

Alexander M Mebel

List of Publications by Year in descending order

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473
papers

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citing authors

#	ARTICLE	IF	CITATIONS
1	The Reaction of C_6H_4 Benzyne with Vinylacetylene: An Unexplored Way to Produce Naphthalene. <i>ChemPhysChem</i> , 2022, 23, .	2.1	7
2	Combustion chemistry of alkenes and alkadienes. <i>Progress in Energy and Combustion Science</i> , 2022, 90, 100983.	31.2	28
3	The Role of Methylaryl Radicals in the Growth of Polycyclic Aromatic Hydrocarbons: The Formation of Five-Membered Rings. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1233-1244.	2.5	9
4	Unconventional excited-state dynamics in the concerted benzyl (C_7H_7) radical self-reaction to anthracene ($\text{C}_{14}\text{H}_{10}$). <i>Nature Communications</i> , 2022, 13, 786.	12.8	17
5	Radicalâ€“Radical Reaction Dynamics Probed Using Millimeterwave Spectroscopy: Propargyl + NH_2 . <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 91-97.	4.6	2
6	Density Functional Theory Study of the Oxygen Reduction Reaction Mechanism on Graphene Doped with Nitrogen and a Transition Metal. <i>ACS Omega</i> , 2022, 7, 7066-7073.	3.5	11
7	Gas-Phase Study of the Elementary Reaction of the D1-Ethynyl Radical (C_2D); Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Single-Collision Conditions. <i>Journal of Physical Chemistry A</i> , 2022, 126, 1889-1898.	2.5	3
8	Hierarchical porous N-doped carbon-supported PtCu nanoparticles as an efficient catalyst for oxygen reduction reaction. <i>Journal of Power Sources</i> , 2022, 533, 231270.	7.8	8
9	Formation of Benzene and Naphthalene through Cyclopentadienyl-Mediated Radicalâ€“Radical Reactions. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 208-213.	4.6	14
10	Direct H abstraction by molecular oxygen from unsaturated C_3 â€“ C_5 hydrocarbons: A theoretical study. <i>International Journal of Chemical Kinetics</i> , 2022, 54, 203-217.	1.6	4
11	Mechanism of E-bridge formation by various PAH molecules: A theoretical study. <i>Chemical Physics Letters</i> , 2022, 799, 139637.	2.6	5
12	Gas-Phase Preparation of Subvalent Germanium Monoxide (GeO , X^1 ¹ Î£ ⁺) via Non-Adiabatic Reaction Dynamics in the Exit Channel. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4589-4597.	4.6	2
13	Probing the Intermediates of Catalyzed Dehydration Reactions of Primary Amide to Nitrile in Plasmonic Junctions. <i>ACS Catalysis</i> , 2022, 12, 7737-7747.	11.2	13
14	Chromatographic framework for coffee ring effect-driven separation of small molecules in surface enhanced Raman spectroscopy analysis. <i>Talanta</i> , 2022, 250, 123688.	5.5	2
15	Formation of phenanthrenyl radicals via the reaction of acenaphthyl with acetylene. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 1441-1448.	3.9	12
16	Directed Gas Phase Formation of the Elusive Silylgermylidyne Radical (H_3SiGe , X^2 A^2 E^2). <i>ChemPhysChem</i> , 2021, 22, 184-191.	2.1	3
17	Experimental and numerical studies of downward flame spread over PMMA with and without addition of tri phenyl phosphate. <i>Proceedings of the Combustion Institute</i> , 2021, 38, 4867-4875.	3.9	15
18	A molecular beam and computational study on the barrierless gas phase formation of (iso)quinoline in low temperature extraterrestrial environments. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18495-18505.	2.8	5

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19	Gas-Phase Formation of C ₅ H ₆ Isomers via the Crossed Molecular Beam Reaction of the Methylidyne Radical (CH; X ²⁺) with 1,2-Butadiene (CH ₃ CHCCH ₂ ; X ¹⁺). Journal of Physical Chemistry A, 2021, 125, 126-138.	2.5	6
20	Low-temperature gas-phase formation of indene in the interstellar medium. Science Advances, 2021, 7, .	10.3	42
21	Gas-phase pyrolysis of <i>trans</i> -3-pentenitrile: competition between direct and isomerization-mediated dissociation. Physical Chemistry Chemical Physics, 2021, 23, 6462-6471.	2.8	5
22	Mechanism and kinetics of the oxidation of 1,3-butadien-1-yl (n-C ₄ H ₅): a theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 9198-9210.	2.8	2
23	On the Synthesis of the Astronomically Elusive 1-Ethynyl-3-Silacyclopropenylidene (c-SiC ₄ H ₂) Molecule in Circumstellar Envelopes of Carbon-rich Asymptotic Giant Branch Stars and Its Potential Role in the Formation of the Silicon Tetracarbide Chain (SiC ₄). Astrophysical Journal Letters, 2021, 908, L40.	8.3	7
24	Transformation of an Embedded Five-Membered Ring in Polycyclic Aromatic Hydrocarbons via the Hydrogen-Abstraction ⁺ Acetylene-Addition Mechanism: A Theoretical Study. Journal of Physical Chemistry A, 2021, 125, 3341-3354.	2.5	10
25	Theoretical Study of the Phenoxy Radical Recombination with the O(³ P) Atom, Phenyl plus Molecular Oxygen Revisited. Journal of Physical Chemistry A, 2021, 125, 3965-3977.	2.5	11
26	Gas-phase synthesis of benzene via the propargyl radical self-reaction. Science Advances, 2021, 7, .	10.3	34
27	Combined Crossed Molecular Beams and Ab Initio Study of the Bimolecular Reaction of Ground State Atomic Silicon (Si; 3 P) with Germane (GeH ₄ ; X ^{1A1}). ChemPhysChem, 2021, 22, 1497-1504.	2.1	1
28	Theoretical Study of the Mechanism and Kinetics of the Oxidation of Cyclopenta[<i>a</i>]Naphthalenyl Radical C ₁₃ H ₉ with Molecular Oxygen. Journal of Physical Chemistry A, 2021, 125, 6796-6804.	2.5	3
29	On the Mechanism of Soot Nucleation. III. The Fate and Facility of the E-Bridge. Journal of Physical Chemistry A, 2021, 125, 6789-6795.	2.5	6
30	Directed Gas-Phase Formation of Aminosilylene (HSiNH ₂ ; X ¹⁺): The Simplest Silicon Analogue of an Aminocarbene, under Single-Collision Conditions. Journal of the American Chemical Society, 2021, 143, 14227-14234.	13.7	6
31	Gas-phase synthesis of corannulene – a molecular building block of fullerenes. Physical Chemistry Chemical Physics, 2021, 23, 5740-5749.	2.8	10
32	Theoretical Study of the Reaction of the Methylidyne Radical (CH; X ²⁺) with 1-Butyne (CH ₃ CH ₂ CCH; X ¹⁺). Journal of Physical Chemistry A, 2021, 125, 9536-9547.	2.5	2
33	Ozone destruction due to the recombination of oxygen atoms. Journal of Chemical Physics, 2021, 155, 164307.	3.0	4
34	Gas-phase Synthesis of Silaformaldehyde (H ₂ SiO) and Hydroxysilylene (HSiOH) in Outflows of Oxygen-rich Asymptotic Giant Branch Stars. Astrophysical Journal Letters, 2021, 921, L7.	8.3	0
35	A chemical dynamics study of the reaction of the methylidyne radical (CH, X ²⁺) with dimethylacetylene (CH ₃ CCCH ₃ , X ¹⁺). Physical Chemistry Chemical Physics, 2021, 24, 578-593.	2.8	12
36	Conversion of acenaphthalene to phenalene via methylation: A theoretical study. Combustion and Flame, 2020, 213, 302-313.	5.2	24

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37	A Unified Mechanism on the Formation of Acenes, Helicenes, and Phenacenes in the Gas Phase. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 4051-4058.	13.8	18
38	Iodoindenes: Synthesis and application to cross-coupling. <i>Tetrahedron Letters</i> , 2020, 61, 152427.	1.4	2
39	Formation of Phenanthrene via Recombination of Indenyl and Cyclopentadienyl Radicals: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9933-9941.	2.5	17
40	A chemical dynamics study on the gas-phase formation of triplet and singlet C ₅ H ₂ carbenes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 30142-30150.	7.1	16
41	Formation of phenanthrene via H ₂ -assisted isomerization of 2-ethynylbiphenyl produced in the reaction of phenyl with phenylacetylene. <i>International Journal of Chemical Kinetics</i> , 2020, 52, 875-883.	1.6	12
42	Gas phase formation of cyclopentanaphthalene (benzindene) isomers via reactions of 5- and 6-indenyl radicals with vinylacetylene. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 22493-22500.	2.8	13
43	Gas Phase Synthesis of the Elusive Trisilacyclopropyl Radical (Si ₃ H ₅) via Unimolecular Decomposition of Chemically Activated Doublet Trisilapropyl Radicals (Si ₃ H ₇). <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 7874-7881.	4.6	0
44	A chemical dynamics study on the gas phase formation of thioformaldehyde (H ₂ CS) and its thiohydroxycarbene isomer (HCSH). <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 22712-22719.	7.1	18
45	Energies and molecular parameters involved in the reaction of CH + 1, 3-butadiene. <i>AIP Conference Proceedings</i> , 2020, , .	0.4	0
46	Gas-Phase Synthesis of 3-Vinylcyclopropene via the Crossed Beam Reaction of the Methylidyne Radical (CH; X 2 Å) with 1,3-Butadiene (CH ₂ CHCHCH ₂ ; X 1 Å g). <i>ChemPhysChem</i> , 2020, 21, 1295-1309.	2.1	7
47	Kinetics of Reactions of 1- and 2-Naphthyl with Propyne and Allene. <i>Bulletin of the Lebedev Physics Institute</i> , 2020, 47, 97-100.	0.6	1
48	Gas Phase Identification of the Elusive <i>i</i> -N-Hydroxyoxaziridine (c-H ₂ CON(OH)): A Chiral Molecule. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5383-5389.	4.6	8
49	Directed Gas Phase Formation of Silene (H ₂ SiCH ₂). <i>Chemistry - A European Journal</i> , 2020, 26, 13584-13589.	3.3	4
50	Theoretical study of the reaction mechanism and kinetics of the phenyl + propargyl association. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 6868-6880.	2.8	22
51	A Unified Mechanism on the Formation of Acenes, Helicenes, and Phenacenes in the Gas Phase. <i>Angewandte Chemie</i> , 2020, 132, 4080-4087.	2.0	5
52	Gas phase formation of phenalene via 10 π -aromatic, resonantly stabilized free radical intermediates. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 15381-15388.	2.8	15
53	Gas Phase Formation of Methylgermylene (HGeCH ₃). <i>ChemPhysChem</i> , 2020, 21, 1898-1904.	2.1	4
54	On the mechanism of soot nucleation. II. E-bridge formation at the PAH bay. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 17196-17204.	2.8	14

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55	Revisiting diacetyl and acetic acid flames: The role of the ketene+OH reaction. <i>Combustion and Flame</i> , 2020, 218, 28-41.	5.2	13
56	The Elusive Ketene (H ₂ CCO) Channel in the Infrared Multiphoton Dissociation of Solid 1,3,5-Trinitro-1,3,5-Triazinane (RDX). <i>ChemPhysChem</i> , 2020, 21, 837-842.	2.1	7
57	On the mechanism of soot nucleation. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5314-5331.	2.8	136
58	Gas-Phase Formation of Fulvenallene (C ₇ H ₆) via the Jahn-Teller Distorted Tropylium (C ₇ H ₇) Radical Intermediate under Single-Collision Conditions. <i>Journal of the American Chemical Society</i> , 2020, 142, 3205-3213.	13.7	15
59	A Free-Radical Prompted Barrierless Gas-Phase Synthesis of Pentacene. <i>Angewandte Chemie</i> , 2020, 132, 11430-11434.	2.0	5
60	A Free-Radical Prompted Barrierless Gas-Phase Synthesis of Pentacene. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 11334-11338.	13.8	16
61	Spectroscopic and Theoretical Insights into Surprisingly Effective Sm(III) Extraction from Alkaline Aqueous Media by <i>o</i> -Phenylenediamine-Derived Sulfonamides. <i>Inorganic Chemistry</i> , 2020, 59, 6884-6894.	4.0	2
62	The oxidation of cyclopenta[b]naphthalene C ₁₃ H ₉ radical at the combustion conditions. <i>AIP Conference Proceedings</i> , 2020, , .	0.4	1
63	Rate constants for the formation of the vinylidene bridge bond between naphthalene and acenaphthalene: A theoretical study. <i>AIP Conference Proceedings</i> , 2020, , .	0.4	0
64	The study of indenyl + cyclopentadienyl reaction. <i>AIP Conference Proceedings</i> , 2020, , .	0.4	0
65	Aceanthracene-anthracene dimerization with the formation of an E-bridge bond. <i>AIP Conference Proceedings</i> , 2020, , .	0.4	0
66	Calculation of Potential Energy Curves for Ar*He Collision Complex. <i>Bulletin of the Lebedev Physics Institute</i> , 2020, 47, 300-302.	0.6	0
67	On the low-temperature limit of HACA. <i>Proceedings of the Combustion Institute</i> , 2019, 37, 969-976.	3.9	62
68	Molecular mass growth through ring expansion in polycyclic aromatic hydrocarbons via radical-radical reactions. <i>Nature Communications</i> , 2019, 10, 3689.	12.8	59
69	Directed Gas-Phase Synthesis of Triafulvene under Single-Collision Conditions. <i>Angewandte Chemie</i> , 2019, 131, 15634-15641.	2.0	2
70	Surface-enhanced Raman spectroscopy, Raman, and density functional theoretical analyses of fentanyl and six analogs. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 1405-1415.	2.5	24
71	How to add a five-membered ring to polycyclic aromatic hydrocarbons (PAHs) - molecular mass growth of the 2-naphthyl radical (C ₁₀ H ₇) to benzindenes (C ₁₃ H ₁₀) as a case study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16737-16750.	2.8	26
72	Directed Gas-Phase Synthesis of Triafulvene under Single-Collision Conditions. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 15488-15495.	13.8	9

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73	Gas-Phase Formation of 1-Methylcyclopropene and 3-Methylcyclopropene via the Reaction of the Methylidyne Radical (CH^{\bullet}) with Propylene ($\text{CH}_2=\text{CHCH}_3$); Tj ETQq1 1 0.784314 rgBT /Overlock	2.1	13
74	Gas-Phase Synthesis of Triphenylene ($\text{C}_{18}\text{H}_{12}$). ChemPhysChem, 2019, 20, 791-797.	2.1	13
75	Elucidating the Chemical Dynamics of the Elementary Reactions of the 1-Propynyl Radical ($\text{CH}_3\text{C}\equiv\text{C}^{\bullet}$) with Methylacetylene ($\text{H}_3\text{C}-\text{C}\equiv\text{C}-\text{CH}_3$); Tj ETQq1 1 0.784314 rgBT /Overlock	2.5	25
76	Gas Phase Formation of the Interstellar Molecule Methyltriacetylene. ChemPhysChem, 2019, 20, 1912-1917.	2.1	2
77	Scission of the Five-Membered Ring in 1-Inden-1-one $\text{C}_9\text{H}_6\text{O}$ and Indenyl C_9H_7 in the Reactions with H and O Atoms. Journal of Physical Chemistry A, 2019, 123, 5741-5752.	2.5	13
78	Combined Experimental and Computational Study on the Reaction Dynamics of the 1-Propynyl ($\text{CH}_3\text{C}\equiv\text{C}^{\bullet}$) + 1,3-Butadiene ($\text{CH}_2=\text{CHCH}=\text{CH}_2$) System and the Formation of Toluene under Single Collision Conditions. Journal of Physical Chemistry A, 2019, 123, 4104-4118.	2.5	13
79	Aggregation induced emission enhancement (AIEE) of tripodal pyrazole derivatives for sensing of nitroaromatics and vapor phase detection of picric acid. New Journal of Chemistry, 2019, 43, 7251-7258.	2.8	23
80	Reactivity of the Indenyl Radical (C_9H_7) with Acetylene (C_2H_2) and Vinylacetylene (C_4H_4). ChemPhysChem, 2019, 20, 1437-1447.	2.1	21
81	The mechanism and rate constants for oxidation of indenyl radical C_9H_7 with molecular oxygen O_2 : a theoretical study. Physical Chemistry Chemical Physics, 2019, 21, 8915-8924.	2.8	15
82	Gas phase synthesis of [4]-helicene. Nature Communications, 2019, 10, 1510.	12.8	27
83	Micro Solid Phase Extraction Surface-Enhanced Raman Spectroscopy (MSPE/SERS) Screening Test for the Detection of the Synthetic Cannabinoid JWH-018 in Oral Fluid. Analytical Chemistry, 2019, 91, 4780-4789.	6.5	38
84	Directed Gas-Phase Formation of the Germaniumsilylene Butterfly Molecule (GeH_2Si). Journal of Physical Chemistry Letters, 2019, 10, 1264-1271.	4.6	6
85	Theoretical Study of the Reaction Mechanism and Kinetics of the Phenyl + Allyl and Related Benzyl + Vinyl Associations. Journal of Physical Chemistry A, 2019, 123, 1720-1729.	2.5	14
86	Directed Gas-Phase Synthesis of Trifulvene under Single-Collision Conditions (Angew.) Tj ETQq0 0 0 rgBT /Overlock	2.0	0
87	$\text{O}_2(\text{b}^1\Sigma_g^+)$ removal by I ₂ and NO at temperatures of 297–750 K. Chemical Physics Letters, 2019, 735, 1367746	4.6	0
88	A combined experimental and computational study on the reaction dynamics of the 1-propynyl radical ($\text{CH}_3\text{C}\equiv\text{C}^{\bullet}$) with ethylene ($\text{H}_2\text{C}=\text{CH}_2$); Tj ETQq0 0 0 rgBT /Overlock	2.8	8
89	($\text{CH}_2\text{CHCCCH}_3$; X^{\bullet}). Physical Chemistry Chemical Physics, 2019, 21, 22308-22319.	3.3	7
89	A Barrierless Pathway Accessing the C_9H_9 and C_9H_8 Potential Energy Surfaces via the Elementary Reaction of Benzene with 1-Propynyl. Scientific Reports, 2019, 9, 17595.	3.3	7
90	Computational investigation of energy transfer and line broadening for $\text{Ar}^* + \text{He}$ collisions. Journal of Chemical Physics, 2019, 151, 224306.	3.0	6

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91	Reaction mechanism, rate constants, and product yields for the oxidation of embedded five-member ring radicals with atomic oxygen. <i>Chemical Physics</i> , 2019, 519, 101-109.	1.9	5
92	Mechanism and rate constants of the CH ₂ + CH ₂ CO reactions in triplet and singlet states: A theoretical study. <i>Journal of Computational Chemistry</i> , 2019, 40, 387-399.	3.3	12
93	Product channels of the reactions of O ₂ (b ¹ Σ ^{g+}). <i>Chemical Physics</i> , 2019, 521, 85-91.	1.9	4
94	Directed gas phase formation of silicon dioxide and implications for the formation of interstellar silicates. <i>Nature Communications</i> , 2018, 9, 774.	12.8	23
95	A combined crossed molecular beams and computational study on the formation of distinct resonantly stabilized C ₅ H ₃ radicals <i>via</i> chemically activated C ₅ H ₄ and C ₆ H ₆ intermediates. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 10906-10925.	2.8	5
96	Pyrene synthesis in circumstellar envelopes and its role in the formation of 2D nanostructures. <i>Nature Astronomy</i> , 2018, 2, 413-419.	10.1	62
97	Oxidation of cyclopentadienyl radical with molecular oxygen: A theoretical study. <i>Combustion and Flame</i> , 2018, 191, 309-319.	5.2	22
98	Mechanism and Rate Constants of the CH ₃ + CH ₂ CO Reaction: A Theoretical Study. <i>International Journal of Chemical Kinetics</i> , 2018, 50, 273-284.	1.6	23
99	Collisional relaxation of O ₂ (a ¹ Δ ^g , j=1, 2, 3) by CO ₂ . <i>Chemical Physics Letters</i> , 2018, 691, 456-461.	2.6	7
100	VUV Photoionization Study of the Formation of the Simplest Polycyclic Aromatic Hydrocarbon: Naphthalene (C ₁₀ H ₈). <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 2620-2626.	4.6	57
101	Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates III: Butylbenzene Isomers (n-, s-, and t-C ₁₄ H ₁₀). <i>Journal of Physical Chemistry A</i> , 2018, 122, 3980-4001.	2.5	16
102	Quantum-Chemical Calculations of the Primary Reactions of Thermal Decomposition of Cyclopentadienone. <i>Combustion, Explosion and Shock Waves</i> , 2018, 54, 9-15.	0.8	1
103	Combined Experimental and Computational Investigation of the Elementary Reaction of Ground State Atomic Carbon (C(³ P _j)) with Pyridine (C ₅ H ₅ N): T _j = 0.784314 ± 0.00014 K. <i>Journal of Physical Chemistry A</i> , 2018, 122, 3128-3139.	2.5	7
104	Reaction mechanism, rate constants, and product yields for the oxidation of Cyclopentadienyl and embedded five-member ring radicals with hydroxyl. <i>Combustion and Flame</i> , 2018, 187, 147-164.	5.2	24
105	Raman spectra of thiolated arsenicals with biological importance. <i>Talanta</i> , 2018, 179, 520-530.	5.5	9
106	Detailed, sterically-resolved modeling of soot oxidation: Role of O atoms, interplay with particle nanostructure, and emergence of inner particle burning. <i>Combustion and Flame</i> , 2018, 188, 284-306.	5.2	81
107	Kinetics of C ₁₀ H ₇ Br Pyrolysis. <i>Bulletin of the Lebedev Physics Institute</i> , 2018, 45, 314-317.	0.6	1
108	Rate constants for collision-induced emission of O ₂ (a ¹ Δ ^g) with He, Ne, Ar, Kr, N ₂ , CO ₂ and SF ₆ as collisional partners. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 29677-29683.	2.8	3

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109	Potential Energy Surface for Oxidation of Indenyl C ₉ H ₇ . Bulletin of the Lebedev Physics Institute, 2018, 45, 291-294.	0.6	1
110	Theoretical Calculation of Products Distribution in the Reaction of Atomic Carbon with Pyridine. Bulletin of the Lebedev Physics Institute, 2018, 45, 299-302.	0.6	0
111	Low-temperature formation of polycyclic aromatic hydrocarbons in Titan's atmosphere. Nature Astronomy, 2018, 2, 973-979.	10.1	72
112	Functional Relationships between Kinetic, Flow, and Geometrical Parameters in a High-Temperature Chemical Microreactor. Journal of Physical Chemistry A, 2018, 122, 8819-8827.	2.5	27
113	A Theoretical Study of Pyrolysis of <i>exo</i> -Tetrahydrodicyclopentadiene and Its Primary and Secondary Unimolecular Decomposition Products. Journal of Physical Chemistry A, 2018, 122, 4920-4934.	2.5	28
114	O ₂ (b ¹ g ⁺) Removal by H ₂ , CO, N ₂ O, CH ₄ , and C ₂ H ₄ in the 300–800 K Temperature Range. Journal of Physical Chemistry A, 2018, 122, 5283-5288.	2.5	5
115	A Combined Experimental and Computational Study on the Reaction Dynamics of the 1-Propynyl (CH ₃ CC≡C)–Acetylene (HCCH) System and the Formation of Methylidyne (CH ₃ CCCCH). Journal of Physical Chemistry A, 2018, 122, 6663-6672.	2.5	12
116	Vibrationally Excited Ozone Relaxation by CO. Bulletin of the Lebedev Physics Institute, 2018, 45, 67-70.	0.6	0
117	Fundamental study of the ultrasonic induced degradation of the popular antihistamine, diphenhydramine (DPH). Water Research, 2018, 144, 265-273.	11.3	15
118	Bimolecular Reaction Dynamics in the Phenyl–Silane System: Exploring the Prototype of a Radical Substitution Mechanism. Journal of Physical Chemistry Letters, 2018, 9, 5135-5142.	4.6	3
119	1,3,5-Tris-(4-(iso-propyl)-phenylsulfamoylmethyl)benzene as a potential Am(III) extractant: experimental and theoretical study of Sm(III) complexation and extraction and theoretical correlation with Am(III). Molecular Physics, 2018, 116, 2719-2727.	1.7	2
120	Combined Experimental and Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates. I. <i>n</i> -Decane (<i>n</i> -C ₁₀ H ₂₂). Journal of Physical Chemistry A, 2017, 121, 1261-1280.	2.5	34
121	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
122	Combined Experimental and Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates. II: <i>n</i> -Dodecane (<i>n</i> -C ₁₂ H ₂₆). Journal of Physical Chemistry A, 2017, 121, 1281-1297.	2.5	26
123	A vacuum ultraviolet photoionization study on high-temperature decomposition of JP-10 (<i>exo</i> -tetrahydrodicyclopentadiene). Physical Chemistry Chemical Physics, 2017, 19, 15780-15807.	2.8	38
124	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
125	Reaction mechanism and product branching ratios of the CH + C ₃ H ₄ reactions: a theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 14543-14554.	2.8	23
126	A Free-Radical Pathway to Hydrogenated Phenanthrene in Molecular Clouds—Low Temperature Growth of Polycyclic Aromatic Hydrocarbons. ChemPhysChem, 2017, 18, 1971-1976.	2.1	12

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127	HACA's Heritage: A Free-Radical Pathway to Phenanthrene in Circumstellar Envelopes of Asymptotic Giant Branch Stars. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 4515-4519.	13.8	48
128	HACA's Heritage: A Free-Radical Pathway to Phenanthrene in Circumstellar Envelopes of Asymptotic Giant Branch Stars. <i>Angewandte Chemie</i> , 2017, 129, 4586-4590.	2.0	20
129	$O_2(b^1\Sigma_g^+)$ Quenching by O_2 , CO_2 , H_2O , and N_2 at Temperatures of 300–800 K. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7343-7348.	2.5	12
130	Kinetic, product, and computational studies of the ultrasonic induced degradation of 4-methylcyclohexanemethanol (MCHM). <i>Water Research</i> , 2017, 126, 164-171.	11.3	19
131	Gas-Phase Synthesis of the Elusive Cyclooctatetraenyl Radical (C_8H_7) via Triplet Aromatic Cyclooctatetraene (C_8H_8) and Non-Aromatic Cyclooctatriene (C_8H_8) Intermediates. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 13655-13660.	13.8	2
132	Gas-Phase Synthesis of the Elusive Cyclooctatetraenyl Radical (C_8H_7) via Triplet Aromatic Cyclooctatetraene (C_8H_8) and Non-Aromatic Cyclooctatriene (C_8H_8) Intermediates. <i>Angewandte Chemie</i> , 2017, 129, 13843-13848.	2.0	3
133	Rate constants for H abstraction from benzo(a)pyrene and chrysene: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 25401-25413.	2.8	37
134	Remarkably selective NH_4^+ binding and fluorescence sensing by tripodal tris(pyrazolyl) receptors derived from 1,3,5-triethylbenzene: structural and theoretical insights on the role of ion pairing. <i>New Journal of Chemistry</i> , 2017, 41, 14835-14838.	2.8	15
135	Kinetics of the $CH_3 + C_5H_5$ Reaction: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2017, 121, 9191-9200.	2.5	27
136	Temperature- and pressure-dependent rate coefficients for the HACA pathways from benzene to naphthalene. <i>Proceedings of the Combustion Institute</i> , 2017, 36, 919-926.	3.9	115
137	Product channels of the reactions of $Rb(62P)$ with H_2 , CH_4 and C_2H_6 . <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2017, 196, 46-52.	2.3	2
138	Analysis of Geologically Relevant Metal Porphyrins Using Trapped Ion Mobility Spectrometry–Mass Spectrometry and Theoretical Calculations. <i>Energy & Fuels</i> , 2016, 30, 10341-10347.	5.1	21
139	PENTACARBON DIOXIDE (C_5O_2) FORMATION AND ITS ROLE AS A TRACER OF SOLAR SYSTEM EVOLUTION. <i>Astrophysical Journal Letters</i> , 2016, 818, L30.	8.3	10
140	Oxidation of the <i>p</i> -Tolyl Radical by Molecular Oxygen under Single-Collision Conditions: Formation of the <i>p</i> -Toloxyl Radical. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 5121-5127.	4.6	5
141	Ab initio calculations of transition dipole moments of $(O_2)^+_2$ complex. , 2016, , .		0
142	Hydrogen-Abstraction/Acetylene-Addition Exposed. <i>Angewandte Chemie</i> , 2016, 128, 15207-15211.	2.0	7
143	Hydrogen-Abstraction/Acetylene-Addition Exposed. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 14983-14987.	13.8	48
144	Pressure-dependent rate constants for PAH growth: formation of indene and its conversion to naphthalene. <i>Faraday Discussions</i> , 2016, 195, 637-670.	3.2	76

#	ARTICLE	IF	CITATIONS
145	On the Formation of N ₃ H ₃ Isomers in Irradiated Ammonia Bearing Ices: Triazene (H ₂ NNNH) or Triimide (HNHNNH). <i>ChemPhysChem</i> , 2016, 17, 2726-2735.	2.1	21
146	Reaction Mechanism and Product Branching Ratios of the CH + C ₃ H ₆ Reaction: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1800-1812.	2.5	20
147	Removal of Rb(6 ² P) by H ₂ , CH ₄ , and C ₂ H ₆ . <i>Optics Letters</i> , 2016, 41, 669.	3.3	11
148	Luminescence of the (O ₂ (<i>a</i> ¹ _g)) ₂ collisional complex in the temperature range of 90-315 K: Experiment and theory. <i>Journal of Chemical Physics</i> , 2015, 143, 244315.	3.0	7
149	Formation of resonantly stabilised free radicals via the reactions of atomic carbon, dicarbon, and tricarbon with unsaturated hydrocarbons: theory and crossed molecular beams experiments. <i>International Reviews in Physical Chemistry</i> , 2015, 34, 461-514.	2.3	40
150	Formation of 5- and 6-methyl-1H-indene (C ₁₀ H ₁₀) via the reactions of the para-tolyl radical (C ₆ H ₄ CH ₃) with allene (H ₂ CCCH ₂) and methylacetylene (HCCCH ₃) under single collision conditions. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10510-10519.	2.8	11
151	Formation of 2- and 1-methyl-1,4-dihydronaphthalene isomers via the crossed beam reactions of phenyl radicals (C ₆ H ₅) with isoprene (CH ₂ C(CH ₃)CHCH ₂) and 1,3-pentadiene (CH ₂ CHCHCH ₂). <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 530-540.	2.8	9
152	Reaction Dynamics in Astrochemistry: Low-Temperature Pathways to Polycyclic Aromatic Hydrocarbons in the Interstellar Medium. <i>Annual Review of Physical Chemistry</i> , 2015, 66, 43-67.	10.8	109
153	Rate coefficients and product branching ratios for the oxidation of phenyl and naphthyl radicals: A theoretical RRKM-ME study. <i>Proceedings of the Combustion Institute</i> , 2015, 35, 1861-1869.	3.9	34
154	Toward the Oxidation of the Phenyl Radical and Prevention of PAH Formation in Combustion Systems. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7145-7154.	2.5	41
155	Reaction mechanism and rate constants of the CH+CH ₄ reaction: a theoretical study. <i>Molecular Physics</i> , 2015, 113, 1865-1872.	1.7	12
156	Oxidation of Graphene-Edge Six- and Five-Member Rings by Molecular Oxygen. <i>Journal of Physical Chemistry A</i> , 2015, 119, 7528-7547.	2.5	46
157	GAS PHASE SYNTHESIS OF (ISO)QUINOLINE AND ITS ROLE IN THE FORMATION OF NUCLEOBASES IN THE INTERSTELLAR MEDIUM. <i>Astrophysical Journal</i> , 2015, 803, 53.	4.5	29
158	A crossed molecular beam and ab initio study on the formation of 5- and 6-methyl-1,4-dihydronaphthalene (C ₁₁ H ₁₂) via the reaction of meta-tolyl (C ₇ H ₇) with 1,3-butadiene (C ₄ H ₆). <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 7699-7706.	2.8	7
159	On the formation of ethynylbiphenyl (C ₁₄ D ₅ H ₅ ; C ₆ D ₅ C ₆ H ₄ CCH) isomers in the reaction of D ₅ -phenyl radicals (C ₆ D ₅ ; X ₂ A ₁) with phenylacetylene (C ₆ H ₅ C ₂ H; X ₁ A ₁) under single collision conditions. <i>Chemical Physics Letters</i> , 2014, 595-596, 230-236.	2.6	13
160	Roaming dynamics in radical addition-elimination reactions. <i>Nature Communications</i> , 2014, 5, 4064.	12.8	47
161	Understanding the chemical dynamics of the reactions of dicarbon with 1-butyne, 2-butyne, and 1,2-butadiene toward the formation of resonantly stabilized free radicals. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 12150-12163.	2.8	9
162	Reaction dynamics of the 4-methylphenyl radical (C ₆ H ₄ CH ₃ ; p-tolyl) with isoprene (C ₅ H ₈) toward the formation of dimethyldihydronaphthalenes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16805-16814.	2.8	6

#	ARTICLE	IF	CITATIONS
163	The role of isovalency in the reactions of the cyano (CN), boron monoxide (BO), silicon nitride (SiN), and ethynyl (C ₂ H) radicals with unsaturated hydrocarbons acetylene (C ₂ H ₂) and ethylene (C ₂ H ₄). <i>Chemical Society Reviews</i> , 2014, 43, 2701-2713.	38.1	27
164	Reaction Mechanism and Product Branching Ratios of the CH + C ₃ H ₈ Reaction: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9080-9086.	2.5	12
165	Directed Gas-Phase Formation of the Ethynylsulfidoboron Molecule. <i>Journal of the American Chemical Society</i> , 2014, 136, 8387-8392.	13.7	5
166	Crossed Beam Reactions of the Phenyl (C ₆ H ₅ ; X ² A ₁) and Phenyl- <i>d</i> ₅ Radical (C ₆ D ₅ ; X ² A ₁) with 1,2-Butadiene (H ₂ CCCHCH ₃ ; X ¹ Å ²). <i>Journal of Physical Chemistry A</i> , 2014, 118, 4372-4381.	2.5	5
167	Reaction Dynamics of the 4-Methylphenyl Radical (<i>p</i> -Tolyl) with 1,2-Butadiene (1-Methylallene): Are Methyl Groups Purely Spectators?. <i>Journal of Physical Chemistry A</i> , 2014, 118, 6181-6190.	2.5	7
168	Dynamics of Chlorine Atom Reactions with Hydrocarbons: Insights from Imaging the Radical Product in Crossed Beams. <i>Journal of Physical Chemistry A</i> , 2014, 118, 9281-9295.	2.5	27
169	An experimental and theoretical investigation of the formation of C ₇ H ₇ isomers in the bimolecular reaction of dicarbon molecules with 1,3-pentadiene. <i>Chemical Physics Letters</i> , 2014, 607, 92-99.	2.6	7
170	Gas-Phase Synthesis of the Benzyl Radical (C ₆ H ₅ CH ₂). <i>Angewandte Chemie - International Edition</i> , 2014, 53, 4608-4613.	13.8	22
171	A Combined Experimental and Theoretical Study on the Gas-Phase Synthesis of Toluene under Single Collision Conditions. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 7186-7189.	13.8	13
172	A VUV photoionization study of the multichannel reaction of phenyl radicals with 1,3-butadiene under combustion relevant conditions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 341-347.	2.8	49
173	Ionization/dissociation processes of methyl-substituted derivatives of cyclopentanone in intense femtosecond laser field. <i>Chemical Physics Letters</i> , 2013, 586, 21-28.	2.6	10
174	Formation Mechanism of Polycyclic Aromatic Hydrocarbons beyond the Second Aromatic Ring. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4794-4816.	2.5	146
175	A Combined Crossed Beam and Ab Initio Investigation of the Gas Phase Reaction of Dicarbon Molecules (C ₂ ; X ¹ Î ^g + C ³ u) with Propene (C ₃ H ₆ ; X ¹ Å ²): Identification of the Resonantly Stabilized Free Radicals 1- and 3-Vinylpropargyl. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11783-11793.	2.5	16
176	H/D kinetic isotope effect in HCOOH cis-Å ^{trans} conversion of formic acid in noble gas matrices. <i>Chemical Physics Letters</i> , 2013, 574, 47-50.	2.6	2
177	Low-Temperature Mechanisms for the Formation of Substituted Azanaphthalenes through Consecutive CN and C ₂ H Additions to Styrene and <i>N</i> -Methylenebenzamine: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2013, 135, 7251-7263.	13.7	14
178	Gas-Phase Synthesis of Phenyl Oxoborane (C ₆ H ₅ BO) via the Reaction of Boron Monoxide with Benzene. <i>Journal of Organic Chemistry</i> , 2013, 78, 11896-11900.	3.2	15
179	Theoretical Investigation of the Mechanism and Product Branching Ratios of the Reactions of Cyano Radical with 1- and 2-Butyne and 1,2-Butadiene. <i>Journal of Physical Chemistry A</i> , 2013, 117, 741-755.	2.5	14
180	A Crossed Beam and ab Initio Investigation on the Formation of Boronyldiacetylene (HCCCC ¹¹ BO; <i>X</i> ¹ Î ⁺) via the Reaction of the Boron Monoxide Radical (C ¹¹ BO; <i>X</i> ² Î ⁺) with Diacetylene (C ₄ H ₂ ; <i>X</i> ¹ Î ^g + C ⁺). <i>Journal of Physical Chemistry A</i> , 2013, 117, 8189-8198.	2.5	6

#	ARTICLE	IF	CITATIONS
181	Low temperature formation of naphthalene and its role in the synthesis of PAHs (Polycyclic Aromatic) Tj ETQq1 1 0.784314 rgBT /Ove United States of America, 2012, 109, 53-58.	7.1	192
182	AN EXPERIMENTAL AND THEORETICAL STUDY OF THE IONIZATION ENERGIES OF $\text{SiC}_{2x}\text{H}_x$ ($x = 0, 1, 2$) ISOMERS. <i>Astrophysical Journal</i> , 2012, 761, 178.	4.5	30
183	Gas-Phase Synthesis of the Silaisocynoethylene Molecule ($\text{C}_2\text{H}_3\text{NSi}$). <i>Journal of Organic Chemistry</i> , 2012, 77, 8574-8580.	3.2	6
184	Separation mechanism of chiral impurities, ephedrine and pseudoephedrine, found in amphetamine-type substances using achiral modifiers in the gas phase. <i>Analytical and Bioanalytical Chemistry</i> , 2012, 404, 2407-2416.	3.7	14
185	PAH Formation under Single Collision Conditions: Reaction of Phenyl Radical and 1,3-Butadiene to Form 1,4-Dihydronaphthalene. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4248-4258.	2.5	56
186	Crossed beam reaction of phenyl and D5-phenyl radicals with propene and deuterated counterparts competing atomic hydrogen and methyl loss pathways. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 720-729.	2.8	23
187	Reaction Mechanism of Naphthyl Radicals with Molecular Oxygen. 1. Theoretical Study of the Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2012, 116, 1571-1585.	2.5	24
188	On the formation of polyacetylenes and cyanopolyacetylenes in Titan's atmosphere and their role in astrobiology. <i>Chemical Society Reviews</i> , 2012, 41, 5490.	38.1	40
189	On the formation of phenyldiacetylene ($\text{C}_6\text{H}_5\text{CCCH}$) and D5-phenyldiacetylene ($\text{C}_6\text{D}_5\text{CCCH}$) studied under single collision conditions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 2997.	2.8	10
190	Reaction of Phenyl Radical with Propylene as a Possible Source of Indene and Other Polycyclic Aromatic Hydrocarbons: An Ab Initio/RRKM-ME Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4176-4191.	2.5	37
191	Synthesis of the Silaisocynoacetylene Molecule. <i>Journal of the American Chemical Society</i> , 2012, 134, 13896-13901.	13.7	11
192	Investigation of reactions postulated to occur during inhibition of ribonucleotide reductases by 2-azido-2-deoxynucleotides. <i>Tetrahedron</i> , 2012, 68, 5655-5667.	1.9	1
193	Product branching ratios in photodissociation of phenyl radical: A theoretical ab initio/Rice-Ramsperger-Kassel-Marcus study. <i>Journal of Chemical Physics</i> , 2012, 136, 234305.	3.0	14
194	On the electron-induced isotope fractionation in low temperature O_2 / O_3 as a case study. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 421-427.	2.8	13
195	A Crossed Molecular Beams and Ab Initio Study on the Formation of C_6H_3 Radicals. An Interface between Resonantly Stabilized and Aromatic Radicals. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10251-10258.	2.5	9
196	Reactions of C_2H with 1- and 2-Butynes: An Ab Initio/RRKM Study of the Reaction Mechanism and Product Branching Ratios. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2196-2207.	2.5	13
197	A VUV Photoionization Study of the Formation of the Indene Molecule and Its Isomers. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1731-1735.	4.6	79
198	A CROSSED MOLECULAR BEAM, LOW-TEMPERATURE KINETICS, AND THEORETICAL INVESTIGATION OF THE REACTION OF THE CYANO RADICAL (CN) WITH 1,3-BUTADIENE (C_4H_6). A ROUTE TO COMPLEX NITROGEN-BEARING MOLECULES IN LOW-TEMPERATURE EXTRATERRESTRIAL ENVIRONMENTS. <i>Astrophysical Journal</i> , 2011, 742, 26.	4.5	45

#	ARTICLE	IF	CITATIONS
199	An ab initio/RRKM study of the reaction mechanism and product branching ratios of the reactions of ethynyl radical with 1,2-butadiene. <i>Chemical Physics Letters</i> , 2011, 518, 29-37.	2.6	5
200	On the Formation of Resonantly Stabilized C ₅ H ₃ Radicals—A Crossed Beam and Ab Initio Study of the Reaction of Ground State Carbon Atoms with Vinylacetylene. <i>Journal of Physical Chemistry A</i> , 2011, 115, 593-601.	2.5	11
201	Indene Formation under Single-Collision Conditions from the Reaction of Phenyl Radicals with Allene and Methylacetylene—A Crossed Molecular Beam and Ab Initio Study. <i>Chemistry - an Asian Journal</i> , 2011, 6, 3035-3047.	3.3	45
202	ON THE FORMATION OF ORTHO-BENZYNE (o-C ₆ H ₄) UNDER SINGLE COLLISION CONDITIONS AND ITS ROLE IN INTERSTELLAR CHEMISTRY. <i>Astrophysical Journal</i> , 2011, 728, 141.	4.5	34
203	Modeling of the ribonucleotide reductases substrate reaction. Hydrogen atom abstraction by a thiyl free radical and detection of the ribosyl-based carbon radical by pulse radiolysis. <i>Collection of Czechoslovak Chemical Communications</i> , 2011, 76, 1223-1238.	1.0	6
204	Formation of benzene in the interstellar medium. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 452-457.	7.1	131
205	Addition of one and two units of C ₂ H to styrene: A theoretical study of the C ₁₀ H ₉ and C ₁₂ H ₉ systems and implications toward growth of polycyclic aromatic hydrocarbons at low temperatures. <i>Journal of Chemical Physics</i> , 2011, 134, 024302.	3.0	17
206	COSMIC-RAY-MEDIATED FORMATION OF BENZENE ON THE SURFACE OF SATURN'S MOON TITAN. <i>Astrophysical Journal</i> , 2010, 718, 1243-1251.	4.5	42
207	PHOTODISSOCIATION OF THE DIACETYLENE DIMER AND IMPLICATIONS FOR HYDROCARBON GROWTH IN TITAN'S ATMOSPHERE. <i>Astrophysical Journal</i> , 2010, 714, 1249-1255.	4.5	11
208	AN EXPERIMENTAL AND THEORETICAL STUDY ON THE IONIZATION ENERGIES OF POLYYNES (H-(C≡C) _n -H; n = 1-9). <i>Astrophysical Journal</i> , 2010, 719, 1884-1889.	4.5	52
209	Effect of the Medium on Intramolecular H-Atom Tunneling: Cis-Trans Conversion of Formic Acid in Solid Matrixes of Noble Gases. <i>Journal of Physical Chemistry B</i> , 2010, 114, 17102-17112.	2.6	6
210	On the ionization energies of C ₄ H ₃ isomers. <i>Chemical Physics Letters</i> , 2010, 485, 281-285.	2.6	21
211	Ab Initio/RRKM-ME Study on the Mechanism and Kinetics of the Reaction of Phenyl Radical with 1,2-Butadiene. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7682-7692.	2.5	13
212	UV Photodissociation of Ethylamine Cation: A Combined Experimental and Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 13296-13302.	2.5	9
213	Spectroscopic and Thermochemical Consequences of Site-Specific H-Atom Addition to Naphthalene. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6255-6262.	2.5	35
214	On the Directed Gas Phase Synthesis of the Imidoborane Molecule (HNBH) — An Isoelectronic Molecule of Acetylene (HCCH). <i>Journal of Physical Chemistry A</i> , 2010, 114, 12148-12154.	2.5	14
215	Hydroxyl Radical Substitution in Halogenated Carbonyls: Oxalic Acid Formation. <i>Journal of Physical Chemistry A</i> , 2010, 114, 2806-2820.	2.5	6
216	Formation of the Phenyl Radical [C ₆ H ₅ (X ² A ₁)] under Single Collision Conditions: A Crossed Molecular Beam and ab Initio Study. <i>Journal of the American Chemical Society</i> , 2010, 132, 2672-2683.	13.7	38

#	ARTICLE	IF	CITATIONS
217	An ab initio/RRKM study of the reaction mechanism and product branching ratios of the reactions of ethynyl radical with allene and methylacetylene. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 2606.	2.8	24
218	Isomer specific spectroscopy of C ₁₀ H _n , n = 8–12: Exploring pathways to naphthalene in Titan's atmosphere. <i>Faraday Discussions</i> , 2010, 147, 231.	3.2	23
219	Untangling the chemical evolution of Titan's atmosphere and surface—from homogeneous to heterogeneous chemistry. <i>Faraday Discussions</i> , 2010, 147, 429.	3.2	118
220	Crossed Molecular Beam Study on the Formation of Phenylacetylene and Its Relevance to Titan's Atmosphere. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5256-5262.	2.5	18
221	Mechanisms of formation of nitrogen-containing polycyclic aromatic compounds in low-temperature environments of planetary atmospheres: A theoretical study. <i>Faraday Discussions</i> , 2010, 147, 479.	3.2	34
222	Chemical dynamics of triacetylene formation and implications to the synthesis of polyynes in Titan's atmosphere. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 16078-16083.	7.1	39
223	Matrix reorganization with intramolecular tunneling of H atom: Formic acid in Ar matrix. <i>Journal of Chemical Physics</i> , 2009, 130, 144502.	3.0	14
224	A crossed beams and <i>ab initio</i> investigation on the formation of cyanodiacetylene in the reaction of cyano radicals with diacetylene. <i>Journal of Chemical Physics</i> , 2009, 130, 234308.	3.0	13
225	Quantum chemical modeling of photoadsorption properties of the nitrogen vacancy point defect in diamond. <i>Journal of Computational Chemistry</i> , 2009, 30, 119-131.	3.3	36
226	On the calculation of the dissociation rate constant of the water dimer by the ab initio anharmonic RRKM theory. <i>Chemical Physics Letters</i> , 2009, 470, 210-214.	2.6	33
227	Reaction dynamics of the phenyl radical with 1,2-butadiene. <i>Chemical Physics Letters</i> , 2009, 474, 51-56.	2.6	12
228	Reaction dynamics of the phenyl radical (C ₆ H ₅) with 1-butyne (HCCC ₂ H ₅) and 2-butyne (CH ₃ CCCH ₃). <i>Chemical Physics Letters</i> , 2009, 481, 46-53.	2.6	6
229	A Theoretical Study of the Reaction Mechanism and Product Branching Ratios of C ₂ H + C ₂ H ₄ and Related Reactions on the C ₄ H ₅ Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11112-11128.	2.5	21
230	Formation of the 1,3,5-Hexatriynyl Radical (C ₆ H(X ²)) via the Crossed Beams Reaction of Dicarbon (C ₂ (X ¹)g ⁺ /a ³ u), with Diacetylene (C ₄ H ₂ (X ¹)g ⁺), <i>Journal of Physical Chemistry A</i> , 2009, 113, 1210-1217.	2.5	19
231	Quantum Chemical Modeling of Photoabsorption Properties of Two- and Three-Nitrogen Vacancy Point Defects in Diamond. <i>Journal of Physical Chemistry C</i> , 2009, 113, 10432-10440.	3.1	25
232	Ionization and Dissociation Processes of Pyrrolidine in Intense Femtosecond Laser Field. <i>Journal of Physical Chemistry C</i> , 2009, 113, 11805-11815.	3.1	22
233	Crossed Molecular Beams Study on the Formation of Vinylacetylene in Titan's Atmosphere. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11167-11173.	2.5	25
234	UV Photodissociation of Cyanoacetylene: A Combined Ion Imaging and Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11182-11186.	2.5	10

#	ARTICLE	IF	CITATIONS
235	An ab Initio/Rice-Ramsperger-Kassel-Marcus Study of the Reactions of Propenols with OH. Mechanism and Kinetics of H Abstraction Channels. Journal of Physical Chemistry A, 2009, 113, 10667-10677.	2.5	19
236	Dissociation Rate Constant of the Hydrogen Fluoride Dimer by the ab Initio Anharmonic RRKM Theory. Journal of Physical Chemistry A, 2009, 113, 14664-14669.	2.5	22
237	Can the $C_{10}H_9 + C_{10}H_9 \rightarrow C_{10}H_{10} + C_{10}H_8 + H_2$ Reaction Produce Naphthalene? An Ab Initio/RRKM Study. Journal of Physical Chemistry A, 2009, 113, 9825-9833.	2.5	68
238	A CROSSED MOLECULAR BEAMS STUDY ON THE FORMATION OF THE EXOTIC CYANOETHYNYL RADICAL IN TITAN'S ATMOSPHERE. Astrophysical Journal, 2009, 701, 1797-1803.	4.5	18
239	Chemistry of Energetically Activated Cumulenes—From Allene (H_2CCCH_2) to Hexapentaene ($H_2CCCCCH_2$). ChemPhysChem, 2008, 9, 350-369.	2.1	42
240	First detection of the Cs symmetric isomer of carbon hexaoxide (CO ₆) at 10K. Chemical Physics Letters, 2008, 450, 312-317.	2.6	12
241	Theoretical study of the reaction mechanism of ethynyl radical with benzene and related reactions on the C ₈ H ₇ potential energy surface. Chemical Physics Letters, 2008, 459, 54-59.	2.6	22
242	Potential energy surfaces for the lowest excited states of the nitrogen-vacancy point defects in diamonds: A quantum chemical study. Chemical Physics Letters, 2008, 462, 251-255.	2.6	7
243	On the formation of higher carbon oxides in extreme environments. Chemical Physics Letters, 2008, 465, 1-9.	2.6	17
244	H elimination and metastable lifetimes in the UV photoexcitation of diacetylene. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12713-12718.	7.1	22
245	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
246	Theoretical study of multiphoton ionization of cyclohexadienes and unimolecular decomposition of their mono- and dications. Physical Chemistry Chemical Physics, 2008, 10, 2321.	2.8	12
247	An Ab Initio G3-Type/Statistical Theory Study of the Formation of Indene in Combustion Flames. II. The Pathways Originating from Reactions of Cyclic C ₅ SpeciesCyclopentadiene and Cyclopentadienyl Radicals. Journal of Physical Chemistry A, 2008, 112, 700-716.	2.5	57
248	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
249	Theoretical study of the C ₆ H ₃ potential energy surface and rate constants and product branching ratios of the $C_2H(\Sigma^+)+C_4H_2(\Sigma^+)$ and $C_4H(\Sigma^+)+C_2H_2(\Sigma^+)$ reactions. Journal of Chemical Physics, 2008, 128, 214301.	3.0	30
250	Theoretical study of unimolecular decomposition of allene cations. Journal of Chemical Physics, 2008, 129, 224311.	3.0	50
251	Chapter 4 Ab Initio Calculations of Electronic Transitions and Photoabsorption and Photoluminescence Spectra of Silica and Germania Nanoparticles. Thin Films and Nanostructures, 2007, 34, 67-120.	0.1	3
252	Prediction of product branching ratios in the $C(P_3)+C_2H_2 \rightarrow C_3H+H \rightarrow C_3H+H \rightarrow C_3+H_2$ 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

#	ARTICLE	IF	CITATIONS
271	A crossed molecular beams study on the formation and energetics of the resonantly stabilized free $i\text{-C}_4\text{H}_3(\text{X}_2\text{A}\hat{\epsilon}^2)$ radical and its isotopomers. <i>Chemical Physics</i> , 2007, 335, 95-108.	1.9	12
272	Computational modeling of biodegradable blends of starch amylose and poly-propylene carbonate. <i>Polymer</i> , 2007, 48, 3893-3901.	3.8	27
273	Reaction dynamics of carbon-bearing radicals in circumstellar envelopes of carbon stars. <i>Faraday Discussions</i> , 2006, 133, 245.	3.2	103
274	Ab initio and RRKM study of photodissociation of azulene cation. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 1404.	2.8	44
275	Unimolecular Decomposition of Chemically Activated Pentatetraene ($\text{H}_2\text{CCCCCH}_2$) Intermediates: A Crossed Beams Study of Dicarbon Molecule Reactions with Allene. <i>Journal of Physical Chemistry A</i> , 2006, 110, 10699-10707.	2.5	19
276	Potential Energy Surface and Product Branching Ratios for the Reaction of Dicarbon, $\text{C}_2(\text{X}\hat{\epsilon}^g+)$, with Methylacetylene, $\text{CH}_3\text{CCH}(\text{X}_1\text{A}_1)$: An Ab Initio/RRKM Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2421-2433.	2.5	24
277	Chemical Dynamics of the Formation of the 1,3-Butadiynyl Radical ($\text{C}_4\text{H}(\text{X}_2\hat{\epsilon}^g+)$) and Its Isotopomers. <i>Journal of Physical Chemistry A</i> , 2006, 110, 11265-11278.	2.5	33
278	Investigating the Formation of Intermediates in the Reactions of Carbon Dioxide (CO_2) with Suprathermal Oxygen and Nitrogen Atoms. <i>AIP Conference Proceedings</i> , 2006, .	0.4	0
279	Absorption Cross Sections of NH_3 , NH_2D , NHD_2 , and ND_3 in the Spectral Range 140-220 nm and Implications for Planetary Isotopic Fractionation. <i>Astrophysical Journal</i> , 2006, 647, 1535-1542.	4.5	65
280	Acetylene Elimination in Photodissociation of Neutral Azulene and Its Cation: An Ab Initio and RRKM Study. <i>Journal of the Chinese Chemical Society</i> , 2006, 53, 161-168.	1.4	10
281	Understanding the Kinetics and Dynamics of Radiation-Induced Reaction Pathways in Carbon Monoxide Ice at 10 K. <i>Astrophysical Journal, Supplement Series</i> , 2006, 163, 184-206.	7.7	127
282	Theoretical study of isomerism, structure, and stability of dimers of C-doped aluminide clusters (C@Al_2) ₂ and (C@Al_2)(L@Al_2) (L = Si, Ge). <i>Russian Journal of Inorganic Chemistry</i> , 2006, 51, 599-607.	1.3	3
283	Quantum-chemical study of crystal formation of supramolecular silver compounds with trans-1,2-Bis(4-pyridyl)ethylene and their electronic absorption spectra. <i>Russian Journal of Inorganic Chemistry</i> , 2006, 51, 925-940.	1.3	2
284	Theoretical study of host-guest interaction and its manifestations in the properties of model endohedral fullerenes with small covalent molecules inside the C_n and C_nH_m cages. <i>Russian Journal of Inorganic Chemistry</i> , 2006, 51, S1-S27.	1.3	8
285	Identification of the D_{3h} Isomer of Carbon Trioxide (CO_3) and Its Implications for Atmospheric Chemistry. <i>ChemPhysChem</i> , 2006, 7, 2508-2513.	2.1	38
286	Ab initio/Rice-Ramsperger-Kassel-Marcus study of the singlet C_4H_4 potential energy surface and of the reactions of $\text{C}_2(\text{X}\hat{\epsilon}^g+)$ with $\text{C}_4\text{H}_4(\text{X}_1\text{g}+1)$ and $\text{C}(\text{D}1)$ with C_3H_4 (allene and methylacetylene). <i>Journal of Chemical Physics</i> , 2006, 125, 133113.	3.0	33
287	A Combined Experimental and Theoretical Study of the Reaction of Dicarbon (C_2) with D_1 -Acetylene (HCCD): Possible Mechanisms for Deuterium Enrichment in the Interstellar D_1 -Butadiynyl Radical, $\text{CCCCD}(\text{X}_2\hat{\epsilon}^g+)$. <i>Astrophysical Journal</i> , 2006, 653, 1577-1582.	4.5	7
288	A Computational Study of End-Group Conformational Energy Barriers in Carotenoids. <i>FASEB Journal</i> , 2006, 20, A1060.	0.5	0

#	ARTICLE	IF	CITATIONS
289	Investigating the Mechanism for the Formation of Nitrous Oxide [N ₂ O(X ¹ Σ ⁺)] in Extraterrestrial Ices. <i>Astrophysical Journal</i> , 2005, 624, 436-447.	4.5	49
290	An improved potential energy surface for the F+H ₂ reaction. <i>Chemical Physics</i> , 2005, 308, 259-266.	1.9	40
291	Potential energy surface and product branching ratios for the reaction of F(2P) with the methyl radical: An ab initio/RRKM study. <i>Chemical Physics Letters</i> , 2005, 406, 60-74.	2.6	9
292	Bond lengths and diameters of armchair single wall carbon nanotubes. <i>Chemical Physics Letters</i> , 2005, 407, 266-271.	2.6	96
293	Fragmentation of heme and hemin+ with sequential loss of carboxymethyl groups: A DFT and mass-spectrometry study. <i>Chemical Physics Letters</i> , 2005, 415, 362-369.	2.6	37
294	Potential energy surfaces in Coulomb explosion of polyatomic molecules: Benzene and cyclohexane trications and acetylene dication. <i>International Journal of Quantum Chemistry</i> , 2005, 102, 506-519.	2.0	19
295	Temperature and pressure dependences of tunneling rate constant: Density-functional theory potential-energy surface for H-atom transfer in the fluorene-acridine system. <i>Journal of Chemical Physics</i> , 2005, 123, 114508.	3.0	12
296	A matrix isolation study of the Cs symmetric OCNO(X ² A [−]) radical. <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 4089.	2.8	16
297	The Reaction of Phenyl Radical with Molecular Oxygen: A G2M Study of the Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6114-6127.	2.5	126
298	Photodissociation of Azulene at 193 nm: Ab Initio and RRKM Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8774-8784.	2.5	27
299	The C ₂ H ₃ + O ₂ Reaction Revisited: Is Multireference Treatment of the Wave Function Really Critical?. <i>Journal of Physical Chemistry A</i> , 2005, 109, 6993-6997.	2.5	18
300	Two-photon vibronic spectroscopy of allene at 7.0–10.5 eV: experiment and theory. <i>Molecular Physics</i> , 2005, 103, 229-248.	1.7	1
301	Hydrogen Abstraction Acetylene Addition and Diels-Alder Mechanisms of PAH Formation: A Detailed Study Using First Principles Calculations. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 908-924.	5.3	141
302	Photodissociation dynamics of pyridine. <i>Journal of Chemical Physics</i> , 2005, 123, 054309.	3.0	38
303	Theoretical study of isomerization and dissociation of acetylene dication in the ground and excited electronic states. <i>Journal of Chemical Physics</i> , 2005, 123, 134320.	3.0	69
304	Photodissociation of benzene under collision-free conditions: An ab initio/Rice-Ramsperger-Kassel-Marcus study. <i>Journal of Chemical Physics</i> , 2004, 120, 7008-7017.	3.0	133
305	Analytic-numerical approach to calculate electronic nonadiabatic coupling terms: Study of the C ₂ H molecule and the H ₂ + H system. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 594-604.	2.0	3
306	Rate constant for H-atom tunneling in the fluorene-acridine system based on DFT potential energy surface. <i>Chemical Physics</i> , 2004, 303, 107-113.	1.9	5

#	ARTICLE	IF	CITATIONS
307	Theoretical study of the reaction mechanism of nitrogen hydrogenation on transition metal oxides (TiO, VO, and CuO). <i>Chemical Physics</i> , 2004, 304, 301-313.	1.9	3
308	Dissociation pathways of cyclohexane trication. <i>Chemical Physics Letters</i> , 2004, 393, 470-477.	2.6	10
309	Reaction mechanism of hydrogenation of carbon dioxide to formic acid in the presence of scandium oxide: a density functional study. <i>Chemical Physics Letters</i> , 2004, 396, 75-82.	2.6	6
310	Ab Initio/RRKM Study of the O(1D) + NH ₃ Reaction: Prediction of Product Branching Ratios. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11644-11650.	2.5	18
311	Theoretical Study of the Reaction Mechanism of BO, B ₂ O ₂ , and BS with H ₂ . <i>Journal of Physical Chemistry A</i> , 2004, 108, 473-483.	2.5	27
312	Theoretical Study of TiO-Catalyzed Hydrogenation of Carbon Dioxide to Formic Acid. <i>Journal of Physical Chemistry A</i> , 2004, 108, 10245-10251.	2.5	9
313	Photoisomerization and Photodissociation of Aniline and 4-Methylpyridine. <i>Journal of the American Chemical Society</i> , 2004, 126, 8760-8768.	13.7	40
314	Untangling the formation of the cyclic carbon trioxide isomer in low temperature carbon dioxide ices. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 735.	2.8	156
315	Theoretical Study of Oxygen Isotope Exchange and Quenching in the O(1D) + CO ₂ Reaction. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7983-7994.	2.5	45
316	Performance of time-dependent density functional and Green functions methods for calculations of excitation energies in radicals and for Rydberg electronic states. <i>Journal of Computational Chemistry</i> , 2003, 24, 692-700.	3.3	13
317	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. <i>Chemistry - A European Journal</i> , 2003, 9, 726-740.	3.3	45
318	A crossed beam and ab initio study of the C ₂ (X ¹ Σ ^{g+} + /a ³ Σ ^u)+C ₂ H ₂ (X ¹ Σ ^{g+}) reactions. <i>Chemical Physics Letters</i> , 2003, 382, 112-119.	2.6	59
319	The Curl "Divergence equations for the electronic non-adiabatic coupling terms: study of the C ₂ H molecule and the H ₂ +H system. <i>Chemical Physics Letters</i> , 2003, 367, 177-185.	2.6	4
320	Absorption cross-section of the C ₂ H molecule: proper treatment of the conical intersection. <i>Chemical Physics Letters</i> , 2003, 372, 1-7.	2.6	14
321	Reaction mechanism of nitrogen hydrogenation in the presence of scandium oxide: a density functional study. <i>Chemical Physics Letters</i> , 2003, 375, 17-25.	2.6	8
322	Theoretical study of the reaction mechanism of boron atom with carbon dioxide. <i>Chemical Physics Letters</i> , 2003, 375, 670-675.	2.6	10
323	Experimental and calculational consequences of phases in molecules with multiple conical intersections. <i>International Journal of Quantum Chemistry</i> , 2003, 92, 135-151.	2.0	8
324	A theoretical study of isomerism in doped aluminum MAI ₂ and MAI ₂ X ₁₂ clusters with 40 and 50 valence electrons Electronic supplementary information (ESI) available: Selected geometric parameters of clusters. See http://www.rsc.org/suppdata/fd/b2/b211114d/ . <i>Faraday Discussions</i> , 2003, 124, 215.	3.2	28

#	ARTICLE	IF	CITATIONS
325	Ab Initio/RRKM Study of the Potential Energy Surface of Triplet Ethylene and Product Branching Ratios of the C(3P) + CH ₄ Reaction. <i>Journal of Physical Chemistry A</i> , 2003, 107, 1788-1796.	2.5	35
326	Potential Energy Surface and Product Branching Ratios for the Reaction of C(3P _j) with the Allyl Radical: An ab Initio/RRKM Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2990-2999.	2.5	9
327	A Combined Quantum Chemistry and RRKM Calculation Predicts the O(1D) + C ₂ H ₆ Reaction Can Produce Water Molecule in a Collision-Free Crossed Molecular Beam Environment. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6986-6994.	2.5	6
328	Photodissociation Dynamics of Fluorobenzene. <i>Journal of the American Chemical Society</i> , 2003, 125, 9814-9820.	13.7	27
329	Reaction Mechanism of N ₂ /H ₂ Conversion to NH ₃ : A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 2865-2874.	2.5	69
330	Azido-Nitrene Is Probably the N ₄ Molecule Observed in Mass Spectrometric Experiments. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5452-5460.	2.5	29
331	Reaction Mechanism of the Synthesis of Ammonia in the N ₂ /H ₂ /BeO and N ₂ /H ₂ /FeO Systems: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5092-5100.	2.5	9
332	Influence of distortion and Duschinsky effects on Marcus-type theories of electron transfer rate. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 4656.	2.8	19
333	Accurate prediction of excitation energies to high-lying Rydberg electronic states: Rydberg states of acetylene as a case study. <i>Journal of Chemical Physics</i> , 2003, 119, 6581-6587.	3.0	10
334	H and CH ₃ eliminations in the photodissociation of chlorotoluene. <i>Journal of Chemical Physics</i> , 2003, 119, 7701-7704.	3.0	14
335	Quantum chemical modeling of photoabsorption and photoluminescence of the [AlO ₄] ⁰ defect in bulk SiO ₂ . <i>Journal of Chemical Physics</i> , 2003, 119, 11408-11414.	3.0	11
336	A survey of ab initio conical intersections for the H+H ₂ system. <i>Journal of Chemical Physics</i> , 2003, 118, 3052-3064.	3.0	45
337	Quantization of the 3 ⁺ —3 nonadiabatic coupling matrix for three coupled states of the C ₂ H molecule. <i>Journal of Chemical Physics</i> , 2002, 117, 991-1000.	3.0	35
338	Experimental and theoretical investigations of the O(¹ D) reaction with cyclopropane. <i>Journal of Chemical Physics</i> , 2002, 116, 8292.	3.0	9
339	Stripping dynamics in the reactions of electronically excited carbon atoms, C(1D), with ethylene and propylene: production of propargyl and methylpropargyl radicals. <i>Journal of Chemical Physics</i> , 2002, 116, 1318-1324.	3.0	25
340	Ab initio study of the reaction mechanism of CO ₂ with Ti atom in the ground and excited electronic states. <i>Journal of Chemical Physics</i> , 2002, 116, 5633-5642.	3.0	25
341	Prediction of absolute rate coefficients and product branching ratios for the C(3P)+allene reaction system. <i>Journal of Chemical Physics</i> , 2002, 117, 7055-7067.	3.0	8
342	A globally smooth ab initio potential surface of the 1 ⁺ state for the reaction S(1D)+H ₂ . <i>Journal of Chemical Physics</i> , 2002, 116, 4124-4134.	3.0	84

#	ARTICLE	IF	CITATIONS
343	The reactivity of ground-state carbon atoms with unsaturated hydrocarbons in combustion flames and in the interstellar medium. <i>International Reviews in Physical Chemistry</i> , 2002, 21, 307-356.	2.3	81
344	The Formation of Interstellar C ₂ N Isomers in Circumstellar Envelopes of Carbon Stars: An Ab Initio Study. <i>Astrophysical Journal</i> , 2002, 564, 787-791.	4.5	42
345	Ab Initio and DFT Study of the Formation Mechanisms of Polycyclic Aromatic Hydrocarbons: The Phenanthrene Synthesis from Biphenyl and Naphthalene. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6171-6182.	2.5	35
346	Necessary Conditions for a Rigorous Minimal Diabatic Potential Matrix. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6499-6507.	2.5	9
347	Ab Initio Study of the Reaction Mechanisms of NiO and NiS with H ₂ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 520-528.	2.5	15
348	Activation of Methane by Neutral Transition Metal Oxides (ScO, NiO, and PdO): A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 12072-12083.	2.5	39
349	Theoretical Study of Complexes of Closo-Borane, Alane, and Gallane Anions with Cations of Light Metals Inside and Outside of Icosahedral Clusters [A ₁₂ H ₁₂] ⁻ (A = B, Al, and Ga). <i>Journal of Physical Chemistry A</i> , 2002, 106, 11594-11602.	2.5	23
350	Red and near-infrared photoluminescence from silica-based nanoscale materials: Experimental investigation and quantum-chemical modeling. <i>Journal of Chemical Physics</i> , 2002, 116, 281.	3.0	44
351	An ab initio/Rice-Ramsperger-Kassel-Marcus study of photodissociation of carbonyl cyanide. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 566-574.	2.0	6
352	Curl equations as substratum for the derivation of the electronic nonadiabatic coupling terms. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 1577-1585.	2.0	13
353	Conical intersection revisited: extension to an elliptic form. <i>Chemical Physics Letters</i> , 2002, 354, 243-250.	2.6	24
354	Photoluminescence from mesoporous silica akin to that from nanoscale silicon: the nature of light-emitters. <i>Chemical Physics Letters</i> , 2002, 358, 180-186.	2.6	41
355	Theoretical study on the reaction mechanism of Sc atoms with carbon dioxide. <i>Chemical Physics Letters</i> , 2002, 357, 51-58.	2.6	27
356	Ab initio non-adiabatic coupling elements: the conical intersection between the 2 ² A ⁺ and the 3 ² A ⁺ of the H+H ₂ system. <i>Chemical Physics Letters</i> , 2002, 358, 163-169.	2.6	29
357	Dissociation pathways of benzene trication. <i>Chemical Physics Letters</i> , 2002, 359, 253-261.	2.6	20
358	An ab initio study on the formation of interstellar tricarbon isomers l-C ₃ (X ¹ g ⁺) and c-C ₃ (X ³ A ⁺). <i>Chemical Physics Letters</i> , 2002, 360, 139-143.	2.6	25
359	Ab initio study of excited electronic states and vibronic spectra of phenyl radical. <i>Chemical Physics Letters</i> , 2002, 361, 421-431.	2.6	24
360	Theoretical study of the reaction mechanism of platinum oxide with methane. <i>Chemical Physics Letters</i> , 2002, 365, 140-147.	2.6	20

#	ARTICLE	IF	CITATIONS
361	A theoretical study of isomerism in doped aluminum XAl_2 clusters ($X=B, Al, Ga, C, Si, Ge$) with 40 valence electrons. <i>Chemical Physics Letters</i> , 2002, 365, 494-504.	2.6	41
362	Photoluminescence of silanone and dioxasilirane groups in silicon oxides: A theoretical study. <i>Journal of Chemical Physics</i> , 2002, 116, 9889-9896.	3.0	32
363	DISSOCIATION, ISOMERIZATION, AND ISOTOPE SCRAMBLING OF BENZENE: A THEORETICAL VIEW. , 2002, , 340-358.		6
364	Unimolecular decomposition of chemically activated triplet C_4H_3 complexes: A combined crossed-beam and ab initio study. <i>Journal of Chemical Physics</i> , 2001, 115, 5117-5125.	3.0	11
365	Structure of the acetone liquid/vapor interface. <i>Journal of Chemical Physics</i> , 2001, 114, 1837-1843.	3.0	89
366	The role of the ground and excited potential energy surfaces in the $O(1D) + SiH_4$ reactions: A theoretical study. <i>Journal of Chemical Physics</i> , 2001, 114, 10816-10834.	3.0	13
367	Chemical dynamics of cyclopropynylidyne ($c-C_3H; \tilde{X}^2B_2$) formation from the reaction of $C([sup 1]D)$ with acetylene, $C_2H_2(\tilde{X}^1\Sigma_g^+)$. <i>Journal of Chemical Physics</i> , 2001, 114, 231.	3.0	49
368	Product Branching Ratios of the $C(3P) + C_2H_3(2A^-)$ and $CH(2\tilde{I}) + C_2H_2(1\tilde{I}g^+)$ Reactions and Photodissociation of $H_2CC^+CH(2B_1)$ at 193 and 242 nm: An ab Initio/RRKM Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 11549-11559.	2.5	47
369	Theoretical Study of Icosahedralcloso-Borane, -Alane, and -Gallane Dianions ($A_{12}H_{12}^{2-}$; $A = B, Al, Ga$) with Endohedral Noble Gas Atoms ($Ng = He, Ne, Ar, \text{ and } Kr$) and Their Lithium Salts ($Li[Ng@A_{12}H_{12}]^-$ and $Tl[ETQq_4@A_{12}H_{12}]^+$)		7
370	Conversion of CO to Formaldehyde Catalyzed by BeO : A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 10433-10438.	2.5	7
371	A Combined Crossed Molecular Beam and ab Initio Study of the Reactions $C_2(X^1g^+, a^3\tilde{u}) + C_2H_4 \rightarrow n-C_4H_3(X^2A^-) + H(2S_{1/2})$. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9813-9818.	2.5	58
372	Ab Initio MO Study of the Triplet C_3H_4 Potential Energy Surface and the Reaction of $C(3P_j)$ with Ethylene, C_2H_4 . <i>Journal of Physical Chemistry A</i> , 2001, 105, 1847-1856.	2.5	41
373	A Computational Study of the $OH(OD) + CO$ Reactions: Effects of Pressure, Temperature, and Quantum-Mechanical Tunneling on Product Formation. <i>Journal of Physical Chemistry A</i> , 2001, 105, 11249-11259.	2.5	72
374	A Theoretical Investigation of the Triplet Carbon Atom $C(3P) +$ Vinyl Radical $C_2H_3(2A^-)$ Reaction and Thermochemistry of $C_3H_n(n=1-4)$ Species. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3284-3299.	2.5	55
375	Theoretical Study of the Reaction Mechanism of Fe Atoms with H_2O, H_2S, O_2 and H^+ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 7460-7467.	2.5	30
376	The Formation of C_5H_5 Isomers as Potential Key Intermediates to Polycyclic Aromatic Hydrocarbon-like Molecules. <i>Astrophysical Journal</i> , 2001, 548, 852-860.	4.5	16
377	A Theory of Coulomb Explosion of Molecules. <i>Journal of the Chinese Chemical Society</i> , 2001, 48, 963-969.	1.4	3
378	An Ab Initio Investigation of Reactions of Carbon Atoms, $C(3P_j)$, with C_2H_4 and C_3H_6 in the Interstellar Medium. <i>Astrophysical Journal</i> , 2001, 561, 858-863.	4.5	23

#	ARTICLE	IF	CITATIONS
379	Thermochemistry of cyclopentadienylidene (c-C ₅ H ₄ ,C _{2v} ,3B ₁), cyclopentadienyl radical (c-C ₅ H ₅ ?,C _{2v} ,2B ₁) and 1,3-cyclopentadiene (c-C ₅ H ₆ ,C _{2v} ,1A ₁): a theoretical study by the G2M(RCC,MP2) method. Journal of Physical Organic Chemistry, 2001, 14, 131-138.	1.9	16
380	Ab initio study of C ₄ H ₃ potential energy surface and reaction of ground-state carbon atom with propargyl radical. Journal of Computational Chemistry, 2001, 22, 1522-1535.	3.3	27
381	Ab initio study of nonadiabatic coupling matrix elements between excited 2A ⁺ and 3A ⁺ electronic states of C ₂ H. Chemical Physics Letters, 2001, 336, 135-142.	2.6	14
382	Theoretical study of the reaction mechanism of ScO with molecular hydrogen. Chemical Physics Letters, 2001, 341, 393-399.	2.6	15
383	Theoretical study of the reaction of beryllium oxide with methane. Chemical Physics Letters, 2001, 348, 303-310.	2.6	25
384	A theoretical re-evaluation of the heat of formation of phenylcarbene. Chemical Physics Letters, 2001, 349, 571-577.	2.6	16
385	Intermolecular potential and equilibrium orientational states for dimers of non-polar molecules. Molecular Physics, 2001, 99, 1883-1897.	1.7	12
386	A combined crossed beam and ab initio investigation on the reaction of carbon species with C ₄ H ₆ isomers. III. 1,2-butadiene, H ₂ CCCH(CH ₃) (X ⁺ and ⁺) a non-Rice-Ramsperger-Kassel-Marcus system? Journal of Chemical Physics, 2001, 115, 5107-5116.	3.0	29
387	Branching ratios of C ₂ products in the photodissociation of C ₂ H at 193 nm. Journal of Chemical Physics, 2001, 114, 9821-9831.	3.0	20
388	O(1D) reaction with cyclopropane: Evidence of O atom insertion into the C-C bond. Journal of Chemical Physics, 2001, 115, 7-10.	3.0	13
389	Reaction dynamics of S(¹ D)+H ₂ /D ₂ on a new ab initio potential surface. Journal of Chemical Physics, 2001, 114, 320.	3.0	58
390	Ab initio molecular orbital/Rice-Ramsperger-Kassel-Marcus theory study of multichannel rate constants for the unimolecular decomposition of benzene and the H+C ₆ H ₅ reaction over the ground electronic state. Journal of Chemical Physics, 2001, 114, 8421-8435.	3.0	53
391	Computational formulas for symmetry-forbidden vibronic spectra and their application to n [*] transition in neat acetone. Journal of Chemical Physics, 2001, 115, 4080-4094.	3.0	25
392	The study of conical intersections between consecutive pairs of the five lowest 2A ⁺ states of the C ₂ H molecule. Journal of Chemical Physics, 2001, 115, 3673-3689.	3.0	34
393	Degenerate conical intersections: The interaction between the 3 ⁺ and 4 ⁺ electronic states of C ₂ H as a case study. Journal of Chemical Physics, 2001, 114, 5109-5112.	3.0	16
394	Theoretical study on the reversible storage of H ₂ by BeO. Chemical Physics Letters, 2000, 321, 95-100.	2.6	13
395	Ab initio study of H photodetachment from the ethyl radical. Chemical Physics Letters, 2000, 323, 441-447.	2.6	22
396	Theoretical study on reforming of CO ₂ catalyzed with Be. Chemical Physics Letters, 2000, 325, 639-644.	2.6	11

#	ARTICLE	IF	CITATIONS
397	Reaction mechanism of CO ₂ with Ca atom: A theoretical study. <i>Chemical Physics Letters</i> , 2000, 331, 526-532.	2.6	12
398	Two-dimensional Ga-induced magic clusters on the Si surface: a density functional study. <i>Chemical Physics Letters</i> , 2000, 318, 27-34.	2.6	5
399	Ab initio study of spin-forbidden unimolecular decomposition of carbon dioxide. <i>Chemical Physics</i> , 2000, 256, 169-176.	1.9	39
400	Ab initio study of the reaction mechanism of singlet and triplet N ₂ O and their intersystem crossing. <i>Chemical Physics</i> , 2000, 259, 89-97.	1.9	23
401	Heats of formation of small bicyclic hydrocarbons, spiropentadiene (C ₅ H ₄), spiropentane (C ₅ H ₈) and bicyclo[1.1.0]but-1(3)-ene (C ₄ H ₄): a theoretical study by the G2M(RCC,MP2) method. <i>Chemical Physics Letters</i> , 2000, 326, 468-476.	2.6	9
402	Rydberg states of propyne at 6.8–10.5 eV studied by two-photon resonant ionization spectroscopy and theoretical calculation. <i>Journal of Chemical Physics</i> , 2000, 112, 7384-7393.	3.0	30
403	A combined crossed beam and ab initio investigation on the reaction of carbon species with C ₄ H ₆ isomers. I. The 1,3-butadiene molecule, H ₂ CCHCH ₂ (X ¹ A ₁ ⁺). <i>Journal of Chemical Physics</i> , 2000, 113, 9622-9636.	3.0	37
404	A combined crossed beam and ab initio investigation on the reaction of carbon species with C ₄ H ₆ isomers. II. The dimethylacetylene molecule, H ₃ CCCCH ₃ (X ¹ A ₁ g). <i>Journal of Chemical Physics</i> , 2000, 113, 9637-9648.	3.0	26
405	Probing the nature of surface intersection by ab initio calculations of the nonadiabatic coupling matrix elements: A conical intersection due to bending motion in C ₂ H. <i>Journal of Chemical Physics</i> , 2000, 112, 10703-10706.	3.0	37
406	Theoretical Study on the Reaction Mechanism of Nickel Atoms with Carbon Dioxide. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11622-11627.	2.5	30
407	Theoretical Study of the Reversible Storage of H ₂ by BeS. <i>Journal of the American Chemical Society</i> , 2000, 122, 11406-11410.	13.7	12
408	Ab Initio MO Study of the Global Potential Energy Surface of C ₄ H ₄ in Triplet Electronic State and the Reactions of C(3P _j) with C ₃ H ₄ (Allene and Propyne) and C ₂ (A ³ Π _u) with C ₂ H ₄ (X ¹ A ₁ g ⁺). <i>Journal of the American Chemical Society</i> , 2000, 122, 1776-1788.	13.7	39
409	Theoretical Study on the Reaction Mechanism of CO ₂ with Mg. <i>Journal of Physical Chemistry A</i> , 2000, 104, 7646-7650.	2.5	22
410	Toward the understanding of ethylene photodissociation: Theoretical study of energy partition in products and rate constants. <i>Journal of Chemical Physics</i> , 1999, 110, 10810-10820.	3.0	65
411	Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. <i>Journal of Applied Physics</i> , 1999, 85, 7064-7069.	2.5	25
412	Ab initio study of the addition of atomic carbon with water. <i>Chemical Physics</i> , 1999, 244, 143-149.	1.9	18
413	Ab initio molecular orbital and density functional study of the C ₆ H ₆ ...I ₂ complex in the ground and excited electronic states. <i>International Journal of Quantum Chemistry</i> , 1999, 72, 307-318.	2.0	18
414	Ab Initio Calculations of Vibronic Spectra and Dynamics for Small Polyatomic Molecules: A Role of Duschinsky Effect. <i>Journal of Physical Chemistry A</i> , 1999, 103, 10674-10690.	2.5	139

#	ARTICLE	IF	CITATIONS
415	Ab initio study of the $n\text{-}\tilde{\epsilon}^*$ electronic transition in acetone: Symmetry-forbidden vibronic spectra. <i>Journal of Chemical Physics</i> , 1999, 111, 205-215.	3.0	58
416	Crossed-beam reaction of carbon atoms with hydrocarbon molecules. V. Chemical dynamics of $n\text{-C}_4\text{H}_3$ formation from reaction of $\text{C}(^3\text{P}_j)$ with allene, H_2CCCH_2 ($X\tilde{\epsilon}^1\text{A}_1$). <i>Journal of Chemical Physics</i> , 1999, 110, 10330-10344.	3.0	60
417	Prediction of Absolute Rate Constants for the Reactions of NH_2 with Alkanes from ab Initio G2M/TST Calculations. <i>Journal of Physical Chemistry A</i> , 1999, 103, 2088-2096.	2.5	38
418	The Fragmentation of Melamine: A Study via Electron-Impact Ionization, Laser-Desorption Ionization, Collision-Induced Dissociation, and Density Functional Calculations of Potential Energy Surface. <i>Journal of Physical Chemistry B</i> , 1999, 103, 582-596.	2.6	25
419	Potential energy surfaces of excited states of H_2^+ . <i>Chemical Physics Letters</i> , 1998, 285, 114-120.	2.6	7
420	Ab initio calculations of potential energy surface and rate constants for ethylene photodissociation at 193 and 157 nm. <i>Chemical Physics Letters</i> , 1998, 287, 301-306.	2.6	39
421	Ab initio MO and TST calculations for the rate constant of the $\text{HNO} + \text{NO}_2 \rightarrow \text{HONO} + \text{NO}$ reaction. <i>International Journal of Chemical Kinetics</i> , 1998, 30, 729-736.	1.6	18
422	Ab initio calculations of radiationless transitions between excited and ground singlet electronic states of ethylene. <i>Journal of Chemical Physics</i> , 1998, 108, 2044-2055.	3.0	69
423	Structure and Nonrigidity of $\text{B}_9\text{H}_9^{2-}$ and $\text{B}_9\text{H}_{10}^-$. Comparisons of $\text{B}_n\text{H}_n^{2-}$ and $\text{B}_n\text{H}_{n+1}^-$ Systems. <i>Inorganic Chemistry</i> , 1998, 37, 1693-1703.	4.0	19
424	Rate Constant of the $\text{HONO} + \text{HONO} \rightarrow \text{H}_2\text{O} + \text{NO} + \text{NO}_2$ Reaction from ab Initio MO and TST Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1803-1807.	2.5	50
425	Photodissociation Dynamics of Propyne and Allene: A View from ab Initio Calculations of the C_3H_n ($n = 1, 2$) ETQq1 1 0.784314 rgBT / 13.7 125 1998, 120, 5751-5763.	13.7	125
426	The Largecloso-Borane Dianions, $\text{B}_n\text{H}_n^{2-}$ ($n = 13 \sim 17$) Are Aromatic, Why Are They Unknown? <i>Inorganic Chemistry</i> , 1998, 37, 6765-6772.	4.0	157
427	Ab initio/RRKM approach toward the understanding of ethylene photodissociation. <i>Journal of Chemical Physics</i> , 1998, 109, 2748-2761.	3.0	102
428	Ab initio study on the reaction mechanism of ozone with the chlorine atom. <i>Journal of Chemical Physics</i> , 1998, 109, 10847-10852.	3.0	33
429	Reactions of NO with nitrogen hydrides x. <i>International Reviews in Physical Chemistry</i> , 1997, 16, 249-266.	2.3	19
430	Experimental and Theoretical Studies of the Unimolecular Decomposition of Nitrosobenzene: High-Pressure Rate Constants and the $\text{C}\tilde{\epsilon}^1\text{N}$ Bond Strength. <i>Journal of Physical Chemistry A</i> , 1997, 101, 6043-6047.	2.5	39
431	Theoretical Study of the Structure, Energetics, and the $n\tilde{\epsilon}^*$ Electronic Transition of the Acetone + $n\text{H}_2\text{O}$ ($n = 1 \sim 3$) Complexes. <i>Journal of Physical Chemistry A</i> , 1997, 101, 9925-9934.	2.5	36
432	Theoretical Study on the Mechanism of the Dissociation of Benzene. The $\text{C}_5\text{H}_3 + \text{CH}_3$ Product Channel. <i>Journal of Physical Chemistry A</i> , 1997, 101, 6781-6789.	2.5	50

#	ARTICLE	IF	CITATIONS
433	Theoretical Study of Potential Energy Surface and Thermal Rate Constants for the C ₆ H ₅ + H ₂ and C ₆ H ₆ + H Reactions. <i>Journal of Physical Chemistry A</i> , 1997, 101, 3189-3196.	2.5	116
434	Using ab Initio MO Calculations To Understand the Photodissociation Dynamics of CH ₂ CCH ₂ and CH ₂ C ₂ . <i>Journal of Physical Chemistry A</i> , 1997, 101, 6638-6646.	2.5	29
435	Ab Initio Study of the H + HONO Reaction: Direct Abstraction versus Indirect Exchange Processes. <i>Journal of Physical Chemistry A</i> , 1997, 101, 60-66.	2.5	40
436	IR spectroscopy and theoretical vibrational calculation of the melamine molecule. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997, 93, 3445-3451.	1.7	81
437	Theoretical study of vibronic spectra and photodissociation pathways of methane. <i>Journal of Chemical Physics</i> , 1997, 106, 2612-2620.	3.0	49
438	Excited electronic states of the methyl radical. Ab initio molecular orbital study of geometries, excitation energies and vibronic spectra. <i>Chemical Physics</i> , 1997, 215, 329-341.	1.9	41
439	Can chlorine anion catalyze the reaction of HOCl with HCl?. <i>Chemical Physics Letters</i> , 1997, 270, 395-398.	2.6	9
440	Ab initio calculations of vibronic coupling. Applications to symmetry-forbidden vibronic spectra and internal conversion in ethylene. <i>Chemical Physics Letters</i> , 1997, 274, 281-292.	2.6	40
441	Ab initio molecular orbital study of excited electronic states of the vinyl radical. <i>Chemical Physics Letters</i> , 1997, 275, 19-27.	2.6	47
442	Ab Initio and RRKM Calculations for Multichannel Rate Constants of the C ₂ H ₃ + O ₂ Reaction. <i>Journal of the American Chemical Society</i> , 1996, 118, 9759-9771.	13.7	161
443	On the theoretical investigation of vibronic spectra of ethylene by ab initio calculations of the Franck-Condon factors. <i>Journal of Chemical Physics</i> , 1996, 105, 9007-9020.	3.0	68
444	Ab Initio Study of the Mechanism for the Thermal Decomposition of the Phenoxy Radical. <i>The Journal of Physical Chemistry</i> , 1996, 100, 9314-9322.	2.9	111
445	Theoretical Study of the Reaction of HCl with ClONO ₂ Catalyzed by NO ₃ -. Attachment-Detachment Mechanism for the Anion-Catalyzed Neutral Reactions. <i>The Journal of Physical Chemistry</i> , 1996, 100, 2985-2992.	2.9	19
446	Theoretical study of the thermal isomerization of fulvene to benzene. <i>Journal of Physical Organic Chemistry</i> , 1996, 9, 801-810.	1.9	52
447	Theoretical study of reactions of N ₂ O with NO and OH radicals. <i>International Journal of Chemical Kinetics</i> , 1996, 28, 693-703.	1.6	24
448	$\tilde{\nu}(\tilde{\nu}^{\wedge})$ – vibronic spectrum of ethylene from ab initio calculations of the Franck-Condon factors. <i>Chemical Physics Letters</i> , 1996, 258, 53-62.	2.6	57
449	The CH ₃ +C ₅ H ₅ reaction: A potential source of benene at high temperatures. <i>Proceedings of the Combustion Institute</i> , 1996, 26, 521-526.	0.3	71
450	Ab initio molecular orbital study of the HCO+O ₂ reaction: Direct versus indirect abstraction channels. <i>Journal of Chemical Physics</i> , 1996, 105, 2346-2352.	3.0	82

#	ARTICLE	IF	CITATIONS
451	A density functional study of the global potential energy surfaces of the [H,C,N,O] system in singlet and triplet states. <i>Journal of Chemical Physics</i> , 1996, 105, 6439-6454.	3.0	105
452	Density functional study of the global potential energy surfaces of the [H,C,N,O]+system in doublet and quartet states. <i>Journal of Chemical Physics</i> , 1996, 105, 3187-3205.	3.0	22
453	Theoretical study of the thermal isomerization of fulvene to benzene. <i>Journal of Physical Organic Chemistry</i> , 1996, 9, 801-810.	1.9	1
454	Theoretical study of reactions of N ₂ O with NO and OH radicals. <i>International Journal of Chemical Kinetics</i> , 1996, 28, 693-703.	1.6	18
455	Ab initio molecular orbital studies of elementary reactions and homogeneous catalytic cycles with organometallic compounds. <i>Pure and Applied Chemistry</i> , 1995, 67, 257-263.	1.9	28
456	Reaction of phenoxy radical with nitric oxide. <i>Journal of Physical Organic Chemistry</i> , 1995, 8, 47-53.	1.9	29
457	Ab initio molecular orbital study of the O + C ₆ H ₅ O reaction. <i>Journal of Physical Organic Chemistry</i> , 1995, 8, 407-420.	1.9	28
458	An ab initio molecular orbital study of potential energy surface of the NH ₂ +NO ₂ reaction. <i>Journal of Chemical Physics</i> , 1995, 103, 5640-5649.	3.0	37
459	Ab initio molecular orbital study of potential energy surface for the reaction of C ₂ H ₃ with H ₂ and related reactions. <i>Journal of Chemical Physics</i> , 1995, 103, 3440-3449.	3.0	49
460	A Theoretical Study of Rectangular Tetrasulfur in a Gas Phase and in the Tetranuclear [Rh ₂ (η ⁵ -C ₅ Me ₅) ₂ (μ-CH ₂) ₂ (μ-S ₄)] ₂ ⁺ Complex. <i>Inorganic Chemistry</i> , 1995, 34, 1208-1211.	4.0	13
461	Modification of the gaussian ² theoretical model: The use of coupled cluster energies, density functional geometries, and frequencies. <i>Journal of Chemical Physics</i> , 1995, 103, 7414-7421.	3.0	468
462	Ab initio molecular orbital study of potential energy surface for the NH+NO ₂ reaction. <i>Journal of Chemical Physics</i> , 1994, 101, 3916-3922.	3.0	34
463	Propargylene. <i>Journal of the American Chemical Society</i> , 1994, 116, 8229-8237.	13.7	57
464	Ab Initio MO Study of Cluster Rearrangements in Pentagonal Pyramidal Clusters: B ₆ H ₁₀ Borane and [(IrB ₅ H ₈)(CO)(PH ₃) ₂] Metallaborane. <i>Journal of the American Chemical Society</i> , 1994, 116, 3932-3942.	13.7	10
465	Ab Initio Molecular Orbital Calculations of C ₆ H ₅ O ₂ Isomers. <i>Journal of the American Chemical Society</i> , 1994, 116, 9577-9584.	13.7	51
466	An ab initio molecular orbital study of the mechanism of the rhodium(I)-catalyzed olefin hydroboration reaction. <i>Journal of the American Chemical Society</i> , 1994, 116, 10693-10702.	13.7	106
467	Ab initio molecular orbital study of structure and NMR ¹¹ B chemical shifts of Lewis base adducts of CO, NH ₃ , PF ₃ , and PH ₃ with small nido-boranes, B ₃ H ₇ and B ₄ H ₈ . <i>Chemical Physics Letters</i> , 1993, 214, 69-76.	2.6	9
468	An alternative mechanism of BH ₂ SH formation in the reaction of B ₂ H ₆ with SH ₂ : concerted elimination of BH ₃ and H ₂ from H ₂ S · B ₂ H ₆ . Ab initio MO study. <i>Chemical Physics Letters</i> , 1993, 216, 313-318.	2.6	2

#	ARTICLE	IF	CITATIONS
469	Structure and nonrigidity of undecahydrodecaborate(1-). An ab initio/IGLO/NMR study. Inorganic Chemistry, 1993, 32, 463-468.	4.0	31
470	Theoretical prediction of the structure and nonrigidity of octahydroheptaborate(1-). Application of the ab initio/IGLO/NMR method. Inorganic Chemistry, 1993, 32, 469-473.	4.0	19
471	Metallaboranes with Group 8 and 9 Transition Metals. Is Accurate ab initio Molecular Orbital Calculation of Structure, Stability, and NMR Chemical Shifts Possible?. Bulletin of the Chemical Society of Japan, 1993, 66, 3259-3270.	3.2	12
472	The structure of octahydrooctaborate(2-) in solution. Is nonahydrooctaborate(1-) also involved? An ab initio/IGLO/NMR study. Inorganic Chemistry, 1992, 31, 3769-3775.	4.0	24
473	Cleavage of an aromatic ring and radical migration. Faraday Discussions, 0, , .	3.2	1