

Albert SolÃ©

List of Publications by Year in descending order

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60
papers

1,500
citations

304368

22
h-index

344852

36
g-index

62
all docs

62
docs citations

62
times ranked

1251
citing authors

#	ARTICLE	IF	CITATIONS
1	Unimolecular Isomerizations and Oxygen Atom Loss in Formaldehyde and Acetaldehyde Carbonyl Oxides. A Theoretical Investigation. <i>Journal of the American Chemical Society</i> , 1996, 118, 4636-4647.	6.6	137
2	Impact of the water dimer on the atmospheric reactivity of carbonyl oxides. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17698-17712.	1.3	78
3	The Mechanism of Methoxy Radical Oxidation by O ₂ in the Gas Phase. Computational Evidence for Direct H Atom Transfer Assisted by an Intermolecular Noncovalent O...O Bonding Interaction. <i>Journal of the American Chemical Society</i> , 1999, 121, 1337-1347.	6.6	77
4	Ab Initio Calculations of the Potential Surface for the Thermal Decomposition of the Phenoxy Radical. <i>The Journal of Physical Chemistry</i> , 1995, 99, 10549-10556.	2.9	67
5	Mechanism of the Hydrogen Transfer from the OH Group to Oxygen-Centered Radicals: Proton-Coupled Electron-Transfer versus Radical Hydrogen Abstraction. <i>Chemistry - A European Journal</i> , 2004, 10, 3404-3410.	1.7	63
6	A theoretical investigation of the thermal ring opening of cyclopropyl radical into allyl radical. Evidence for a highly nonsymmetric transition state. <i>Journal of the American Chemical Society</i> , 1990, 112, 2160-2167.	6.6	61
7	Mechanistic Study of the CH ₃ O ₂ + HO ₂ → CH ₃ O ₂ H + O ₂ Reaction in the Gas Phase. Computational Evidence for the Formation of a Hydrogen-Bonded Diradical Complex. <i>Journal of Physical Chemistry A</i> , 2006, 110, 6073-6082.	1.1	58
8	New Insight into the Gas-Phase Bimolecular Self-Reaction of the HOO Radical. <i>Journal of Physical Chemistry A</i> , 2007, 111, 1695-1704.	1.1	46
9	On the Dissociation of Ground State trans-HOOO Radical: A Theoretical Study. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2743-2750.	2.3	42
10	Theoretical Mechanistic Study of the Oxidative Degradation of Benzene in the Troposphere: Reaction of Benzene + HO Radical Adduct with O ₂ . <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1607-1623.	2.3	41
11	Ab-initio mechanistic studies of radical reactions. Directive effects in the addition of methyl radical to unsymmetrical fluoroethenes. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1986, , 1517-1524.	0.9	39
12	The reaction between HO and (H ₂ O) _n (n = 1, 3) clusters: reaction mechanisms and tunneling effects. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 579-592.	0.5	37
13	Theoretical Investigation of the Low-Lying Electronic States of Dioxirane: Ring Opening to Dioxymethane and Dissociation into CO ₂ and H ₂ . <i>Journal of Physical Chemistry A</i> , 1998, 102, 3398-3406.	1.1	36
14	Unimolecular Reactions of Ionized Alkanes: Theoretical Study of the Potential Energy Surface for CH ₃ · and CH ₄ Losses from Ionized Butane and Isobutane. <i>Journal of the American Chemical Society</i> , 1994, 116, 11078-11088.	6.6	35
15	Ab Initio Calculations on the Mechanism of the Oxidation of the Hydroxymethyl Radical by Molecular Oxygen in the Gas Phase: A Significant Reaction for Environmental Science. <i>Chemistry - A European Journal</i> , 2001, 7, 3377-3386.	1.7	35
16	Hydrogen Transfer between Sulfuric Acid and Hydroxyl Radical in the Gas Phase: Competition among Hydrogen Atom Transfer, Proton-Coupled Electron-Transfer, and Double Proton Transfer. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1982-1990.	1.1	33
17	Molecular and electronic structure of the low-lying electronic states of cycloalkenylidenes: cyclopropenylidene. <i>Journal of the American Chemical Society</i> , 1988, 110, 1694-1700.	6.6	26
18	The reaction of formaldehyde carbonyl oxide with the methyl peroxy radical and its relevance in the chemistry of the atmosphere. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 18921.	1.3	26

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19	4-31G ab initio and MNDO semi-empirical calculations on bicyclic CN ₇ and N ₈ species, and n.m.r. and i.r. studies on ¹⁵ N-labelled CN ₇ . Journal of the Chemical Society Chemical Communications, 1986, , 959-961.	2.0	25
20	Potential energy curves for the HeAr ⁺ and NeAr ⁺ ions. Chemical Physics Letters, 1986, 126, 245-250.	1.2	25
21	Small-ring cyclic alkynes: ab initio molecular orbital study of cyclohexyne. Journal of Organic Chemistry, 1987, 52, 4160-4163.	1.7	23
22	Unimolecular Decomposition of β -Hydroxyethylperoxy Radicals in the HO ₂ -Initiated Oxidation of Ethene: A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 11651-11663.	1.1	23
23	Molecular and electronic structure of the low-lying electronic states of cycloalkenylidenes. Cyclopentadienylidene. Journal of the American Chemical Society, 1988, 110, 3740-3746.	6.6	22
24	Unimolecular Decompositions of Ionized Isopropyl Methyl Ether: An ab Initio and RRKM Study. Journal of the American Chemical Society, 1995, 117, 2557-2564.	6.6	21
25	Theoretical Analysis of the Unimolecular Gas-Phase Decompositions of the Propane Molecular Ion. Journal of Physical Chemistry A, 1998, 102, 10798-10804.	1.1	21
26	Ab Initio Calculations on the 5-exo versus 6-endo Cyclization of 1,3-Hexadiene-5-yn-1-yl Radical: Formation of the First Aromatic Ring in Hydrocarbon Combustion. Journal of the American Chemical Society, 2000, 122, 11416-11422.	6.6	20
27	The 1,2,4-Triazolyl Cation: Thermolytic and Photolytic Studies. Journal of Organic Chemistry, 2001, 66, 1242-1251.	1.7	20
28	Mechanism of 1,3-Migration in Allylperoxy Radicals: Computational Evidence for the Formation of a Loosely Bound Radical-Dioxygen Complex. Journal of the American Chemical Society, 2003, 125, 10641-10650.	6.6	20
29	Theoretical Study of the Low-Lying Electronic States of 4-Oxo-2,5-cyclohexadienylidene and Their Formation from 1H-Bicyclo[3.1.0]hexa-3,5-dien-2-one. The Journal of Physical Chemistry, 1995, 99, 5934-5944.	2.9	19
30	Mechanisms for the Reactions of Hydroxyl Radicals with Acrolein: A Theoretical Study. Journal of Chemical Theory and Computation, 2008, 4, 941-950.	2.3	19
31	Ab initio mechanistic studies of radical reactions. Addition of methyl radical to acetylene and ethylene. Chemical Physics Letters, 1985, 118, 573-579.	1.2	18
32	Kinetic interpretation of aromaticity: a theoretical study. Journal of Organic Chemistry, 1988, 53, 5148-5149.	1.7	18
33	Methane Elimination from Ionized Propane through an Ion-Neutral Complex: An ab Initio Study. Journal of the American Chemical Society, 1996, 118, 9368-9376.	6.6	18
34	Thermal and Photochemical Rearrangement of Bicyclo[3.1.0]hex-3-en-2-one to the Ketonic Tautomer of Phenol. Computational Evidence for the Formation of a Diradical Rather than a Zwitterionic Intermediate. Journal of the American Chemical Society, 2002, 124, 15375-15384.	6.6	18
35	Atmospheric formation of the NO ₃ radical from gas-phase reaction of HNO ₃ acid with the NH ₂ radical: proton-coupled electron-transfer versus hydrogen atom transfer mechanisms. Physical Chemistry Chemical Physics, 2014, 16, 19437-19445.	1.3	17
36	Substituent Effects on the Low-Lying Singlet and Triplet States of Methylene. Journal of Computational Chemistry, 1986, 7, 428-442.	1.5	15

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37	B(2P)+ H ₂ O (X1A1): a quasi-classical 3D trajectory calculation. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1057-1068.	1.7	15
38	Unexpected Reactivity of Amidogen Radical in the Gas Phase Degradation of Nitric Acid. Journal of the American Chemical Society, 2014, 136, 6834-6837.	6.6	15
39	The Atmospheric Oxidation of HONO by OH, Cl, and ClO Radicals. Journal of Physical Chemistry A, 2017, 121, 9698-9707.	1.1	15
40	Small-ring cyclic alkynes: ab initio molecular orbital study of cyclopentyne. Journal of the American Chemical Society, 1986, 108, 6884-6888.	6.6	14
41	Molecular and electronic structure of the low-lying electronic states of the 1-pyrazolyl and 1-imidazolyl radicals. Journal of the American Chemical Society, 1989, 111, 7740-7746.	6.6	14
42	HBO osculating complex in the B(2P)+ OH(2̂) reaction. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 37-44.	1.7	12
43	Crossed molecular beams study of the M+(1S)+Na(3 2S)â†'M+(1S)+Na(3 2P) collision systems (M+=Li+, Na+), Tj ETQq1 1 0.784314 12	1.2	12
44	New Selective Haloform-type Reaction Yielding 3-Hydroxy-2,2-difluoroacids:Â Theoretical Study of the Mechanism. Journal of the American Chemical Society, 2005, 127, 2620-2627.	6.6	12
45	Photochemical Rearrangements of Norbornadiene Pausonâ€™Khand Cycloadducts. Angewandte Chemie - International Edition, 2007, 46, 5943-5946.	7.2	12
46	Theoretical studies on the ring-opening reactions of bicycloalkyl radicals: homolytic .beta.-scission in bicyclo[1.1.0]but-2-yl radical. Journal of the American Chemical Society, 1991, 113, 87-94.	6.6	10
47	MNDO-CI theoretical study of [2 + 2] cycloaddition of cyclopentyne with ethylene. Journal of the Chemical Society Perkin Transactions II, 1986, , 613-617.	0.9	9
48	Theoretical studies of the ring-opening reactions of bicycloalkyl radicals: electrocyclic and degenerate rearrangements in the bicyclo[3.1.0]hex-3-en-2-yl radical. Journal of the American Chemical Society, 1991, 113, 8628-8633.	6.6	9
49	Theoretical study of the reaction H + ClCH ₃ â†' HCl + CH ₃ . Chemical Physics, 1985, 93, 265-275.	0.9	7
50	Tropospheric oxidation of methyl hydrotrioxide (CH ₃ OOOH) by hydroxyl radical. Physical Chemistry Chemical Physics, 2018, 20, 27406-27417.	1.3	7
51	Unimolecular reactions of the enolic tautomer of ionized acetic acid in the gas phase: an ab initio and RRKM study. The Journal of Physical Chemistry, 1988, 92, 3336-3341.	2.9	6
52	Attempted generation and structure of the 4-(1,2,4-triazoyl) cation. Tetrahedron Letters, 1994, 35, 2321-2324.	0.7	6
53	The gas phase oxidation of HCOOH by Cl and NH ₂ radicals. Proton coupled electron transfer versus hydrogen atom transfer. Molecular Physics, 2019, 117, 1430-1441.	0.8	6
54	Theoretical and Experimental Studies on the Mechanism of Norbornadiene Pausonâ€™Khand Cycloadducts Photorearrangement. Is There a Pathway on the Excited Singlet Potential Energy Surface?. Journal of the American Chemical Society, 2008, 130, 16898-16907.	6.6	5

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55	Theoretical investigation of the energy, structure, vibrational frequencies, and infrared intensities of low-lying electronic states of the symmetric azacyclopentadienylidenes. <i>The Journal of Physical Chemistry</i> , 1991, 95, 10623-10630.	2.9	4
56	Small-ring cyclic alkynes: ab initio molecular orbital study of 1,4-dioxacyclohexyne (p-dioxyne). <i>Journal of the American Chemical Society</i> , 1987, 109, 5600-5605.	6.6	3
57	Quantum Chemistry Laboratory at Home. <i>Journal of Chemical Education</i> , 2008, 85, 1288.	1.1	3
58	Dynamical study of the collinear C(3P) + HF(1 $\hat{\Sigma}$ +) $\hat{\rightarrow}$ CF(2 $\hat{\Sigma}$) + H(2S) reaction. <i>Chemical Physics</i> , 1988, 123, 277-293.	0.9	2
59	Theoretical study of regioselectivity in methyl radical additions to fluoroethenes. <i>Journal of the Chemical Society Chemical Communications</i> , 1985, , 1331-1332.	2.0	1
60	Theoretical Characterization of Transition State Dynamical Resonances in Heavy $\hat{\leftrightarrow}$ Light $\hat{\leftrightarrow}$ Heavy Reactions. <i>Laser Chemistry</i> , 1991, 11, 291-302.	0.5	0