Alexander M Mebel

List of Publications by Year
in descending order

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473 papers	13,656 citations	26630 56 h-index	54911 84 g-index
479 all docs	479 docs citations	479 times ranked	6859 citing authors

#	Article	IF	Citations
1	Modification of the gaussianâ”2 theoretical model: The use of coupledâ€cluster energies, densityâ€functional geometries, and frequencies. Journal of Chemical Physics, 1995, 103, 7414-7421.	3.0	468
2	Low temperature formation of naphthalene and its role in the synthesis of PAHs (Polycyclic Aromatic) Tj ETQq0 0 0 rgBT /Overlock 10 Tf United States of America, 2012, 109, 53-58.	7.1	192
3	Ab Initio and RRKM Calculations for Multichannel Rate Constants of the C2H3+ O2Reaction. Journal of the American Chemical Society, 1996, 118, 9759-9771.	13.7	161
4	The Largecloso-Borane Dianions, BnHn2-(n= 13â”17) Are Aromatic, Why Are They Unknown?â€. Inorganic Chemistry, 1998, 37, 6765-6772.	4.0	157
5	Untangling the formation of the cyclic carbon trioxide isomer in low temperature carbon dioxide ices. Physical Chemistry Chemical Physics, 2004, 6, 735.	2.8	156
6	Formation Mechanism of Polycyclic Aromatic Hydrocarbons beyond the Second Aromatic Ring. Journal of Physical Chemistry A, 2013, 117, 4794-4816.	2.5	146
7	Hydrogen Abstraction Acetylene Addition and Dielsâ”Alder Mechanisms of PAH Formation:Â A Detailed Study Using First Principles Calculations. Journal of Chemical Theory and Computation, 2005, 1, 908-924.	5.3	141
8	Ab Initio Calculations of Vibronic Spectra and Dynamics for Small Polyatomic Molecules:Â Role of Duschinsky Effect. Journal of Physical Chemistry A, 1999, 103, 10674-10690.	2.5	139
9	On the mechanism of soot nucleation. Physical Chemistry Chemical Physics, 2020, 22, 5314-5331.	2.8	136
10	Photodissociation of benzene under collision-free conditions: An ab initio/Riceâ€“Ramspergerâ€“Kasselâ€“Marcus study. Journal of Chemical Physics, 2004, 120, 7008-7017.	3.0	133
11	Formation of benzene in the interstellar medium. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 452-457.	7.1	131
12	Formation Mechanisms of Naphthalene and Indene: From the Interstellar Medium to Combustion Flames. Journal of Physical Chemistry A, 2017, 121, 901-926.	2.5	130
13	Understanding the Kinetics and Dynamics of Radiationâ€induced Reaction Pathways in Carbon Monoxide Ice at 10 K. Astrophysical Journal, Supplement Series, 2006, 163, 184-206.	7.7	127
14	The Reaction of Phenyl Radical with Molecular Oxygen:Â A G2M Study of the Potential Energy Surface. Journal of Physical Chemistry A, 2005, 109, 6114-6127.	2.5	126
15	Photodissociation Dynamics of Propyne and Allene:â€‰ A View from ab Initio Calculations of the C3Hn (n) Tj ETQq1 1 0.784314 rgBT /O 1998, 120, 5751-5763.	13.7	125
16	Untangling the chemical evolution of Titan's atmosphere and surfaceâ€“from homogeneous to heterogeneous chemistry. Faraday Discussions, 2010, 147, 429.	3.2	118
17	Theoretical Study of Potential Energy Surface and Thermal Rate Constants for the C6H5 + H2 and C6H6 + H Reactions. Journal of Physical Chemistry A, 1997, 101, 3189-3196.	2.5	116
18	Temperature- and pressure-dependent rate coefficients for the HACA pathways from benzene to naphthalene. Proceedings of the Combustion Institute, 2017, 36, 919-926.	3.9	115

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19	Ab Initio Study of the Mechanism for the Thermal Decomposition of the Phenoxy Radical. The Journal of Physical Chemistry, 1996, 100, 9314-9322.	2.9	111
20	Reaction Dynamics in Astrochemistry: Low-Temperature Pathways to Polycyclic Aromatic Hydrocarbons in the Interstellar Medium. Annual Review of Physical Chemistry, 2015, 66, 43-67.	10.8	109
21	An ab initio molecular orbital study of the mechanism of the rhodium(I)-catalyzed olefin hydroboration reaction. Journal of the American Chemical Society, 1994, 116, 10693-10702.	13.7	106
22	A density functional study of the global potential energy surfaces of the [H,C,N,O] system in singlet and triplet states. Journal of Chemical Physics, 1996, 105, 6439-6454.	3.0	105
23	Reaction dynamics of carbon-bearing radicals in circumstellar envelopes of carbon stars. Faraday Discussions, 2006, 133, 245.	3.2	103
24	Ab initio/RRKM approach toward the understanding of ethylene photodissociation. Journal of Chemical Physics, 1998, 109, 2748-2761.	3.0	102
25	Bond lengths and diameters of armchair single wall carbon nanotubes. Chemical Physics Letters, 2005, 407, 266-271.	2.6	96
26	Structure of the acetone liquid/vapor interface. Journal of Chemical Physics, 2001, 114, 1837-1843.	3.0	89
27	A globally smooth ab initio potential surface of the 1â€‰Aâ€² state for the reaction S(1D)+H2. Journal of Chemical Physics, 2002, 116, 4124-4134.	3.0	84
28	Abinitiomolecular orbital study of the HCO+O2reaction: Direct versus indirect abstraction channels. Journal of Chemical Physics, 1996, 105, 2346-2352.	3.0	82
29	IR spectroscopy and theoretical vibrational calculation of the melamine molecule. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 3445-3451.	1.7	81
30	The reactivity of ground-state carbon atoms with unsaturated hydrocarbons in combustion flames and in the interstellar medium. International Reviews in Physical Chemistry, 2002, 21, 307-356.	2.3	81
31	Photoinduced Mechanism of Formation and Growth of Polycyclic Aromatic Hydrocarbons in Low-Temperature Environments via Successive Ethynyl Radical Additions. Journal of the American Chemical Society, 2008, 130, 13618-13629.	13.7	81
32	Detailed, sterically-resolved modeling of soot oxidation: Role of O atoms, interplay with particle nanostructure, and emergence of inner particle burning. Combustion and Flame, 2018, 188, 284-306.	5.2	81
33	A VUV Photoionization Study of the Formation of the Indene Molecule and Its Isomers. Journal of Physical Chemistry Letters, 2011, 2, 1731-1735.	4.6	79
34	Pressure-dependent rate constants for PAH growth: formation of indene and its conversion to naphthalene. Faraday Discussions, 2016, 195, 637-670.	3.2	76
35	A Computational Study of the OH(OD) + CO Reactions:Â Effects of Pressure, Temperature, and Quantum-Mechanical Tunneling on Product Formation. Journal of Physical Chemistry A, 2001, 105, 11249-11259.	2.5	72
36	Low-temperature formation of polycyclic aromatic hydrocarbons in Titanâ€™s atmosphere. Nature Astronomy, 2018, 2, 973-979.	10.1	72

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37	The CH3+C5H5 reaction: A potential source of benene at high temperatures. Proceedings of the Combustion Institute, 1996, 26, 521-526.	0.3	71
38	Ab initio calculations of radiationless transitions between excited and ground singlet electronic states of ethylene. Journal of Chemical Physics, 1998, 108, 2044-2055.	3.0	69
39	Reaction Mechanism of N2/H2 Conversion to NH3:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2003, 107, 2865-2874.	2.5	69
40	Theoretical study of isomerization and dissociation of acetylene dication in the ground and excited electronic states. Journal of Chemical Physics, 2005, 123, 134320.	3.0	69
41	Ab Initio G3-type/Statistical Theory Study of the Formation of Indene in Combustion Flames. I. Pathways Involving Benzene and Phenyl Radicalâ€. Journal of Physical Chemistry A, 2007, 111, 3922-3931.	2.5	69
42	The Formation of Naphthalene, Azulene, and Fulvalene from Cyclic C₅ Species in Combustion:â€‰ An Ab Initio/RRKM Study of 9-H-Fulvalenyl (C₅H₅â”C₅H₄) Radical Rearrangements. Journal of Physical Chemistry A, 2007, 111, 9532-9543.	2.5	69
43	On the theoretical investigation of vibronic spectra of ethylene by ab initio calculations of the Franckâ€“Condon factors. Journal of Chemical Physics, 1996, 105, 9007-9020.	3.0	68
44	Can the C₅H₅ + C₅H₅ â†’ C₁₀H₁₀ â†’ C₁₀H₉ + H/C₁₀H₈ + H₂ Reaction Produce Naphthalene? An Ab Initio/RRKM Study. Journal of Physical Chemistry A, 2009, 113, 9825-9833.	2.5	68
45	Toward the understanding of ethylene photodissociation: Theoretical study of energy partition in products and rate constants. Journal of Chemical Physics, 1999, 110, 10810-10820.	3.0	65
46	Absorption Cross Sections of NH3, NH2D, NHD2, and ND3in the Spectral Range 140â€“220 nm and Implications for Planetary Isotopic Fractionation. Astrophysical Journal, 2006, 647, 1535-1542.	4.5	65
47	Pyrene synthesis in circumstellar envelopes and its role in the formation of 2D nanostructures. Nature Astronomy, 2018, 2, 413-419.	10.1	62
48	On the low-temperature limit of HACA. Proceedings of the Combustion Institute, 2019, 37, 969-976.	3.9	62
49	Crossed-beam reaction of carbon atoms with hydrocarbon molecules. V. Chemical dynamics of n-C4H3 formation from reaction of C(3Pj) with allene, H2CCCH2(Xâ€Š1A1). Journal of Chemical Physics, 1999, 110, 10330-10344.	3.0	60
50	A crossed beam and ab initio study of the C2(X1Î£g+ /a3âˆ‘u)+C2H2(X1Î£g+) reactions. Chemical Physics Letters, 2003, 382, 112-119.	2.6	59
51	Molecular mass growth through ring expansion in polycyclic aromatic hydrocarbons via radicalâ€“radical reactions. Nature Communications, 2019, 10, 3689.	12.8	59
52	Ab initio study of the n-Ï€* electronic transition in acetone: Symmetry-forbidden vibronic spectra. Journal of Chemical Physics, 1999, 111, 205-215.	3.0	58
53	A Combined Crossed Molecular Beam and ab Initio Study of the Reactions C2(X1âˆ‘g+, a3Îu) + C2H4â†’n-C4H3(X2Aâ€˜) + H(2S1/2). Journal of Physical Chemistry A, 2001, 105, 9813-9818.	2.5	58
54	Reaction dynamics of S([sup 1]D)+H[sub 2]/D[sub 2] on a new ab initio potential surface. Journal of Chemical Physics, 2001, 114, 320.	3.0	58

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55	Propargylene. Journal of the American Chemical Society, 1994, 116, 8229-8237.	13.7	57
56	Ï€·Ï€âˆ— vibronic spectrum of ethylene from ab initio calculations of the Franck-Condon factors. Chemical Physics Letters, 1996, 258, 53-62.	2.6	57
57	An Ab Initio G3-Type/Statistical Theory Study of the Formation of Indene in Combustion Flames. II. The Pathways Originating from Reactions of Cyclic C5SpeciesCyclopentadiene and Cyclopentadienyl Radicals. Journal of Physical Chemistry A, 2008, 112, 700-716.	2.5	57
58	VUV Photoionization Study of the Formation of the Simplest Polycyclic Aromatic Hydrocarbon: Naphthalene (C₁₀H₈). Journal of Physical Chemistry Letters, 2018, 9, 2620-2626.	4.6	57
59	PAH Formation under Single Collision Conditions: Reaction of Phenyl Radical and 1,3-Butadiene to Form 1,4-Dihydronaphthalene. Journal of Physical Chemistry A, 2012, 116, 4248-4258.	2.5	56
60	A Theoretical Investigation of the Triplet Carbon Atom C(3P) + Vinyl Radical C2H3(2Aâ€˜) Reaction and Thermochemistry of C3Hn(n= 1â€“4) Species. Journal of Physical Chemistry A, 2001, 105, 3284-3299.	2.5	55
61	Ab initio molecular orbital/Riceâ€“Ramspergerâ€“Kasselâ€“Marcus theory study of multichannel rate constants for the unimolecular decomposition of benzene and the H+C6H5 reaction over the ground electronic state. Journal of Chemical Physics, 2001, 114, 8421-8435.	3.0	53
62	Theoretical study of the thermal isomerization of fulvene to benzene. Journal of Physical Organic Chemistry, 1996, 9, 801-810.	1.9	52
63	AN EXPERIMENTAL AND THEORETICAL STUDY ON THE IONIZATION ENERGIES OF POLYYNES (H-(Câ‰¡C)_n-H;n= 1-9). Astrophysical Journal, 2010, 719, 1884-1889.	4.5	52
64	Ab Initio Molecular Orbital Calculations of C6H5O2 Isomers. Journal of the American Chemical Society, 1994, 116, 9577-9584.	13.7	51
65	Theoretical Study on the Mechanism of the Dissociation of Benzene. The C5H3+ CH3Product Channel. Journal of Physical Chemistry A, 1997, 101, 6781-6789.	2.5	50
66	Rate Constant of the HONO + HONO â†' H2O + NO + NO2 Reaction from ab Initio MO and TST Calculations. Journal of Physical Chemistry A, 1998, 102, 1803-1807.	2.5	50
67	Theoretical study of unimolecular decomposition of allene cations. Journal of Chemical Physics, 2008, 129, 224311.	3.0	50
68	Ab initio molecular orbital study of potential energy surface for the reaction of C2H3 with H2 and related reactions. Journal of Chemical Physics, 1995, 103, 3440-3449.	3.0	49
69	Theoretical study of vibronic spectra and photodissociation pathways of methane. Journal of Chemical Physics, 1997, 106, 2612-2620.	3.0	49
70	Chemical dynamics of cyclopropynylidyne (c-C[sub 3]H;â€ŠX[sup 2]B[sub 2]) formation from the reaction of C([sup 1]D) with acetylene, C[sub 2]H[sub 2](Xâ€‰[sup 1]Î£[sub g][sup +]). Journal of Chemical Physics, 2001, 114, 231.	3.0	49
71	Investigating the Mechanism for the Formation of Nitrous Oxide [N2O(X1Î£+)] in Extraterrestrial Ices. Astrophysical Journal, 2005, 624, 436-447.	4.5	49
72	A VUV photoionization study of the multichannel reaction of phenyl radicals with 1,3-butadiene under combustion relevant conditions. Physical Chemistry Chemical Physics, 2013, 15, 341-347.	2.8	49

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73	Hydrogenâ€Abstraction/Acetyleneâ€Addition Exposed. Angewandte Chemie - International Edition, 2016, 55, 14983-14987.	13.8	48
74	HACA's Heritage: A Freeâ€Radical Pathway to Phenanthrene in Circumstellar Envelopes of Asymptotic Giant Branch Stars. Angewandte Chemie - International Edition, 2017, 56, 4515-4519.	13.8	48
75	Ab initio molecular orbital study of excited electronic states of the vinyl radical. Chemical Physics Letters, 1997, 275, 19-27.	2.6	47
76	Product Branching Ratios of the C(3P) + C2H3(2Aâ€˜) and CH(2Î) + C2H2(1Î£g+) Reactions and Photodissociation of H2CCâ‹®CH(2B1) at 193 and 242 nm:Â an ab Initio/RRKM Study. Journal of Physical Chemistry A, 2001, 105, 11549-11559.	2.5	47
77	Roaming dynamics in radical additionâ€“elimination reactions. Nature Communications, 2014, 5, 4064.	12.8	47
78	Oxidation of Graphene-Edge Six- and Five-Member Rings by Molecular Oxygen. Journal of Physical Chemistry A, 2015, 119, 7528-7547.	2.5	46
79	An ab Initio/RRKM Study of Product Branching Ratios in the Photodissociation of Buta-1,2- and -1,3-dienes and But-2-yne at 193 nm. Chemistry - A European Journal, 2003, 9, 726-740.	3.3	45
80	A survey ofab initioconical intersections for the H+H2 system. Journal of Chemical Physics, 2003, 118, 3052-3064.	3.0	45
81	Theoretical Study of Oxygen Isotope Exchange and Quenching in the O(1D) + CO2Reactionâ€. Journal of Physical Chemistry A, 2004, 108, 7983-7994.	2.5	45
82	Hydroxyl Radical Mediated Degradation of Phenylarsonic Acid. Journal of Physical Chemistry A, 2007, 111, 7819-7824.	2.5	45
83	Anharmonic Effect on Unimolecular Reactions with Application to the Photodissociation of Ethyleneâ€. Journal of Physical Chemistry A, 2007, 111, 6722-6729.	2.5	45
84	A CROSSED MOLECULAR BEAM, LOW-TEMPERATURE KINETICS, AND THEORETICAL INVESTIGATION OF THE REACTION OF THE CYANO RADICAL (CN) WITH 1,3-BUTADIENE (C₄H₆). A ROUTE TO COMPLEX NITROGEN-BEARING MOLECULES IN LOW-TEMPERATURE EXTRATERRESTRIAL ENVIRONMENTS. Astrophysical Journal, 2011, 742, 26.	4.5	45
85	Indene Formation under Singleâ€Collision Conditions from the Reaction of Phenyl Radicals with Allene and Methylacetyleneâ€”A Crossed Molecular Beam and Ab Initio Study. Chemistry - an Asian Journal, 2011, 6, 3035-3047.	3.3	45
86	Red and near-infrared photoluminescence from silica-based nanoscale materials: Experimental investigation and quantum-chemical modeling. Journal of Chemical Physics, 2002, 116, 281.	3.0	44
87	Ab initio and RRKM study of photodissociation of azulene cation. Physical Chemistry Chemical Physics, 2006, 8, 1404.	2.8	44
88	The Formation of Interstellar C2N Isomers in Circumstellar Envelopes of Carbon Stars: An Ab Initio Study. Astrophysical Journal, 2002, 564, 787-791.	4.5	42
89	Chemistry of Energetically Activated Cumulenesâ€”From Allene (H₂CCCH₂) to Hexapentaene (H₂CCCCCCH₂). ChemPhysChem, 2008, 9, 350-369.	2.1	42
90	COSMIC-RAY-MEDIATED FORMATION OF BENZENE ON THE SURFACE OF SATURNâ€™S MOON TITAN. Astrophysical Journal, 2010, 718, 1243-1251.	4.5	42

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91	Low-temperature gas-phase formation of indene in the interstellar medium. Science Advances, 2021, 7, .	10.3	42
92	Excited electronic states of the methyl radical. Ab initio molecular orbital study of geometries, excitation energies and vibronic spectra. Chemical Physics, 1997, 215, 329-341.	1.9	41
93	Ab Initio MO Study of the Triplet C3H4 Potential Energy Surface and the Reaction of C(3Pj) with Ethylene, C2H4. Journal of Physical Chemistry A, 2001, 105, 1847-1856.	2.5	41
94	Photoluminescence from mesoporous silica akin to that from nanoscale silicon: the nature of light-emitters. Chemical Physics Letters, 2002, 358, 180-186.	2.6	41
95	A theoretical study of isomerism in doped aluminum XAl12 clusters (X=B, Al, Ga, C, Si, Ge) with 40 valence electrons. Chemical Physics Letters, 2002, 365, 494-504.	2.6	41
96	Toward the Oxidation of the Phenyl Radical and Prevention of PAH Formation in Combustion Systems. Journal of Physical Chemistry A, 2015, 119, 7145-7154.	2.5	41
97	Ab Initio Study of the H + HONO Reaction:â€‰ Direct Abstraction versus Indirect Exchange Processes. Journal of Physical Chemistry A, 1997, 101, 60-66.	2.5	40
98	Ab initio calculations of vibronic coupling. Applications to symmetry-forbidden vibronic spectra and internal conversion in ethylene. Chemical Physics Letters, 1997, 274, 281-292.	2.6	40
99	Photoisomerization and Photodissociation of Aniline and 4-Methylpyridine. Journal of the American Chemical Society, 2004, 126, 8760-8768.	13.7	40
100	An improved potential energy surface for the F+H2 reaction. Chemical Physics, 2005, 308, 259-266.	1.9	40
101	On the formation of polyacetylenes and cyanopolyacetylenes in Titan's atmosphere and their role in astrobiology. Chemical Society Reviews, 2012, 41, 5490.	38.1	40
102	Formation of resonantly stabilised free radicals via the reactions of atomic carbon, dicarbon, and tricarbon with unsaturated hydrocarbons: theory and crossed molecular beams experiments. International Reviews in Physical Chemistry, 2015, 34, 461-514.	2.3	40
103	Experimental and Theoretical Studies of the Unimolecular Decomposition of Nitrosobenzene:Â High-Pressure Rate Constants and the Câ^'N Bond Strength. Journal of Physical Chemistry A, 1997, 101, 6043-6047.	2.5	39
104	Ab initio calculations of potential energy surface and rate constants for ethylene photodissociation at 193 and 157 nm. Chemical Physics Letters, 1998, 287, 301-306.	2.6	39
105	Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide. Chemical Physics, 2000, 256, 169-176.	1.9	39
106	Ab Initio MO Study of the Global Potential Energy Surface of C4H4in Triplet Electronic State and the Reactions of C(3Pj) with C3H4(Allene and Propyne) and C2(A3Îu) with C2H4(X1A1g+). Journal of the American Chemical Society, 2000, 122, 1776-1788.	13.7	39
107	Activation of Methane by Neutral Transition Metal Oxides (ScO, NiO, and PdO):â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2002, 106, 12072-12083.	2.5	39
108	Chemical dynamics of triacetylene formation and implications to the synthesis of polyynes in Titan's atmosphere. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 16078-16083.	7.1	39

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109	Prediction of Absolute Rate Constants for the Reactions of NH2 with Alkanes from ab Initio G2M/TST Calculations. Journal of Physical Chemistry A, 1999, 103, 2088-2096.	2.5	38
110	Photodissociation dynamics of pyridine. Journal of Chemical Physics, 2005, 123, 054309.	3.0	38
111	Identification of the D3h Isomer of Carbon Trioxide (CO3) and Its Implications for Atmospheric Chemistry. ChemPhysChem, 2006, 7, 2508-2513.	2.1	38
112	Experimental and Theoretical Investigation of High-Power Laser Ionization and Dissociation of Methane. Journal of Physical Chemistry A, 2007, 111, 9405-9416.	2.5	38
113	A crossed beam investigation of the reactions of tricarbon molecules, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si6.gif" display="inline" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>		

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127	Ab Initio/RRKM Study of the Potential Energy Surface of Triplet Ethylene and Product Branching Ratios of the C(3P) + CH4 Reaction. Journal of Physical Chemistry A, 2003, 107, 1788-1796.	2.5	35
128	Spectroscopic and Thermochemical Consequences of Site-Specific H-Atom Addition to Naphthalene. Journal of Physical Chemistry A, 2010, 114, 6255-6262.	2.5	35
129	Ab initio molecular orbital study of potential energy surface for the NH+NO2 reaction. Journal of Chemical Physics, 1994, 101, 3916-3922.	3.0	34
130	The study of conical intersections between consecutive pairs of the five lowest 2Aâ€² states of the C2H molecule. Journal of Chemical Physics, 2001, 115, 3673-3689.	3.0	34
131	Mechanisms of formation of nitrogen-containing polycyclic aromatic compounds in low-temperature environments of planetary atmospheres: A theoretical study. Faraday Discussions, 2010, 147, 479.	3.2	34
132	ON THE FORMATION OF ORTHO-BENZYNE (o-C₆H₄) UNDER SINGLE COLLISION CONDITIONS AND ITS ROLE IN INTERSTELLAR CHEMISTRY. Astrophysical Journal, 2011, 728, 141.	4.5	34
133	Rate coefficients and product branching ratios for the oxidation of phenyl and naphthyl radicals: A theoretical RRKM-ME study. Proceedings of the Combustion Institute, 2015, 35, 1861-1869.	3.9	34
134	Combined Experimental and Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates. I. n-Decane (n-C₁₀H₂₂). Journal of Physical Chemistry A, 2017, 121, 1261-1280.	2.5	34
135	Gas-phase synthesis of benzene via the propargyl radical self-reaction. Science Advances, 2021, 7, .	10.3	34
136	Ab initio study on the reaction mechanism of ozone with the chlorine atom. Journal of Chemical Physics, 1998, 109, 10847-10852.	3.0	33
137	Chemical Dynamics of the Formation of the 1,3-Butadiynyl Radical (C4H(X2Î£+)) and Its Isotopomers. Journal of Physical Chemistry A, 2006, 110, 11265-11278.	2.5	33
138	Ab initio/Rice-Ramsperger-Kassel-Marcus study of the singlet C4H4 potential energy surface and of the reactions of C2(XÎ£g+1) with C4H4(XA1g+1) and C(D1) with C3H4 (allene and methylacetylene). Journal of Chemical Physics, 2006, 125, 133113.	3.0	33
139	Prediction of product branching ratios in the C(P3)+C2H2â†'l-C3H+Hâˆ•c-C3H+Hâˆ•C3+H2 reaction using ab initio coupled clusters calculations extrapolated to the complete basis set combined with Rice-Ramsperger-Kassel-Marcus and radiationless transition theories. Journal of Chemical Physics, 2007, 126, 204310.	3.0	33
140	On the calculation of the dissociation rate constant of the water dimer by the ab initio anharmonic RRKM theory. Chemical Physics Letters, 2009, 470, 210-214.	2.6	33
141	Photoluminescence of silanone and dioxasilyrane groups in silicon oxides: A theoretical study. Journal of Chemical Physics, 2002, 116, 9889-9896.	3.0	32
142	Experimental and theoretical investigations of ionization/dissociation of cyclopentanone molecule in a femtosecond laser field. Journal of Chemical Physics, 2008, 129, 204302.	3.0	32
143	Reaction mechanism, rate constants, and product yields for unimolecular and H-assisted decomposition of 2,4-cyclopentadienone and oxidation of cyclopentadienyl with atomic oxygen. Combustion and Flame, 2017, 183, 181-193.	5.2	32
144	Structure and nonrigidity of undecahydrodecaborate(1-). An ab initio/IGLO/NMR study. Inorganic Chemistry, 1993, 32, 463-468.	4.0	31

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145	Rydberg states of propyne at 6.8â€“10.5 eV studied by two-photon resonant ionization spectroscopy and theoretical calculation. Journal of Chemical Physics, 2000, 112, 7384-7393.	3.0	30
146	Theoretical Study on the Reaction Mechanism of Nickel Atoms with Carbon Dioxide. Journal of Physical Chemistry A, 2000, 104, 11622-11627.	2.5	30
147	Theoretical Study of the Reaction Mechanism of Fe Atoms with H2O, H2S, O2 and H+. Journal of Physical Chemistry A, 2001, 105, 7460-7467.	2.5	30
148	Theoretical study of the C6H3 potential energy surface and rate constants and product branching ratios of the C2H(Î£+2)+C4H2(Î£g+1) and C4H(Î£+2)+C2H2(Î£g+1) reactions. Journal of Chemical Physics, 2008, 128, 214301.	3.0	30
149	AN EXPERIMENTAL AND THEORETICAL STUDY OF THE IONIZATION ENERGIES OF SiC₂H_x(x= 0, 1, 2) ISOMERS. Astrophysical Journal, 2012, 761, 178.	4.5	30
150	Reaction of phenoxy radical with nitric oxide. Journal of Physical Organic Chemistry, 1995, 8, 47-53.	1.9	29
151	Using ab Initio MO Calculations To Understand the Photodissociation Dynamics of CH2CCH2and CH2C2. Journal of Physical Chemistry A, 1997, 101, 6638-6646.	2.5	29
152	A combined crossed beam and ab initio investigation on the reaction of carbon species with C4H6 isomers. III. 1,2-butadiene, H2CCCH(CH3) (Xâ€Š1Aâ€²)â€”a non-Riceâ€“Ramspergerâ€“Kasselâ€“Marcus system?. Journal of Chemical Physics, 2001, 115, 5107-5116.	3.0	29
153	Ab initio non-adiabatic coupling elements: the conical intersection between the 22Aâ€² and the 32Aâ€² of the H+H2 system. Chemical Physics Letters, 2002, 358, 163-169.	2.6	29
154	Azido-Nitrene Is Probably the N4 Molecule Observed in Mass Spectrometric Experiments. Journal of Physical Chemistry A, 2003, 107, 5452-5460.	2.5	29
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