Shinichi Yamabe

List of Publications by Year
in descending order

104 papers	1,697 citations	304602 22 h-index	360920 35 g-index
106 all docs	106 docs citations	106 times ranked	1994 citing authors

#	Article	IF	Citations
1	Reaction Paths of Ketoâ^'Enol Tautomerization of Î²-Diketones. Journal of Physical Chemistry A, 2004, 108, 2750-2757.	1.1	90
2	Theoretical Study of Hydrolysis and Condensation of Silicon Alkoxides. Journal of Physical Chemistry A, 1998, 102, 3991-3998.	1.1	85
3	A determination of the stabilities and structures of Fâ^'(C6H6) and Fâ^'(C6F6) clusters. Journal of Chemical Physics, 1987, 86, 4102-4105.	1.2	57
4	Reaction Paths of Tautomerization between Hydroxypyridines and Pyridones. Journal of Physical Chemistry A, 2005, 109, 1974-1980.	1.1	57
5	Molecular Interactions between Glycine and H2O Affording the Zwitterion. Journal of Physical Chemistry A, 2003, 107, 7915-7922.	1.1	53
6	Stability and structure of benzene dimer cation (C6H6)+2in the gas phase. Journal of Chemical Physics, 1991, 95, 8413-8418.	1.2	50
7	Is the Beckmann Rearrangement a Concerted or Stepwise Reaction? A Computational Study. Journal of Organic Chemistry, 2005, 70, 10638-10644.	1.7	47
8	A Theoretical Study of the Epoxidation of Olefins by Peracids. Journal of Organic Chemistry, 1996, 61, 616-620.	1.7	46
9	Characteristic Changes of Bond Energies for Gas-Phase Cluster Ions of Halide Ions with Methane and Chloromethanes. Journal of Physical Chemistry A, 2001, 105, 4887-4893.	1.1	41
10	The Role of Hydrogen Bonds in Baeyerâ^'Villiger Reactions. Journal of Organic Chemistry, 2007, 72, 3031-3041.	1.7	41
11	A Three-Center Orbital Interaction in the Dielsâ^'Alder Reactions Catalyzed by Lewis Acids. Journal of Organic Chemistry, 2000, 65, 1830-1841.	1.7	40
12	A mild and efficient Si (111) surface modification via hydrosilylation of activated alkynes. Journal of Materials Chemistry, 2005, 15, 4906.	6.7	40
13	A Mechanism of the Ion Separation of the NaCl Microcrystal via the Association of Water Clusters. Journal of Physical Chemistry B, 2000, 104, 10242-10252.	1.2	38
14	Reaction Paths of the Water-Assisted Neutral Hydrolysis of Ethyl Acetate. Journal of Physical Chemistry A, 2005, 109, 7216-7224.	1.1	36
15	Stability and structure of cluster ions: Halide ions with CO2. Journal of Chemical Physics, 1987, 87, 3647-3652.	1.2	35
16	Synthesis, Characterization, and DFT Investigation of IrIII Tolylterpyridine Complexes. European Journal of Inorganic Chemistry, 2007, 2007, 1911-1919.	1.0	35
17	A FMO-Controlled Reaction Path in the Benzilâ^'Benzilic Acid Rearrangement. Journal of Organic Chemistry, 2006, 71, 1777-1783.	1.7	30
18	Ab Initio Study of Proton Affinities of Three Crown Ethers. The Journal of Physical Chemistry, 1996, 100, 7367-7371.	2.9	29

#	Article	IF	Citations
19	MO Study of the photochemical behavior of the imine bond. International Journal of Quantum Chemistry, 1980, 18, 457-462.	1.0	23
20	How are nitrogen molecules bound to NO+2 and NO+?. Journal of Chemical Physics, 1989, 90, 3268-3273.	1.2	23
21	Reaction ofo-Benzyne with Tropothione Involving Biradical Processesâ€. Journal of Organic Chemistry, 2007, 72, 2832-2841.	1.7	23
22	A Theoretical Study of Curing Reactions of Maleimide Resins through Michael Additions of Amines. Journal of Organic Chemistry, 2000, 65, 1544-1548.	1.7	22
23	Three competitive transition states in the benzoin condensation compared to the clear rate-determining step in the Cannizzaro reaction. Organic and Biomolecular Chemistry, 2009, 7, 951.	1.5	22
24	Formation of the chelate bonds in the cluster Oâ˜'2(CO2)n, COâ˜'3(CO2)n, and NOâ˜'2(CO2)n. Journal of Chemical Physics, 1992, 97, 643-650.	1.2	21
25	[2 + 1] Cycloaddition Reactions of a 1-Seleno-2-silylethene to 2-Sulfonylacrylates:Â Stereoselective Synthesis of Sulfone-Substituted Cyclopropanes. Journal of Organic Chemistry, 1999, 64, 9521-9528.	1.7	21
26	A remarkable difference in the deprotonation steps of the Friedelâ€"Crafts acylation and alkylation reactions. Journal of Physical Organic Chemistry, 2009, 22, 1094-1103.	0.9	21
27	Ï€ Complexes in benzidine rearrangement. Organic and Biomolecular Chemistry, 2009, 7, 4631.	1.5	21
28	A computational study of base-catalyzed reactions between isocyanates and epoxides affording 2-oxazolidones and isocyanurates. Journal of Computational Chemistry, 2001, 22, 316-326.	1.5	20
29	Three Competitive Transition States at the Glycosidic Bond of Sucrose in Its Acid-Catalyzed Hydrolysis. Journal of Organic Chemistry, 2013, 78, 2527-2533.	1.7	20
30	Cluster ions: Gasâ€phase stabilities of NO+(O2)n and NO+(CO2)n with n=1â€"5. Journal of Chemical Physics, 1991, 95, 6800-6805.	1.2	19
31	Chiral Synthesis of Cyclopropanes. Stereoselective [2 + 1] Cycloaddition Reactions of 1-Seleno-2-silylethenes with Di-(â˜')-menthyl Ethene-1,1-dicarboxylates. Journal of Organic Chemistry, 1999, 64, 2367-2374.	1.7	19
32	Tropone Is a Mere Ketone for Cycloadditions to Ketenes. Helvetica Chimica Acta, 2005, 88, 1519-1539.	1.0	19
33	A metal free blue emission by the protonated 2,2â€²:6â€²,2â€³â€terpyridine hexafluorophosphate. Journal of Physical Organic Chemistry, 2009, 22, 410-417.	0.9	19
34	A Novel Strategy for Cyclobutane Formation. Fine Tuning of Cyclobutanation vs Cyclopropanation. Journal of Organic Chemistry, 1998, 63, 3371-3378.	1.7	18
35	A computational study of the role of hydrogen bonds in SN1 and E1 reactions. Journal of Computational Chemistry, 2004, 25, 598-608.	1.5	18
36	Gas-Phase Stability and Structure of the Cluster Ions CF3+(CO)n, CF3+(N2)n, CF3+(CF4)n, and CF4H+(CF4)n. The Journal of Physical Chemistry, 1996, 100, 5245-5251.	2.9	17

#	Article	IF	Citations
37	Anomalous Change of Bond Energies in the Cluster Ion N2H+(H2)n. Journal of Physical Chemistry A, 1998, 102, 1214-1218.	1.1	17
38	Frontier-orbital analyses of ketene [2+2] cycloadditions. Theoretical Chemistry Accounts, 1999, 102, 139-146.	0.5	17
39	Revisiting Hydrogen [1,5] Shifts in Cyclopentadiene and Cycloheptatriene as Bimolecular Reactions. Journal of Chemical Theory and Computation, 2005, 1, 944-952.	2.3	17
40	Dipping probe electrospray ionization/mass spectrometry for direct on-site and low-invasive food analysis. Food Chemistry, 2018, 260, 53-60.	4.2	16
41	Hydrogen bonds in gas-phase clusters between halide ions and olefins. Journal of the American Society for Mass Spectrometry, 2001, 12, 144-149.	1.2	15
42	Gas-phase ion/molecule reactions in octafluorocyclobutane. Journal of Chemical Physics, 2002, 116, 7574-7582.	1.2	15
43	A computational study of interactions between acetic acid and water molecules. Journal of Computational Chemistry, 2003, 24, 939-947.	1.5	15
44	On the formation of the isomeric cluster ions (CO)+n. Journal of Chemical Physics, 1991, 94, 2697-2703.	1.2	14
45	Remarkable emissions in diprotonated 2,2â€²:6â€²,2â€³â€terpyridine derivatives. Journal of Physical Organic Chemistry, 2010, 23, 431-439.	0.9	14
46	S_N1â€S_N2 and S_N2â€S_N3 mechanistic changes revealed by transition states of the hydrolyses of benzyl chlorides and benzenesulfonyl chlorides. Journal of Computational Chemistry, 2014, 35, 1140-1148.	1.5	14
47	Gas Phase Study of the Clustering Reactions of C2H5+,s-C3H7+, andt-C4H9+with CO2and N2O:Â Isomeric Structure of C2H5+, C2H5+(CO2)n, and C2H5+(N2O)n. Journal of Physical Chemistry A, 2003, 107, 775-781.	1.1	13
48	Frontier orbitals and transition states in the oxidation and degradation of<scp>l</scp>-ascorbic acid: a DFT study. Organic and Biomolecular Chemistry, 2015, 13, 4002-4015.	1.5	13
49	Gasâ€phase solvation of NO+, O+2, N2O+, N2OH+, and H3O+ with N2O. Journal of Chemical Physics, 1994, 101, 4073-4082.	1.2	12
50	Role of hydrogen bonds in acid-catalyzed hydrolyses of esters. Theoretical Chemistry Accounts, 2011, 130, 429-438.	0.5	12
51	Active Role of Hydrogen Bonds in Rupe and Meyerâˆ'Schuster Rearrangements. Journal of Chemical Theory and Computation, 2006, 2, 1379-1387.	2.3	11
52	Reaction Paths of the Water-Assisted Solvolysis of N,N-Dimethylformamide. Journal of Physical Chemistry A, 2007, 111, 6296-6303.	1.1	11
53	Proton Transfers along Hydrogen Bonds in the Tautomerization of Purine. Journal of Physical Chemistry A, 2012, 116, 1289-1297.	1.1	11
54	An aniline dication-like transition state in the Bamberger rearrangement. Beilstein Journal of Organic Chemistry, 2013, 9, 1073-1082.	1.3	11

#	Article	IF	Citations
55	Substrate dependent reaction channels of the Wolffâ€“Kishner reduction reaction: A theoretical study. Beilstein Journal of Organic Chemistry, 2014, 10, 259-270.	1.3	11
56	A DFT study of hydride transfers to the carbonyl oxygen of DDQ. International Journal of Quantum Chemistry, 2015, 115, 1533-1542.	1.0	11
57	Experimental and Theoretical Studies of Gas-Phase Ion/Molecule Reactions in SiF4Forming SiFm+(SiF4)nClusters (m= 0â˘3 andn= 0â˘2). Journal of Physical Chemistry A, 1999, 103, 568-572.	1.1	10
58	A computational study on the relationship between formation and electrolytic dissociation of carbonic acid. Theoretical Chemistry Accounts, 2011, 130, 909-918.	0.5	10
59	Biradical processes in reactions between benzyne and tropone. Theoretical Chemistry Accounts, 2011, 130, 981-990.	0.5	10
60	Gas-Phase Ionâ˘Molecule Reactions in C3F6. Journal of Physical Chemistry A, 2002, 106, 603-611.	1.1	9
61	A new intermediate in the Prins reaction. Beilstein Journal of Organic Chemistry, 2013, 9, 476-485.	1.3	9
62	Syntheses, X-ray crystal structures, and emission properties of diprotonated tetrapyridylpyrazine and triprotonated terpyridine. Journal of Physical Organic Chemistry, 2016, 29, 269-275.	0.9	9
63	A theoretical study on the photodissociation of C3O2. Theoretica Chimica Acta, 1979, 52, 257-265.	0.9	8
64	How is the Fluoride Ion Bound to O2, N2, and CO Molecules?. Journal of Physical Chemistry A, 1998, 102, 6916-6920.	1.1	8
65	Theoretical study of the role of solvent H2O in neopentyl and pinacol rearrangements. Journal of Computational Chemistry, 2007, 28, 1561-1571.	1.5	8
66	A significant role of alkaline cations on the Reimerâ€“Tiemann reaction. Organic and Biomolecular Chemistry, 2011, 9, 5109.	1.5	8
67	Theoretical study of photochemical reactions: Electron assignment and the state correlation diagram. International Journal of Quantum Chemistry, 1980, 18, 243-250.	1.0	7
68	Gas-phase stability of cluster ions SF m + (SF6) n with m = 0â€“5 and n = 1â€“3. Journal of the American Society for Mass Spectrometry, 1995, 6, 1137-1142.	1.2	7
69	A DFT study of proton transfers for the reaction of phenol and hydroxyl radical leading to dihydroxybenzene and H₂O in the water cluster. International Journal of Quantum Chemistry, 2018, 118, e25510.	1.0	7
70	Comparative study of the gas-phase bond strengths of CO2 and N2O with the halide ions. Journal of the American Society for Mass Spectrometry, 1993, 4, 58-64.	1.2	6
71	On the Structure and Stability of Gas-Phase Cluster Ions SiF3+(CO)n, SiF3OH2+(SiF4)n, SiF4H+(SiF4)n, and F-(SiF4)n. Journal of Physical Chemistry A, 2000, 104, 8353-8359.	1.1	6
72	Is the neutral Knoevenagel reaction initiated by the carbanion formation?. Journal of Physical Organic Chemistry, 2011, 24, 663-671.	0.9	6

#	Article	IF	Citations
73	Steric effects upon transition states of radical addition polymerizations. Journal of Polymer Science Part A, 1996, 34, 1407-1414.	2.5	5
74	Formation of the trimer ion core in the heterogeneous rare gas cluster ions. Journal of Chemical Physics, 1998, 108, 6689-6697.	1.2	5
75	Detailed Description of the Metal-to-Ligand Charge-Transfer State in Monoterpyridine IrIII Complexes. European Journal of Inorganic Chemistry, 2009, 2009, 2067-2073.	1.0	5
76	Presence or absence of a novel charge-transfer complex in the base-catalyzed hydrolysis of <i>N</i>-ethylbenzamide or ethyl benzoate. Beilstein Journal of Organic Chemistry, 2013, 9, 185-196.	1.3	5
77	Proton transfers in the Strecker reaction revealed by DFT calculations. Beilstein Journal of Organic Chemistry, 2014, 10, 1765-1774.	1.3	5
78	A DFT study on proton transfers in hydrolysis reactions of phosphate dianion and sulfate monoanion. Journal of Computational Chemistry, 2014, 35, 2195-2204.	1.5	5
79	A novel contrast of the reactions of 2,4,6-trinitrotoluene (TNT) in atmospheric-pressure O2 and N2 plasma: Experimental and theoretical study. International Journal of Mass Spectrometry, 2020, 450, 116308.	0.7	5
80	Olefinâ€“olefin reactions mediated by Lewis acids may afford cyclopropanes rather than cyclobutanes: a mechanistic study of cyclopropane formation using a 1-seleno-2-silyletheneâ€Šâ€. Perkin Transactions II RSC, 2001, , 164-173.	1.1	4
81	Norcaradiene intermediates in mass spectral fragmentations of tropone and tropothioneElectronic supplementary information (ESI) available: reaction paths supporting Figs. 3Ã¢â,¬â€œ6. See http://www.rsc.org/suppdata/p2/b1/b102127n/. Perkin Transactions II RSC, 2001, , 2202-2210.	1.1	4
82	Gas-Phase Solvation of O2+, O2-, O4-, O3-, and CO3-with CO. Journal of Physical Chemistry A, 2003, 107, 4817-4825.	1.1	4
83	How Many Elementary Processes Are Involved in Base- and Acid-Promoted Aldol Condensations?. European Journal of Organic Chemistry, 2007, 2007, 6070-6077.	1.2	3
84	DFT Study of the Hydroxyl Radical Addition to 2â€²-Deoxyguanosine and the Guanine Base in Four Double-Stranded B-Form Dimers. Journal of Physical Chemistry B, 2020, 124, 1374-1382.	1.2	3
85	How is vitamin B1 oxidized to thiochrome? Elementary processes revealed by a DFT study. Organic and Biomolecular Chemistry, 2021, 19, 4529-4536.	1.5	3
86	An unsymmetrical behavior of reactant units in the Kolbeâ€“Schmitt reaction. Theoretical Chemistry Accounts, 2011, 130, 891-900.	0.5	2
87	Oneâ€Step Paths of the Alkene Hydration Revealed by a DFT Study. ChemistrySelect, 2017, 2, 6857-6864.	0.7	2
88	The tautomerization and ring closure in the Claisen rearrangement: A DFT study. International Journal of Quantum Chemistry, 2018, 118, e25677.	1.0	2
89	The Problem of Non-Recognition for Dienes in Ketene Reactions. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 1997, 55, 56-64.	0.0	2
90	Corona Discharge and Field Electron Emission in Ambient Air Using a Sharp Metal Needle: Formation and Reactivity of CO₃^{âˆ’â€¢} and O₂^{âˆ’â€¢}. Mass Spectrometry, 2021, 10, A0100-A0100.	0.2	2

#	Article	IF	Citations
91	Symmetry or asymmetry in cheletropic additions forming cyclopropanes. Theoretical Chemistry Accounts, 2005, 113, 95-106.	0.5	1
92	Correlation between the Rate Order and the Number of Molecules in the Reaction of Trimethyl Phosphite with Water in Acetonitrile Solvent. Journal of Physical Chemistry A, 2010, 114, 11699-11707.	1.1	1
93	How is the anionic tetrahedral intermediate involved in the isomerization of aspartyl peptides to iso-aspartyl ones? A DFT study on the tetra-peptide. Organic and Biomolecular Chemistry, 2012, 10, 8007.	1.5	1
94	Ketoâ€Enol Tautomerization Controls the Acidâ€Catalyzed Robinson Annulation â€•A DFT Study. ChemistrySelect, 2019, 4, 4962-4966.	0.7	1
95	A density functional theory study of the reaction mechanism of formation of phenolphthalein and fluorescein. Journal of Physical Organic Chemistry, 2021, 34, e4136.	0.9	1
96	How Is the Oxidation Related to the Tautomerization in Vitamin B9?. Journal of Physical Chemistry A, 2021, 125, 9346-9354.	1.1	1
97	A DFT study on the degradation mechanism of vitamin B2. Food Chemistry Molecular Sciences, 2022, 4, 100080.	0.9	1
98	A Molecular Orbital Calculation of Chemically Interacting Systems.: Interaction between Two Radicals. World Scientific Series in 20th Century Chemistry, 1997, , 341-350.	0.0	0
99	A DFT study of the hydrolysis of hydantoin. International Journal of Chemical Kinetics, 2019, 51, 831-839.	1.0	0
100	The adenine ring influences the adenosine 5â€²â€triphosphate hydrolysis. International Journal of Quantum Chemistry, 2019, 119, e25816.	1.0	0
101	A DFT Study on Transition States of Inhibition of Oxidation by Î±â€Tocopherol. ChemistrySelect, 2020, 5, 9184-9194.	0.7	0
102	A density functional theory study of the hydride shift in the Eschweilerâ€"Clarke reaction. Journal of Physical Organic Chemistry, 2021, 34, e4253.	0.9	0
103	Gas-Phase Ion-Molecule Reactions in Tetrahydrothiophene.. Journal of the Mass Spectrometry Society of Japan, 1998, 46, 442-447.	0.0	0
104	A DFT study of the active role of the phosphate group of an internal aldimine in a transamination reaction. Organic and Biomolecular Chemistry, 0, , .	1.5	0