# Albert SolÃ©

List of Publications by Year
in descending order

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| 60 | 1,500 | 304368 | 344852 |
|---|---|---|---|
| papers | citations | 22 h-index | 36 g-index |

| 62 | 62 | 62 | 1251 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | The gas phase oxidation of HCOOH by Cl and NH2 radicals. Proton coupled electron transfer versus hydrogen atom transfer. Molecular Physics, 2019, 117, 1430-1441. | 0.8 | 6 |
| 2 | Tropospheric oxidation of methyl hydrotrioxide (CH<sub>3</sub>OOOH) by hydroxyl radical. Physical Chemistry Chemical Physics, 2018, 20, 27406-27417. | 1.3 | 7 |
| 3 | The Atmospheric Oxidation of HONO by OH, Cl, and ClO Radicals. Journal of Physical Chemistry A, 2017, 121, 9698-9707. | 1.1 | 15 |
| 4 | Impact of the water dimer on the atmospheric reactivity of carbonyl oxides. Physical Chemistry Chemical Physics, 2016, 18, 17698-17712. | 1.3 | 78 |
| 5 | 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 |
| 6 | Atmospheric formation of the NO<sub>3</sub> radical from gas-phase reaction of HNO<sub>3</sub> acid with the NH<sub>2</sub> radical: proton-coupled electron-transfer versus hydrogen atom transfer mechanisms. Physical Chemistry Chemical Physics, 2014, 16, 19437-19445. | 1.3 | 17 |
| 7 | The reaction of formaldehyde carbonyl oxide with the methyl peroxy radical and its relevance in the chemistry of the atmosphere. Physical Chemistry Chemical Physics, 2013, 15, 18921. | 1.3 | 26 |
| 8 | The reaction between HO and (H2O) n (nÂ=Â1, 3) clusters: reaction mechanisms and tunneling effects. Theoretical Chemistry Accounts, 2011, 128, 579-592. | 0.5 | 37 |
| 9 | On the Dissociation of Ground State trans-HOOO Radical: A Theoretical Study. Journal of Chemical Theory and Computation, 2010, 6, 2743-2750. | 2.3 | 42 |
| 10 | Theoretical Mechanistic Study of the Oxidative Degradation of Benzene in the Troposphere: Reaction of Benzeneâˆ'HO Radical Adduct with O<sub>2</sub>. Journal of Chemical Theory and Computation, 2009, 5, 1607-1623. | 2.3 | 41 |
| 11 | Quantum Chemistry Laboratory at Home. Journal of Chemical Education, 2008, 85, 1288. | 1.1 | 3 |
| 12 | Theoretical and Experimental Studies on the Mechanism of Norbornadiene Pausonâˆ'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 |
| 13 | 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 |
| 14 | New Insight into the Gas-Phase Bimolecular Self-Reaction of the HOO Radical. Journal of Physical Chemistry A, 2007, 111, 1695-1704. | 1.1 | 46 |
| 15 | Photochemical Rearrangements of Norbornadiene Pausonâ€"Khand Cycloadducts. Angewandte Chemie - International Edition, 2007, 46, 5943-5946. | 7.2 | 12 |
| 16 | Hydrogen Transfer between Sulfuric Acid and Hydroxyl Radical in the Gas Phase:â€‰ Competition among Hydrogen Atom Transfer, Proton-Coupled Electron-Transfer, and Double Proton Transfer. Journal of Physical Chemistry A, 2006, 110, 1982-1990. | 1.1 | 33 |
| 17 | Mechanistic Study of the CH3O2â€¢+ HO2â€¢â†' CH3O2H + O2Reaction in the Gas Phase. Computational Evidence for the Formation of a Hydrogen-Bonded Diradical Complex. Journal of Physical Chemistry A, 2006, 110, 6073-6082. | 1.1 | 58 |
| 18 | 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 |

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|---|---|---|---|
| 19 | Mechanism of the Hydrogen Transfer from the OH Group to Oxygen-Centered Radicals: Proton-Coupled Electron-Transfer versus Radical Hydrogen Abstraction. Chemistry - A European Journal, 2004, 10, 3404-3410. | 1.7 | 63 |
| 20 | Unimolecular Decomposition of Î²-Hydroxyethylperoxy Radicals in the HOâ€¢-Initiated Oxidation of Ethene:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 11651-11663. | 1.1 | 23 |
| 21 | Mechanism of 1,3-Migration in Allylperoxyl Radicals:â€‰ Computational Evidence for the Formation of a Loosely Bound Radicalâ€¦Dioxygen Complex. Journal of the American Chemical Society, 2003, 125, 10641-10650. | 6.6 | 20 |
| 22 | 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 |
| 23 | The 1,2,4-Triazolyl Cation:Â Thermolytic and Photolytic Studies. Journal of Organic Chemistry, 2001, 66, 1242-1251. | 1.7 | 20 |
| 24 | 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. Chemistry - A European Journal, 2001, 7, 3377-3386. | 1.7 | 35 |
| 25 | Ab InitioCalculations on the 5-exoversus 6-endoCyclization of 1,3-Hexadiene-5-yn-1-yl Radical:Â Formation of the First Aromatic Ring in Hydrocarbon Combustion. Journal of the American Chemical Society, 2000, 122, 11416-11422. | 6.6 | 20 |
| 26 | The Mechanism of Methoxy Radical Oxidation by O2in the Gas Phase. Computational Evidence for Direct H Atom Transfer Assisted by an Intermolecular Noncovalent OÂ·Â·Â·O Bonding Interaction. Journal of the American Chemical Society, 1999, 121, 1337-1347. | 6.6 | 77 |
| 27 | Theoretical Investigation of the Low-Lying Electronic States of Dioxirane:â€‰ Ring Opening to Dioxymethane and Dissociation into CO2 and H2. Journal of Physical Chemistry A, 1998, 102, 3398-3406. | 1.1 | 36 |
| 28 | 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 |
| 29 | Unimolecular Isomerizations and Oxygen Atom Loss in Formaldehyde and Acetaldehyde Carbonyl Oxides. A Theoretical Investigation. Journal of the American Chemical Society, 1996, 118, 4636-4647. | 6.6 | 137 |
| 30 | Methane Elimination from Ionized Propane through an Ionâ€¦Neutral Complex:Â An ab Initio Study. Journal of the American Chemical Society, 1996, 118, 9368-9376. | 6.6 | 18 |
| 31 | Ab Initio Calculations of the Potential Surface for the Thermal Decomposition of the Phenoxyl Radical. The Journal of Physical Chemistry, 1995, 99, 10549-10556. | 2.9 | 67 |
| 32 | 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 |
| 33 | 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 |
| 34 | Crossed molecular beams study of the M+(1S)+Na(3 2S)â†'M+(1S)+Na(3 2P) collision systems (M+=Li+, Na+,) Tj ETQq0 0 0 rgBT /Overl | 1.2 | 12 |
| 35 | Attempted generation and structure of the 4-(1,2,4-triazoyl) cation. Tetrahedron Letters, 1994, 35, 2321-2324. | 0.7 | 6 |
| 36 | Unimolecular Reactions of Ionized Alkanes: Theoretical Study of the Potential Energy Surface for CH3.bul. and CH4 Losses from Ionized Butane and Isobutane. Journal of the American Chemical Society, 1994, 116, 11078-11088. | 6.6 | 35 |

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| 37 | HBO osculating complex in the B(2P)+ OH(2Î) reaction. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 37-44. | 1.7 | 12 |
| 38 | B(2P)+ H2O (X1A1): a quasi-classical 3D trajectory calculation. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1057-1068. | 1.7 | 15 |
| 39 | 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 |
| 40 | 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 |
| 41 | Theoretical Characterization of Transition State Dynamical Resonances in Heavyâ€“Lightâ€“Heavy Reactions. Laser Chemistry, 1991, 11, 291-302. | 0.5 | 0 |
| 42 | Theoretical investigation of the energy, structure, vibrational frequencies, and infrared intensities of low-lying electronic states of the symmetric azacyclopentadienylidenes. The Journal of Physical Chemistry, 1991, 95, 10623-10630. | 2.9 | 4 |
| 43 | A theoretical investigation of the thermal ring opening of cyclopropyl radical into allyl radical. Evidence for a highly nonsymmetric transition state. Journal of the American Chemical Society, 1990, 112, 2160-2167. | 6.6 | 61 |
| 44 | 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 |
| 45 | Dynamical study of the collinear C(3P) + HF(1Î£+)â†'CF(2Î) + H(2S) reaction. Chemical Physics, 1988, 123, 277-293. | 0.9 | 2 |
| 46 | 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 |
| 47 | Kinetic interpretation of aromaticity: a theoretical study. Journal of Organic Chemistry, 1988, 53, 5148-5149. | 1.7 | 18 |
| 48 | 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 |
| 49 | Molecular and electronic structure of the low-lying electronic states of cycloalkenylidenes: cyclopropenylidene. Journal of the American Chemical Society, 1988, 110, 1694-1700. | 6.6 | 26 |
| 50 | Small-ring cyclic alkynes: ab initio molecular orbital study of cyclohexyne. Journal of Organic Chemistry, 1987, 52, 4160-4163. | 1.7 | 23 |
| 51 | Small-ring cyclic alkynes: ab initio molecular orbital study of 1,4-dioxacyclohexyne (p-dioxyne). Journal of the American Chemical Society, 1987, 109, 5600-5605. | 6.6 | 3 |
| 52 | 4-31G ab initio and MNDO semi-empirical calculations on bicyclic CN7â€“and N8species, and n.m.r. and i.r. studies on15N-labelled CN7â€“. Journal of the Chemical Society Chemical Communications, 1986, , 959-961. | 2.0 | 25 |
| 53 | Ab-initio mechanistic studies of radical reactions. Directive effects in the addition of methyl radical to unsymmetrical fluoroethenes. Journal of the Chemical Society Perkin Transactions II, 1986, , 1517-1524. | 0.9 | 39 |
| 54 | MNDO-Cl theoretical study of [2 + 2] cycloaddition of cyclopentyne with ethylene. Journal of the Chemical Society Perkin Transactions II, 1986, , 613-617. | 0.9 | 9 |

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| 55 | Small-ring cyclic alkynes: ab initio molecular orbital study of cyclopentyne. Journal of the American Chemical Society, 1986, 108, 6884-6888. | 6.6 | 14 |
| 56 | Substituent Effects on the Low-Lying Singlet and Triplet States of Methylene. Journal of Computational Chemistry, 1986, 7, 428-442. | 1.5 | 15 |
| 57 | Potential energy curves for the HeAr+ and NeAr+ ions. Chemical Physics Letters, 1986, 126, 245-250. | 1.2 | 25 |
| 58 | Theoretical study of the reaction H + ClCH3 â† HCl + CH3. Chemical Physics, 1985, 93, 265-275. | 0.9 | 7 |
| 59 | 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 |
| 60 | Theoretical study of regioselectivity in methyl radical additions to fluoroethenes. Journal of the Chemical Society Chemical Communications, 1985, , 1331-1332. | 2.0 | 1 |