J Raul Alvarez-Idaboy

List of Publications by Year
in descending order

134 papers	6,092 citations	61984 43 h-index	79698 73 g-index
138 all docs	138 docs citations	138 times ranked	3996 citing authors

#	Article	IF	Citations
1	Chemical repair of damaged leucine and tryptophane by thiophenols at close to diffusionâ€controlled rates: Mechanisms and kinetics. Journal of Computational Chemistry, 2022, , .	3.3	4
2	Free radical scavenging activity of newly designed sesamol derivatives. New Journal of Chemistry, 2021, 45, 11960-11967.	2.8	5
3	Chalcogen effects on the primary antioxidant activity of chrysin and quercetin. New Journal of Chemistry, 2020, 44, 9073-9082.	2.8	24
4	Insights into the Mechanism of Hydroxyl Radical Mediated Oxidations of 2-Aminopurine: A Computational and Sonochemical Product Analysis Study. Journal of Physical Chemistry B, 2020, 124, 6245-6256.	2.6	8
5	Chemical repair mechanisms of damaged tyrosyl and tryptophanyl residues in proteins by the superoxide radical anion. New Journal of Chemistry, 2020, 44, 2505-2513.	2.8	0
6	The Antioxidant Capability of Higenamine: Insights from Theory. Antioxidants, 2020, 9, 358.	5.1	16
7	Computationally Designed Sesamol Derivatives Proposed as Potent Antioxidants. ACS Omega, 2020, 5, 9566-9575.	3.5	21
8	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.	2.0	178
9	Modelling the repair of carbon-centred protein radicals by the antioxidants glutathione and Trolox. New Journal of Chemistry, 2019, 43, 2085-2097.	2.8	7
10	Thiophenols, Promising Scavengers of Peroxyl Radicals: Mechanisms and kinetics. Journal of Computational Chemistry, 2019, 40, 2103-2110.	3.3	43
11	Reinvestigation of Acetophenones Oxidation by Performic Acid in Formic Acid. Journal of Physical Chemistry A, 2019, 123, 1968-1972.	2.5	2
12	Melatonin and its metabolites as chemical agents capable of directly repairing oxidized DNA. Journal of Pineal Research, 2019, 66, e12539.	7.4	37
13	Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently. Chemistry - A European Journal, 2018, 24, 8686-8691.	3.3	15
14	Theoretical and experimental study demonstrates kinetic control in chalcone-flavanone transformation of naphthalene derivatives. Journal of Molecular Structure, 2018, 1157, 631-637.	3.6	2
15	Radical scavenging activity of ascorbic acid analogs: kinetics and mechanisms. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	12
16	Role of purines on the copperâ€catalyzed oxidative damage in biological systems: Protection versus promotion. International Journal of Quantum Chemistry, 2018, 118, e25527.	2.0	11
17	Estimation of empirically fitted parameters for calculating pK a values of thiols in a fast and reliable way. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	16
18	The other side of the superoxide radical anion: its ability to chemically repair DNA oxidized sites. Chemical Communications, 2018, 54, 13710-13713.	4.1	11

#	Article	IF	Citations
19	Theoretical Study of the Reactivity and Selectivity of Various Free Radicals with Cysteine Residues. ACS Omega, 2018, 3, 16519-16528.	3.5	5
20	Comprehensive Investigation of the Antioxidant and Pro-oxidant Effects of Phenolic Compounds: A Double-Edged Sword in the Context of Oxidative Stress?. Journal of Physical Chemistry B, 2018, 122, 6198-6214.	2.6	71
21	Formation mechanism of glyoxal-DNA adduct, a DNA cross-link precursor. International Journal of Biological Macromolecules, 2017, 98, 664-675.	7.5	8
22	Non-covalent Ï€â€“Ï€ stacking interactions turn off non-adiabatic effects in proton-coupled electron transfer reactions. Physical Chemistry Chemical Physics, 2017, 19, 6969-6972.	2.8	20
23	Dual antioxidant/pro-oxidant behavior of the tryptophan metabolite 3-hydroxyanthranilic acid: a theoretical investigation of reaction mechanisms and kinetics. New Journal of Chemistry, 2017, 41, 3829-3845.	2.8	33
24	The role of acidâ€“base equilibria in formal hydrogen transfer reactions: tryptophan radical repair by uric acid as a paradigmatic case. Physical Chemistry Chemical Physics, 2017, 19, 15296-15309.	2.8	24
25	Radical-trapping and preventive antioxidant effects of 2-hydroxymelatonin and 4-hydroxymelatonin: Contributions to the melatonin protection against oxidative stress. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 2206-2217.	2.4	21
26	Rate Constants and Branching Ratios in the Oxidation of Aliphatic Aldehydes by OH Radicals under Atmospheric Conditions. Journal of the Mexican Chemical Society, 2017, 56, .	0.6	2
27	Deprotonation routes of anthocyanidins in aqueous solution, pK_avalues, and speciation under physiological conditions. RSC Advances, 2016, 6, 53421-53429.	3.6	22
28	Primary antioxidant and metal-binding effects of tiopronin: A theoretical investigation of its action mechanism. Computational and Theoretical Chemistry, 2016, 1077, 48-57.	2.5	17
29	Tryptophan versus nitric oxide, nitrogen dioxide and carbonate radicals: differences in reactivity and implications for oxidative damage to proteins. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	7
30	Contrasting reactions of hydrated electron and formate radical with 2-thio analogues of cytosine and uracil. Physical Chemistry Chemical Physics, 2016, 18, 28781-28790.	2.8	9
31	Chemical repair of protein carbon-centred radicals: long-distance dynamic factors. Canadian Journal of Chemistry, 2016, 94, 1119-1126.	1.1	6
32	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.	5.4	97
33	Theoretical study of copper complexes with lipoic and dihydrolipoic acids. RSC Advances, 2016, 6, 107924-107932.	3.6	8
34	Food Antioxidants: Chemical Insights at the Molecular Level. Annual Review of Food Science and Technology, 2016, 7, 335-352.	9.9	294
35	Coumarinâ€“Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. Journal of Chemical Information and Modeling, 2016, 56, 662-670.	5.4	41
36	Hydrogen Abstraction Reactions from Phenolic Compounds by Peroxyl Radicals: Multireference Character and Density Functional Theory Rate Constants. Journal of Physical Chemistry A, 2016, 120, 4634-4642.	2.5	55

#	Article	IF	Citations
37	Assessing the Protective Activity of a Recently Discovered Phenolic Compound against Oxidative Stress Using Computational Chemistry. Journal of Chemical Information and Modeling, 2015, 55, 2552-2561.	5.4	23
38	Site reactivity in the free radicals induced damage to leucine residues: a theoretical study. Physical Chemistry Chemical Physics, 2015, 17, 4970-4976.	2.8	18
39	Free-radical scavenging by tryptophan and its metabolites through electron transfer based processes. Journal of Molecular Modeling, 2015, 21, 213.	1.8	47
40	Modelling the chemical repair of protein carbon-centered radicals formed via oxidative damage with dihydrolipoic acid. RSC Advances, 2015, 5, 96714-96719.	3.6	14
41	A protonâ€“electron sequential transfer mechanism: theoretical evidence about its biological relevance. Physical Chemistry Chemical Physics, 2015, 17, 28525-28528.	2.8	26
42	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.	3.3	211
43	Antioxidant activity of fraxetin and its regeneration in aqueous media. A density functional theory study. RSC Advances, 2014, 4, 52920-52932.	3.6	33
44	Theoretical study on the peroxyl radicals scavenging activity of esculetin and its regeneration in aqueous solution. Physical Chemistry Chemical Physics, 2014, 16, 1197-1207.	2.8	31
45	Dihydroxybenzoic acids as free radical scavengers: mechanisms, kinetics, and trends in activity. New Journal of Chemistry, 2014, 38, 2639.	2.8	37
46	Tryptophan: antioxidant or target of oxidative stress? A quantum chemistry elucidation. RSC Advances, 2014, 4, 56128-56131.	3.6	21
47	An experimental and theoretical study of the kinetics and mechanism of hydroxyl radical reaction with 2-aminopyrimidine. RSC Advances, 2014, 4, 14157.	3.6	17
48	Antioxidant activity of selected natural polyphenolic compounds from soybean via peroxyl radical scavenging. RSC Advances, 2014, 4, 38918-38930.	3.6	30
49	Lipoic Acid and Dihydrolipoic Acid. A Comprehensive Theoretical Study of Their Antioxidant Activity Supported by Available Experimental Kinetic Data. Journal of Chemical Information and Modeling, 2014, 54, 1642-1652.	5.4	37
50	A theoretical and experimental evaluation of imidazolium-based ionic liquids for atmospheric mercury capture. Journal of Molecular Modeling, 2014, 20, 2186.	1.8	6
51	Theoretical study of the complex reaction of O(3P) with trans-2-butene. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	4
52	Antioxidant activity of propyl gallate in aqueous and lipid media: a theoretical study. Physical Chemistry Chemical Physics, 2013, 15, 13137.	2.8	56
53	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.	3.3	289
54	Piceatannol, a better peroxyl radical scavenger than resveratrol. RSC Advances, 2013, 3, 20209.	3.6	85

#	Article	IF	Citations
55	Acid-Catalyzed Nucleophilic Additions to Carbonyl Groups: Is the Accepted Mechanism the Rule or an Exception?. Journal of Organic Chemistry, 2013, 78, 2327-2335.	3.2	16
56	On the Chemical Repair of DNA Radicals by Glutathione: Hydrogen vs Electron Transfer. Journal of Physical Chemistry B, 2012, 116, 9316-9325.	2.6	85
57	On the evolution of one-electron-oxidized deoxyguanosine in damaged DNA under physiological conditions: a DFT and ONIOM study on proton transfer and equilibrium. Physical Chemistry Chemical Physics, 2012, 14, 12476.	2.8	39
58	Influence of the methylation degree on the rate constants of the ^{â€¢}OH addition to alkenes and its temperature dependence. International Journal of Quantum Chemistry, 2012, 112, 3479-3483.	2.0	8
59	Mechanisms and rate constants in the atmospheric oxidation of saturated esters by hydroxyl radicals: A theoretical study. International Journal of Quantum Chemistry, 2012, 112, 3508-3515.	2.0	16
60	Tropospheric degradation of ethylene glycol monovinyl and divinyl ethers: A mechanistic and kinetic study. International Journal of Quantum Chemistry, 2012, 112, 3525-3534.	2.0	12
61	Antioxidant Activity of trans-Resveratrol toward Hydroxyl and Hydroperoxyl Radicals: A Quantum Chemical and Computational Kinetics Study. Journal of Organic Chemistry, 2012, 77, 3868-3877.	3.2	226
62	On the peroxyl scavenging activity of hydroxycinnamic acid derivatives: mechanisms, kinetics, and importance of the acidâ€“base equilibrium. Physical Chemistry Chemical Physics, 2012, 14, 12534.	2.8	68
63	Molecular Description of Indigo Oxidation Mechanisms Initiated by OH and OOH Radicals. Journal of Physical Chemistry A, 2012, 116, 3643-3651.	2.5	17
64	Influence of the Environment on the Protective Effects of Guaiacol Derivatives against Oxidative Stress: Mechanisms, Kinetics, and Relative Antioxidant Activity. Journal of Physical Chemistry B, 2012, 116, 7129-7137.	2.6	33
65	A quantum chemical study on the free radical scavenging activity of tyrosol and hydroxytyrosol. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	38
66	Glutathione: mechanism and kinetics of its non-enzymatic defense action against free radicals. RSC Advances, 2011, 1, 1763.	3.6	136
67	Role of Allyl Group in the Hydroxyl and Peroxyl Radical Scavenging Activity ofS-Allylcysteine. Journal of Physical Chemistry B, 2011, 115, 13408-13417.	2.6	32
68	Hydrolysis of a Chlorambucil Analogue. A DFT study.. Journal of Physical Chemistry A, 2011, 115, 2359-2366.	2.5	16
69	Physicochemical Insights on the Free Radical Scavenging Activity of Sesamol: Importance of the Acid/Base Equilibrium. Journal of Physical Chemistry B, 2011, 115, 13101-13109.	2.6	64
70	Mechanism and Kinetics of the Water-Assisted Formic Acid + OH Reaction under Tropospheric Conditions. Journal of Physical Chemistry A, 2011, 115, 5138-5146.	2.5	57
71	ROS Initiated Oxidation of Dopamine under Oxidative Stress Conditions in Aqueous and Lipidic Environments. Journal of Physical Chemistry B, 2011, 115, 12234-12246.	2.6	119
72	Mechanism and kinetics studies on the antioxidant activity of sinapinic acid. Physical Chemistry Chemical Physics, 2011, 13, 11199.	2.8	80

#	Article	IF	Citations
73	Canolol: A Promising Chemical Agent against Oxidative Stress. Journal of Physical Chemistry B, 2011, 115, 8590-8596.	2.6	77
74	On the possible catalytic role of a single water molecule in the acetoneÂ+ÂOH gas phase reaction: a theoretical pseudo-second-order kinetics study. Theoretical Chemistry Accounts, 2011, 129, 209-217.	1.4	64
75	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.	1.4	130
76	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. Chemical Physics Letters, 2010, 501, 11-15.	2.6	41
77	Mechanism and Branching Ratios of Hydroxy Ethers + ^{â€¢}OH Gas phase Reactions: Relevance of H Bond Interactions. Journal of Physical Chemistry A, 2010, 114, 7525-7536.	2.5	17
78	Can a Single Water Molecule Really Catalyze the Acetaldehyde + OH Reaction in Tropospheric Conditions?. Journal of Physical Chemistry Letters, 2010, 1, 3112-3115.	4.6	108
79	Computational and experimental study of the interactions between ionic liquids and volatile organic compounds. Physical Chemistry Chemical Physics, 2010, 12, 9830.	2.8	51
80	Substituent effects in the Baeyerâ€“Villiger reaction of acetophenones: a theoretical study. Journal of Physical Organic Chemistry, 2009, 22, 643-649.	1.9	23
81	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.	4.6	100
82	Quantum chemistry and TST study of the mechanisms and branching ratios for the reactions of OH with unsaturated aldehydes. Physical Chemistry Chemical Physics, 2009, 11, 7649.	2.8	88
83	OH Radical Gas Phase Reactions with Aliphatic Ethers: A Variational Transition State Theory Study. Journal of Physical Chemistry A, 2009, 113, 13913-13920.	2.5	103
84	The Baeyerâ€“Villiger reaction: solvent effects on reaction mechanisms. Organic and Biomolecular Chemistry, 2009, 7, 3682.	2.8	70
85	Quantum chemistry and TST study of the mechanism and kinetics of the butadiene and isoprene reactions with mercapto radicals. Chemical Physics, 2008, 344, 273-280.	1.9	12
86	Atmospheric Reactions of Oxygenated Volatile Organic Compounds+OH Radicals: Role of Hydrogen-Bonded Intermediates and Transition States. Advances in Quantum Chemistry, 2008, , 245-274.	0.8	16
87	Branching Ratios of Aliphatic Amines + OH Gas-Phase Reactions:â€‰ A Variational Transition-State Theory Study. Journal of Chemical Theory and Computation, 2008, 4, 322-327.	5.3	43
88	Theoretical Explanation of Nonexponential OH Decay in Reactions with Benzene and Toluene under Pseudo-First-Order Conditions. Journal of Physical Chemistry A, 2008, 112, 7608-7615.	2.5	57
89	Reinvestigating the Role of Multiple Hydrogen Transfers in Baeyerâ^•Villiger Reactions. Journal of Organic Chemistry, 2007, 72, 6580-6583.	3.2	28
90	The mechanism of the Baeyerâ€“Villiger rearrangement: quantum chemistry and TST study supported by experimental kinetic data. Organic and Biomolecular Chemistry, 2007, 5, 3682.	2.8	106

#	Article	IF	Citations
91	Non-alkane behavior of cyclopropane and its derivatives: characterization of unconventional hydrogen bond interactions. Theoretical Chemistry Accounts, 2007, 118, 597-606.	1.4	25
92	A New Specific Mechanism for the Acid Catalysis of the Addition Step in the Baeyerâ˜Villiger Rearrangement. Organic Letters, 2006, 8, 1763-1765.	4.6	92
93	Kinetics and mechanism of the Î²-alanine + OH gas phase reaction: A quantum mechanical approach. Physical Chemistry Chemical Physics, 2006, 8, 285-292.	2.8	15
94	Computational Quantum Chemistry: A Reliable Tool in the Understanding of Gas-Phase Reactions. Journal of Chemical Education, 2006, 83, 481.	2.3	8
95	Theoretical Determination of the Rate Constant for OH Hydrogen Abstraction from Toluene. Journal of Physical Chemistry A, 2006, 110, 10155-10162.	2.5	69
96	Isopropylcyclopropane + OH Gas Phase Reaction:â€‰ A Quantum Chemistry + CVT/SCT Approach. Journal of Physical Chemistry A, 2006, 110, 1917-1924.	2.5	17
97	A new approach to counterpoise correction to BSSE. Journal of Computational Chemistry, 2006, 27, 1203-1210.	3.3	105
98	Quantum chemical and conventional TST calculations of rate constants for the OH+alkane reaction. Chemical Physics, 2005, 310, 213-223.	1.9	31
99	Glycolaldehyde + OH Gas Phase Reaction:â€‰ A Quantum Chemistry + CVT/SCT Approach. Journal of Physical Chemistry A, 2005, 109, 169-180.	2.5	65
100	A Possible Mechanism for Furan Formation in the Tropospheric Oxidation of Dienes. Environmental Science & Technology, 2005, 39, 8797-8802.	10.0	22
101	Ab initio study of ÃŸ-alanine conformers in gas phase. Arkivoc, 2005, 2005, 7-18.	0.5	11
102	The Baeyer-Villiger reaction of 23-oxosapogenins. Arkivoc, 2005, 2005, 109-126.	0.5	24
103	Mechanism and Kinetics of the Reaction of OH Radicals with Glyoxal and Methylglyoxal: A Quantum Chemistry+CVT/SCT Approach. ChemPhysChem, 2004, 5, 1379-1388.	2.1	49
104	Quantum mechanical approach to isoleucine+OH gas phase reaction. Mechanism and kinetics. Computational and Theoretical Chemistry, 2004, 676, 97-103.	1.5	13
105	A theoretical investigation of the mechanism of the NO3 addition to alkenes. Computational and Theoretical Chemistry, 2004, 684, 51-59.	1.5	13
106	On the role of s-cis conformers in the reaction of dienes with OH radicals. Physical Chemistry Chemical Physics, 2004, 6, 2237-2244.	2.8	21
107	Structureâ˜Reactivity Relationship in Ketones + OH Reactions:Â A Quantum Mechanical and TST Approach. Journal of Physical Chemistry A, 2004, 108, 2740-2749.	2.5	52
108	Kinetics and mechanism of the gas-phase OH hydrogen abstraction reaction from methionine: A quantum mechanical approach. International Journal of Chemical Kinetics, 2003, 35, 212-221.	1.6	21

#	Article	IF	Citations
109	Rate coefficients and mechanism of the gas phase OH hydrogen abstraction reaction from serine: a quantum mechanical approach. Computational and Theoretical Chemistry, 2003, 629, 165-174.	1.5	20
110	Theoretical study of the initial reaction between OH and isoprene in tropospheric conditions. Physical Chemistry Chemical Physics, 2003, 5, 1392-1399.	2.8	51
111	Rate Coefficient and Mechanism of the Gas Phase OH Hydrogen Abstraction Reaction from Formic Acid:Â A Quantum Mechanical Approach. Journal of Physical Chemistry A, 2002, 106, 9520-9528.	2.5	71
112	Quantum Chemical and Conventional Transition-State Theory Calculations of Rate Constants for the NO3+ Alkane Reaction. Journal of Physical Chemistry A, 2002, 106, 4645-4650.	2.5	48
113	Gas phase reactions of C1â€“C4alcohols with the OH radical: A quantum mechanical approach. Physical Chemistry Chemical Physics, 2002, 4, 4648-4662.	2.8	108
114	Mechanism and rate coefficients of the gas phase OH hydrogen abstraction reaction from asparagine: a quantum mechanical approach. Computational and Theoretical Chemistry, 2002, 617, 77-86.	1.5	32
115	Rate Constant Dependence on the Size of Aldehydes in the NO3+ Aldehydes Reaction. An Explanation via Quantum Chemical Calculations and CTST. Journal of the American Chemical Society, 2001, 123, 8387-8395.	13.7	71
116	Evidence of A Possible Cycloaddition Channel in the Ethene + NO3 Reaction. Journal of Physical Chemistry A, 2001, 105, 9222-9230.	2.5	9
117	A Quantum Chemical and TST Study of the OH Hydrogen-Abstraction Reaction from Substituted Aldehydes:Â FCHO and ClCHO. Journal of Physical Chemistry A, 2001, 105, 9034-9039.	2.5	43
118	OH hydrogen abstraction reactions from alanine and glycine: A quantum mechanical approach. Journal of Computational Chemistry, 2001, 22, 1138-1153.	3.3	57
119	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.	13.7	244
120	A study of the nucleophilic attack of the beta-lactamic bond of antibiotics in water solution. Computational and Theoretical Chemistry, 2001, 539, 233-243.	1.5	5
121	Reaction mechanism of the acyl-enzyme formation in Î²-lactam hydrolysis by means of quantum chemical modeling. Computational and Theoretical Chemistry, 2000, 504, 13-28.	1.5	11
122	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.	13.7	218
123	Mechanism of the OH-propene-O2 reaction: Anabinitio study. International Journal of Chemical Kinetics, 1999, 31, 29-36.	1.6	49
124	Mechanism of the OHâ€“propeneâ€“O2 reaction: An ab initio study. , 1999, 31, 29.		1
125	Formation of 2-hexene by cationic dimerization of propene: an ab initio and density functional theory study. Theoretical Chemistry Accounts, 1997, 97, 277-282.	1.4	4
126	Model Calculations of Matrix Effects on the Conversion of Propene Radical Cations into Allyl Radicals in Halocarbon Matrices.. Acta Chemica Scandinavica, 1997, 51, 242-248.	0.7	0

#	Article	IF	Citations
127	Theoretical Model of Furan and 2-Furancarboxaldehyde. The Molecular Structure and Vibrational Spectra, Including Isotopic Effects. The Journal of Physical Chemistry, 1994, 98, 5607-5613.	2.9	20
128	Model Calculations of Base-Catalysed 1,3-Proton Transfer Reactions in Indene-like Systems.. Acta Chemica Scandinavica, 1994, 48, 423-427.	0.7	2
129	Theoretical investigation of the ethene-ethene radical cation addition reaction. The Journal of Physical Chemistry, 1993, 97, 12737-12741.	2.9	16
130	Theoretical study of reactions of the 1-butene radical cation in frozen halocarbon matrixes. The Journal of Physical Chemistry, 1993, 97, 12742-12744.	2.9	5
131	Theoretical approach to cationic polymerization of alkenylfurans. II. Ab initio and semiempirical study of relevant steps in the reaction mechanism. Journal of Polymer Science Part A, 1992, 30, 2497-2502.	2.3	0
132	Theoretical modelling of the electrophilic substitution mechanism in furan. Computational and Theoretical Chemistry, 1992, 253, 243-259.	1.5	6
133	On the correlation between ionization potentials and bond angles in heterocyclic compounds. Journal of Molecular Structure, 1991, 249, 305-312.	3.6	9
134	Theoretical model of the electrophilic substitution in pentagonal unsaturated heterocycles. Computational and Theoretical Chemistry, 1990, 209, 361-372.	1.5	6