Lawrence B Harding

List of Publications by Year
in descending order

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112 papers	7,381 citations	36303 51 h-index	56724 83 g-index
112 all docs	112 docs citations	112 times ranked	3745 citing authors

#	Article	IF	Citations
1	Substitution Reactions in the Pyrolysis of Acetone Revealed through a Modeling, Experiment, Theory Paradigm. Journal of the American Chemical Society, 2021, 143, 3124-3142.	13.7	28
2	Reaction Profiles and Kinetics for Radicalâ€“Radical Hydrogen Abstraction via Multireference Coupled Cluster Theory. Journal of Chemical Theory and Computation, 2020, 16, 1511-1525.	5.3	8
3	Anharmonic Rovibrational Partition Functions at High Temperatures: Tests of Reduced-Dimensional Models for Systems with up to Three Fluxional Modes. Journal of Physical Chemistry A, 2019, 123, 6210-6228.	2.5	16
4	Active Thermochemical Tables: The Partition Function of Hydroxymethyl (CH2OH) Revisited. Journal of Physical Chemistry A, 2019, 123, 4212-4231.	2.5	13
5	Anharmonic Rovibrational Partition Functions for Fluxional Species at High Temperatures via Monte Carlo Phase Space Integrals. Journal of Physical Chemistry A, 2018, 122, 1727-1740.	2.5	15
6	Nascent energy distribution of the Criegee intermediate CH2OO from direct dynamics calculations of primary ozonide dissociation. Journal of Chemical Physics, 2018, 148, 174306.	3.0	36
7	Accurate Anharmonic Zero-Point Energies for Some Combustion-Related Species from Diffusion Monte Carlo. Journal of Physical Chemistry A, 2017, 121, 4334-4340.	2.5	22
8	Ab Initio Computations and Active Thermochemical Tables Hand in Hand: Heats of Formation of Core Combustion Species. Journal of Physical Chemistry A, 2017, 121, 6580-6602.	2.5	144
9	Time-Resolved Kinetic Chirped-Pulse Rotational Spectroscopy in a Room-Temperature Flow Reactor. Journal of Physical Chemistry Letters, 2017, 8, 6180-6188.	4.6	18
10	Comment on â€œA novel and facile decay path of Criegee intermediates by intramolecular insertion reactions via roaming transition statesâ€•[J. Chem. Phys. 142, 124312 (2015)]. Journal of Chemical Physics, 2015, 143, 167101.	3.0	3
11	Temperature and Pressure-Dependent Rate Coefficients for the Reaction of Vinyl Radical with Molecular Oxygen. Journal of Physical Chemistry A, 2015, 119, 7766-7779.	2.5	88
12	Autobiography of Lawrence B. Harding. Journal of Physical Chemistry A, 2015, 119, 7078-7079.	2.5	0
13	Thermal Dissociation and Roaming Isomerization of Nitromethane: Experiment and Theory. Journal of Physical Chemistry A, 2015, 119, 7872-7893.	2.5	59
14	Resolving Some Paradoxes in the Thermal Decomposition Mechanism of Acetaldehyde. Journal of Physical Chemistry A, 2015, 119, 7724-7733.	2.5	33
15	Secondary channels in the thermal decomposition of monomethylhydrazine (CH3NHNH2). RSC Advances, 2014, 4, 62951-62964.	3.6	3
16	Predictive a priori pressure-dependent kinetics. Science, 2014, 346, 1212-1215.	12.6	142
17	Comparison of multireference configuration interaction potential energy surfaces for HÂ+ÂO2Ââ†’ÂHO2: the effect of internal contraction. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	21
18	Electronic States of the Quasilinear Molecule Propargylene (HCCCH) from Negative Ion Photoelectron Spectroscopy. Journal of the American Chemical Society, 2014, 136, 10361-10372.	13.7	18

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19	Unconventional Peroxy Chemistry in Alcohol Oxidation: The Water Elimination Pathway. Journal of Physical Chemistry Letters, 2013, 4, 350-354.	4.6	38
20	Rate Constant and Branching Fraction for the NH₂ + NO₂ Reaction. Journal of Physical Chemistry A, 2013, 117, 9011-9022.	2.5	37
21	Predictive Theory for the Addition and Insertion Kinetics of ¹CH₂ Reacting with Unsaturated Hydrocarbons. Journal of Physical Chemistry A, 2013, 117, 12677-12692.	2.5	21
22	Separability of Tight and Roaming Pathways to Molecular Decomposition. Journal of Physical Chemistry A, 2012, 116, 6967-6982.	2.5	48
23	Theoretical Determination of the Rate Coefficient for the HO_{2Â}+ HO₂ â†' H₂O₂+O₂ Reaction: Adiabatic Treatment of Anharmonic Torsional Effects. Journal of Physical Chemistry A, 2012, 116, 2089-2100.	2.5	35
24	Statistical Theory for the Kinetics and Dynamics of Roaming Reactions. Journal of Physical Chemistry A, 2011, 115, 14370-14381.	2.5	76
25	Near-threshold H/D exchange in CD3CHO photodissociation. Nature Chemistry, 2011, 3, 443-448.	13.6	60
26	The role of NNH in NO formation and control. Combustion and Flame, 2011, 158, 774-789.	5.2	304
27	The Effect of Spinâ^'Orbit Splitting on the Association Kinetics of Barrierless Halogen Atomâ^'Hydrocarbon Radical Reactions. Journal of Physical Chemistry A, 2010, 114, 5759-5768.	2.5	40
28	Theoretical Validation of Chemical Kinetic Mechanisms: Combustion of Methanol. Journal of Physical Chemistry A, 2010, 114, 8286-8301.	2.5	66
29	Reactions between Resonance-Stabilized Radicals: Propargyl + Allyl. Journal of Physical Chemistry A, 2010, 114, 4881-4890.	2.5	84
30	Roaming Radical Pathways for the Decomposition of Alkanes. Journal of Physical Chemistry Letters, 2010, 1, 3016-3020.	4.6	73
31	Roaming Radical Kinetics in the Decomposition of Acetaldehyde. Journal of Physical Chemistry A, 2010, 114, 765-777.	2.5	125
32	Experimental and Theoretical Investigation of the Self-Reaction of Phenyl Radicals. Journal of Physical Chemistry A, 2010, 114, 8240-8261.	2.5	63
33	Kinetics of CH + N₂ Revisited with Multireference Methods. Journal of Physical Chemistry A, 2008, 112, 522-532.	2.5	62
34	Quantum States of the Endohedral Fullerene Li@C₆₀. Journal of Physical Chemistry A, 2008, 112, 5478-5485.	2.5	31
35	Direct Measurement and Theoretical Calculation of the Rate Coefficient for Cl + CH3in the Range fromT= 202â^'298 K. Journal of Physical Chemistry A, 2007, 111, 1015-1023.	2.5	15
36	Interpolating moving least-squares methods for fitting potential energy surfaces: An application to the H2CN unimolecular reaction. Journal of Chemical Physics, 2007, 126, 104105.	3.0	26

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37	Ab initio methods for reactive potential surfaces. Physical Chemistry Chemical Physics, 2007, 9, 4055.	2.8	158
38	Secondary Kinetics of Methanol Decomposition:â€‰ Theoretical Rate Coefficients for ³CH₂ + OH, ³CH₂ + ³CH₂, and ³CH₂ + CH₃. Journal of Physical Chemistry A, 2007, 111, 8699-8707.	2.5	26
39	Performance of the Spin-Flip and Multireference Methods for Bond Breaking in Hydrocarbons:â€‰ A Benchmark Study. Journal of Physical Chemistry A, 2007, 111, 13264-13271.	2.5	31
40	On the Combination Reactions of Hydrogen Atoms with Resonance-Stabilized Hydrocarbon Radicalsâ€. Journal of Physical Chemistry A, 2007, 111, 3789-3801.	2.5	111
41	Kinetics of the Reaction of Methyl Radical with Hydroxyl Radical and Methanol Decompositionâ€. Journal of Physical Chemistry A, 2007, 111, 3932-3950.	2.5	188
42	Predictive theory for the combination kinetics of two alkyl radicals. Physical Chemistry Chemical Physics, 2006, 8, 1133.	2.8	202
43	Methyl radical:ab initioglobal potential surface, vibrational levels and partition function. Molecular Physics, 2006, 104, 73-81.	1.7	41
44	The determination of molecular properties from MULTIMODE with an application to the calculation of Franckâ€“Condon factors for photoionization of CF3to. Molecular Physics, 2006, 104, 33-45.	1.7	34
45	Predictive Theory for Hydrogen Atomâ^'Hydrocarbon Radical Association Kinetics. Journal of Physical Chemistry A, 2005, 109, 4646-4656.	2.5	176
46	A Global ab Initio Potential Energy Surface for Formaldehydeâ€. Journal of Physical Chemistry A, 2004, 108, 8980-8986.	2.5	135
47	Speciation of C6H6Isomers by Gas Chromatography-Matrix Isolation Fourier Transform Infrared Spectroscopyâ^'Mass Spectrometry. Journal of Physical Chemistry A, 2004, 108, 3403-3405.	2.5	15
48	Implementation of a fast analytic ground state potential energy surface for the N(2D)+H2 reaction. Journal of Chemical Physics, 2003, 119, 3063-3070.	3.0	62
49	A quasiclassical trajectory study of the reaction OH+COâ†'H+CO2. Journal of Chemical Physics, 2003, 119, 5848-5859.	3.0	92
50	Quasiclassical Trajectory Study of Energy and Angular Distributions for the H + CO2â†' OH + CO Reactionâ€. Journal of Physical Chemistry B, 2002, 106, 8148-8160.	2.6	28
51	On the Enthalpy of Formation of Hydroxyl Radical and Gas-Phase Bond Dissociation Energies of Water and Hydroxyl. Journal of Physical Chemistry A, 2002, 106, 2727-2747.	2.5	466
52	Construction of reproducing kernel Hilbert space potential energy surfaces for the 1â€ŠAâ€³ and 1â€ŠAâ€² states of the reaction N(2D)+H2. Journal of Chemical Physics, 2001, 114, 3945-3948.	3.0	19
53	A direct transition state theory based analysis of the branching in NH2 + NO. Faraday Discussions, 2001, 119, 207-222.	3.2	27
54	Evidence for a Lower Enthalpy of Formation of Hydroxyl Radical and a Lower Gas-Phase Bond Dissociation Energy of Water. Journal of Physical Chemistry A, 2001, 105, 1-4.	2.5	175

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55	Theoretical and Experimental Investigation of the Dynamics of the Production of CO from the CH3 + O and CD3 + O Reactions. Journal of Physical Chemistry A, 2001, 105, 8361-8369.	2.5	87
56	Mapping the OH+COâ†'HOCO reaction pathway through IR spectroscopy of the OHâ€"CO reactant complex. Faraday Discussions, 2001, 118, 373-385.	3.2	68
57	Potential Energy Surface of the Ãƒ State of NH2 and the Role of Excited States in the N(2D) + H2 Reaction. Journal of Physical Chemistry A, 2000, 104, 2301-2307.	2.5	74
58	Exploring the OH+CO reaction coordinate via infrared spectroscopy of the OHâ€"CO reactant complex. Journal of Chemical Physics, 2000, 113, 9889-9892.	3.0	97
59	Barrier to Methyl Internal Rotation of Cis- andTrans-2-Methylvinoxy Radicals in the XÌƒ(2Aâ€˜Ââ€˜) and BÌƒ(2Aâ€˜Ââ€˜) States:Â Experiment and Theory. Journal of Physical Chemistry A, 2000, 104, 9906-9913.	2.5	14
60	Barrier to Methyl Internal Rotation of 1-Methylvinoxy Radical in the XÌƒ(2Aâ€˜Ââ€˜) and BÌƒ(2Aâ€˜Ââ€˜) States:Â Experiment and Theoryâ€. Journal of Physical Chemistry A, 2000, 104, 10131-10138.	2.5	19
61	A Summary of â€œA Direct Transition State Theory Based Study of Methyl Radical Recombination Kineticsâ€. Journal of Physical Chemistry A, 2000, 104, 2351-2354.	2.5	9
62	An empirical potential energy surface for the Neâ€"OH/D complexes. Journal of Chemical Physics, 1999, 111, 10053-10060.	3.0	9
63	A theoretical study of the kinetics of C2H3+H. Physical Chemistry Chemical Physics, 1999, 1, 989-997.	2.8	28
64	Potential energy surface and quasiclassical trajectory studies of the N(2D)+H2 reaction. Journal of Chemical Physics, 1999, 110, 9091-9100.	3.0	125
65	A Direct Transition State Theory Based Study of Methyl Radical Recombination Kinetics. Journal of Physical Chemistry A, 1999, 103, 9388-9398.	2.5	77
66	Thermal Rate Constant and Branching Ratio for CN + HD â†' HCN/DCN + D/H fromT= 293 to 375 K. Journal of Physical Chemistry A, 1998, 102, 7653-7661.	2.5	17
67	A theoretical study of solid hydrogens doped with atomic oxygen. Journal of Chemical Physics, 1997, 106, 942-953.	3.0	19
68	A global A-state potential surface for H2O: Influence of excited states on the O(1D)+H2 reaction. Journal of Chemical Physics, 1997, 107, 2340-2350.	3.0	130
69	The influence of hindered rotations on recombination/dissociation kinetics. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1997, 101, 391-399.	0.9	11
70	Potential energy surface and quasiclassical trajectory studies of the CN+H2 reaction. Journal of Chemical Physics, 1996, 105, 558-571.	3.0	100
71	A global H2O potential energy surface for the reaction O(1D)+H2â†'OH+H. Journal of Chemical Physics, 1996, 105, 10472-10486.	3.0	175
72	Importance of hindered rotations in the thermal dissociation of small unsaturated molecules: Classical formulation and application to HCN and HCCH. Journal of Chemical Physics, 1996, 105, 8075-8096.	3.0	20

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73	A Theoretical Study of Reactions on the ClHCN Surface. The Journal of Physical Chemistry, 1996, 100, 10123-10130.	2.9	12
74	Theoretical studies of collisional relaxation of highly excited SO2 in an Ar bath. Faraday Discussions, 1995, 102, 389.	3.2	29
75	The formaldehyde decomposition chain mechanism. International Journal of Chemical Kinetics, 1993, 25, 285-303.	1.6	50
76	Quantum dynamics of Rennerâ€“Teller vibronic coupling: The predissociation of HCO. Journal of Chemical Physics, 1993, 99, 5812-5827.	3.0	69
77	A quasiclassical trajectory study of OH rotational excitation in OH+CO collisions using ab initio potential surfaces. Journal of Chemical Physics, 1992, 96, 7465-7473.	3.0	57
78	Isotope Effects in Addition Reactions of Importance in Combustion. ACS Symposium Series, 1992, , 48-63.	0.5	11
79	Theoretical studies of the hydrogen peroxide potential surface. 2. An ab initio, long-range, hydroxyl(2.PI.) + hydroxyl(2.PI.) potential. The Journal of Physical Chemistry, 1991, 95, 8653-8660.	2.9	50
80	REMPI mass spectrum of the OH radical in the gas phase. Chemical Physics Letters, 1991, 183, 465-470.	2.6	10
81	Theoretical study of the reaction rates of OH+OH â‡” H2O+O. Proceedings of the Combustion Institute, 1989, 22, 983-989.	0.3	19
82	Theoretical studies of the hydrogen peroxide potential surface. 1. An ab initio anharmonic force field. The Journal of Physical Chemistry, 1989, 93, 8004-8013.	2.9	76
83	Polyatomic surface fitting, vibrational-rotational analysis, expectation value and intensity program. Computer Physics Communications, 1988, 51, 257-284.	7.5	39
84	An improved long range potential for O(1D)+H2. Journal of Chemical Physics, 1988, 88, 7653-7661.	3.0	46
85	The electronic states of Si2 and Siâ¯2 as revealed by photoelectron spectroscopy. Journal of Chemical Physics, 1987, 87, 5116-5124.	3.0	96
86	State-to-state chemistry with fast hydrogen atoms. Reaction and collisional excitation in H + CO2. Faraday Discussions of the Chemical Society, 1987, 84, 359.	2.2	180
87	Ab initio calculations of electronic and vibrational energies of HCO and HOC. Journal of Chemical Physics, 1986, 85, 911-921.	3.0	216
88	Coupled channel calculation of resonances in H+CO. Journal of Chemical Physics, 1986, 84, 4888-4893.	3.0	67
89	A quasi-classical trajectory study of collisions of fast H atoms with CO using an accurate ab initio potential surface. Chemical Physics Letters, 1985, 114, 520-525.	2.6	32
90	Polyatomic, anharmonic, vibrational-rotational analysis. Application to accurateab initio results for formaldehyde. Journal of Computational Chemistry, 1985, 6, 13-27.	3.3	103

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91	The photoelectron spectroscopy of HOâ^'2. Journal of Chemical Physics, 1985, 83, 5400-5406.	3.0	41
92	Inclusion and assessment of Rennerâ€"Teller coupling in transition state theory for Î states: Application to O(3P)+H2. Journal of Chemical Physics, 1985, 82, 1866-1872.	3.0	17
93	Vibrational energy levels of formaldehyde. Journal of Chemical Physics, 1985, 82, 4155-4165.	3.0	187
94	Approximate Quantum Approaches to the Calculation of Resonances in Reactive and Nonreactive Scattering. ACS Symposium Series, 1984, , 43-62.	0.5	1
95	Quantum chemical calculations using the floating point systems, Inc. Model 164 attached processor. International Journal of Quantum Chemistry, 1983, 24, 613-622.	2.0	2
96	An ab initio determination of the rate constant for H2+C2Hâ†'H+C2H2. Journal of Chemical Physics, 1982, 76, 5172-5173.	3.0	44
97	An ab initio determination of the rate constant for H+H2CO â†'H2+HCO. Journal of Chemical Physics, 1982, 76, 4296-4297.	3.0	15
98	Proton transfers in hydrogen-bonded systems. 2. Electron correlation effects in diamminehydrogen(1+). Journal of the American Chemical Society, 1981, 103, 2169-2173.	13.7	75
99	Ab initio studies of (1,2)-hydrogen migrations in open-shell hydrocarbons: vinyl radical, ethyl radical, and triplet methylcarbene. Journal of the American Chemical Society, 1981, 103, 7469-7475.	13.7	89
100	Proton transfers in hydrogen bonded systems. Electron correlation effects in (H3NHOH2)+. Chemical Physics Letters, 1981, 79, 39-42.	2.6	20
101	The mechanism of the ene reaction of singlet oxygen with olefins. Journal of the American Chemical Society, 1980, 102, 439-449.	13.7	119
102	Mechanistic implications of the stereochemistry of singlet oxygen-olefin reactions. Tetrahedron Letters, 1978, 19, 747-750.	1.4	26
103	Methylene: ab initio vibronic analysis and reinterpretation of the spectroscopic and negative ion photoelectron experiments. Chemical Physics Letters, 1978, 55, 217-220.	2.6	79
104	Mechanisms of gas-phase and liquid-phase ozonolysis. Journal of the American Chemical Society, 1978, 100, 7180-7188.	13.7	162
105	Abinitiostudies on the singletâ€"triplet splitting of methylene (CH2). Journal of Chemical Physics, 1977, 67, 1777-1779.	3.0	63
106	Ab initio theoretical studies of the Rydberg states of formaldehyde. Journal of the American Chemical Society, 1977, 99, 677-683.	13.7	60
107	Theoretical studies of the low-lying states of vinylidene. Journal of the American Chemical Society, 1977, 99, 2919-2925.	13.7	64
108	Ab initio theoretical results on the stability of cyclic ozone. Journal of Chemical Physics, 1977, 67, 2377.	3.0	43

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109	Intermediates in the chemiluminescent reaction of singlet oxygen with ethylene. Ab initio studies. Journal of the American Chemical Society, 1977, 99, 4520-4523.	13.7	63
110	The generalized valence bond description of the low-lying states of ketene. Journal of the American Chemical Society, 1976, 98, 6093-6099.	13.7	24
111	Triplet states of the amide group. Trapped electron spectra of formamide and related molecules. Chemical Physics Letters, 1975, 36, 589-593.	2.6	53
112	Generalized valence bond description of the valence states of formamide. Journal of the American Chemical Society, 1975, 97, 6300-6305.	13.7	36