivatives: characterization of unconventional hydrogen bond interactions. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 597-606.	0.5	25
66	The role of acid-base equilibria in formal hydrogen transfer reactions: tryptophan radical repair by uric acid as a paradigmatic case. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15296-15309.	1.3	24
67	Chalcogen effects on the primary antioxidant activity of chrysin and quercetin. <i>New Journal of Chemistry</i> , 2020, 44, 9073-9082.	1.4	24
68	The Baeyer-Villiger reaction of 23-oxosapogenins. <i>Arkivoc</i> , 2005, 2005, 109-126.	0.3	24
69	Substituent effects in the Baeyer-Villiger reaction of acetophenones: a theoretical study. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 643-649.	0.9	23
70	Assessing the Protective Activity of a Recently Discovered Phenolic Compound against Oxidative Stress Using Computational Chemistry. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2552-2561.	2.5	23
71	A Possible Mechanism for Furan Formation in the Tropospheric Oxidation of Dienes. <i>Environmental Science & Technology</i> , 2005, 39, 8797-8802.	4.6	22
72	Deprotonation routes of anthocyanidins in aqueous solution, pK _a values, and speciation under physiological conditions. <i>RSC Advances</i> , 2016, 6, 53421-53429.	1.7	22

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73	Kinetics and mechanism of the gas-phase OH hydrogen abstraction reaction from methionine: A quantum mechanical approach. <i>International Journal of Chemical Kinetics</i> , 2003, 35, 212-221.	1.0	21
74	On the role of s-cis conformers in the reaction of dienes with OH radicals. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 2237-2244.	1.3	21
75	Tryptophan: antioxidant or target of oxidative stress? A quantum chemistry elucidation. <i>RSC Advances</i> , 2014, 4, 56128-56131.	1.7	21
76	Radical-trapping and preventive antioxidant effects of 2-hydroxymelatonin and 4-hydroxymelatonin: Contributions to the melatonin protection against oxidative stress. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017, 1861, 2206-2217.	1.1	21
77	Computationally Designed Sesamol Derivatives Proposed as Potent Antioxidants. <i>ACS Omega</i> , 2020, 5, 9566-9575.	1.6	21
78	Theoretical Model of Furan and 2-Furancarboxaldehyde. The Molecular Structure and Vibrational Spectra, Including Isotopic Effects. <i>The Journal of Physical Chemistry</i> , 1994, 98, 5607-5613.	2.9	20
79	Rate coefficients and mechanism of the gas phase OH hydrogen abstraction reaction from serine: a quantum mechanical approach. <i>Computational and Theoretical Chemistry</i> , 2003, 629, 165-174.	1.5	20
80	Non-covalent π - π stacking interactions turn off non-adiabatic effects in proton-coupled electron transfer reactions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6969-6972.	1.3	20
81	Site reactivity in the free radicals induced damage to leucine residues: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4970-4976.	1.3	18
82	Isopropylcyclopropane + OH Gas Phase Reaction: A Quantum Chemistry + CVT/SCT Approach. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1917-1924.	1.1	17
83	Mechanism and Branching Ratios of Hydroxy Ethers + OH Gas phase Reactions: Relevance of H Bond Interactions. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7525-7536.	1.1	17
84	Molecular Description of Indigo Oxidation Mechanisms Initiated by OH and OOH Radicals. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3643-3651.	1.1	17
85	An experimental and theoretical study of the kinetics and mechanism of hydroxyl radical reaction with 2-aminopyrimidine. <i>RSC Advances</i> , 2014, 4, 14157.	1.7	17
86	Primary antioxidant and metal-binding effects of tiopronin: A theoretical investigation of its action mechanism. <i>Computational and Theoretical Chemistry</i> , 2016, 1077, 48-57.	1.1	17
87	Theoretical investigation of the ethene-ethene radical cation addition reaction. <i>The Journal of Physical Chemistry</i> , 1993, 97, 12737-12741.	2.9	16
88	Atmospheric Reactions of Oxygenated Volatile Organic Compounds+OH Radicals: Role of Hydrogen-Bonded Intermediates and Transition States. <i>Advances in Quantum Chemistry</i> , 2008, , 245-274.	0.4	16
89	Hydrolysis of a Chlorambucil Analogue. A DFT study.. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2359-2366.	1.1	16
90	Mechanisms and rate constants in the atmospheric oxidation of saturated esters by hydroxyl radicals: A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3508-3515.	1.0	16

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91	Acid-Catalyzed Nucleophilic Additions to Carbonyl Groups: Is the Accepted Mechanism the Rule or an Exception?. <i>Journal of Organic Chemistry</i> , 2013, 78, 2327-2335.	1.7	16
92	Estimation of empirically fitted parameters for calculating pK _a values of thiols in a fast and reliable way. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	16
93	The Antioxidant Capability of Higenamine: Insights from Theory. <i>Antioxidants</i> , 2020, 9, 358.	2.2	16
94	Kinetics and mechanism of the Î²-alanine + OH gas phase reaction: A quantum mechanical approach. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 285-292.	1.3	15
95	Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently. <i>Chemistry - A European Journal</i> , 2018, 24, 8686-8691.	1.7	15
96	Modelling the chemical repair of protein carbon-centered radicals formed via oxidative damage with dihydrolipoic acid. <i>RSC Advances</i> , 2015, 5, 96714-96719.	1.7	14
97	Quantum mechanical approach to isoleucine+OH gas phase reaction. Mechanism and kinetics. <i>Computational and Theoretical Chemistry</i> , 2004, 676, 97-103.	1.5	13
98	A theoretical investigation of the mechanism of the NO ₃ addition to alkenes. <i>Computational and Theoretical Chemistry</i> , 2004, 684, 51-59.	1.5	13
99	Quantum chemistry and TST study of the mechanism and kinetics of the butadiene and isoprene reactions with mercapto radicals. <i>Chemical Physics</i> , 2008, 344, 273-280.	0.9	12
100	Tropospheric degradation of ethylene glycol monovinyl and divinyl ethers: A mechanistic and kinetic study. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3525-3534.	1.0	12
101	Radical scavenging activity of ascorbic acid analogs: kinetics and mechanisms. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	12
102	Reaction mechanism of the acyl-enzyme formation in Î²-lactam hydrolysis by means of quantum chemical modeling. <i>Computational and Theoretical Chemistry</i> , 2000, 504, 13-28.	1.5	11
103	Role of purines on the copper-catalyzed oxidative damage in biological systems: Protection versus promotion. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25527.	1.0	11
104	The other side of the superoxide radical anion: its ability to chemically repair DNA oxidized sites. <i>Chemical Communications</i> , 2018, 54, 13710-13713.	2.2	11
105	Ab initio study of Î³-alanine conformers in gas phase. <i>Arkivoc</i> , 2005, 2005, 7-18.	0.3	11
106	On the correlation between ionization potentials and bond angles in heterocyclic compounds. <i>Journal of Molecular Structure</i> , 1991, 249, 305-312.	1.8	9
107	Evidence of A Possible Cycloaddition Channel in the Ethene + NO ₃ Reaction. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9222-9230.	1.1	9
108	Contrasting reactions of hydrated electron and formate radical with 2-thio analogues of cytosine and uracil. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28781-28790.	1.3	9

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109	Computational Quantum Chemistry: A Reliable Tool in the Understanding of Gas-Phase Reactions. <i>Journal of Chemical Education</i> , 2006, 83, 481.	1.1	8
110	Influence of the methylation degree on the rate constants of the OH addition to alkenes and its temperature dependence. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 3479-3483.	1.0	8
111	Theoretical study of copper complexes with lipoic and dihydrolipoic acids. <i>RSC Advances</i> , 2016, 6, 107924-107932.	1.7	8
112	Formation mechanism of glyoxal-DNA adduct, a DNA cross-link precursor. <i>International Journal of Biological Macromolecules</i> , 2017, 98, 664-675.	3.6	8
113	Insights into the Mechanism of Hydroxyl Radical Mediated Oxidations of 2-Aminopurine: A Computational and Sonochemical Product Analysis Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 6245-6256.	1.2	8
114	Tryptophan versus nitric oxide, nitrogen dioxide and carbonate radicals: differences in reactivity and implications for oxidative damage to proteins. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	7
115	Modelling the repair of carbon-centred protein radicals by the antioxidants glutathione and Trolox. <i>New Journal of Chemistry</i> , 2019, 43, 2085-2097.	1.4	7
116	Theoretical model of the electrophilic substitution in pentagonal unsaturated heterocycles. <i>Computational and Theoretical Chemistry</i> , 1990, 209, 361-372.	1.5	6
117	Theoretical modelling of the electrophilic substitution mechanism in furan. <i>Computational and Theoretical Chemistry</i> , 1992, 253, 243-259.	1.5	6
118	A theoretical and experimental evaluation of imidazolium-based ionic liquids for atmospheric mercury capture. <i>Journal of Molecular Modeling</i> , 2014, 20, 2186.	0.8	6
119	Chemical repair of protein carbon-centred radicals: long-distance dynamic factors. <i>Canadian Journal of Chemistry</i> , 2016, 94, 1119-1126.	0.6	6
120	Theoretical study of reactions of the 1-butene radical cation in frozen halocarbon matrixes. <i>The Journal of Physical Chemistry</i> , 1993, 97, 12742-12744.	2.9	5
121	A study of the nucleophilic attack of the beta-lactamic bond of antibiotics in water solution. <i>Computational and Theoretical Chemistry</i> , 2001, 539, 233-243.	1.5	5
122	Theoretical Study of the Reactivity and Selectivity of Various Free Radicals with Cysteine Residues. <i>ACS Omega</i> , 2018, 3, 16519-16528.	1.6	5
123	Free radical scavenging activity of newly designed sesamol derivatives. <i>New Journal of Chemistry</i> , 2021, 45, 11960-11967.	1.4	5
124	Formation of 2-hexene by cationic dimerization of propene: an ab initio and density functional theory study. <i>Theoretical Chemistry Accounts</i> , 1997, 97, 277-282.	0.5	4
125	Theoretical study of the complex reaction of $\text{O}(^3\text{P})$ with trans-2-butene. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	4
126	Chemical repair of damaged leucine and tryptophane by thiophenols at close to diffusion-controlled rates: Mechanisms and kinetics. <i>Journal of Computational Chemistry</i> , 2022, , .	1.5	4

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127	Theoretical and experimental study demonstrates kinetic control in chalcone-flavanone transformation of naphthalene derivatives. <i>Journal of Molecular Structure</i> , 2018, 1157, 631-637.	1.8	2
128	Reinvestigation of Acetophenones Oxidation by Performic Acid in Formic Acid. <i>Journal of Physical Chemistry A</i> , 2019, 123, 1968-1972.	1.1	2
129	Rate Constants and Branching Ratios in the Oxidation of Aliphatic Aldehydes by OH Radicals under Atmospheric Conditions. <i>Journal of the Mexican Chemical Society</i> , 2017, 56, .	0.2	2
130	Model Calculations of Base-Catalysed 1,3-Proton Transfer Reactions in Indene-like Systems.. <i>Acta Chemica Scandinavica</i> , 1994, 48, 423-427.	0.7	2
131	Mechanism of the OHâ€“propeneâ€“O ₂ reaction: An ab initio study. , 1999, 31, 29.		1
132	Theoretical approach to cationic polymerization of alkenylfurans. II. Ab initio and semiempirical study of relevant steps in the reaction mechanism. <i>Journal of Polymer Science Part A</i> , 1992, 30, 2497-2502.	2.5	0
133	Chemical repair mechanisms of damaged tyrosyl and tryptophanyl residues in proteins by the superoxide radical anion. <i>New Journal of Chemistry</i> , 2020, 44, 2505-2513.	1.4	0
134	Model Calculations of Matrix Effects on the Conversion of Propene Radical Cations into Allyl Radicals in Halocarbon Matrices.. <i>Acta Chemica Scandinavica</i> , 1997, 51, 242-248.	0.7	0