Weston Thatcher Borden

List of Publications by Year
in descending order

75 papers	3,679 citations	172207 29 h-index	128067 60 g-index
75 all docs	75 docs citations	75 times ranked	2570 citing authors

#	Article	IF	Citations
1	Effects of electron repulsion in conjugated hydrocarbon diradicals. Journal of the American Chemical Society, 1977, 99, 4587-4594.	6.6	623
2	Violations of Hund's Rule in Non-Kekule Hydrocarbons: Theoretical Prediction and Experimental Verification. Accounts of Chemical Research, 1994, 27, 109-116.	7.6	290
3	The Importance of Including Dynamic Electron Correlation inab InitioCalculations. Accounts of Chemical Research, 1996, 29, 67-75.	7.6	240
4	The Interplay of Theory and Experiment in the Study of Phenylnitrene. Accounts of Chemical Research, 2000, 33, 765-771.	7.6	225
5	Carbon Tunneling from a Single Quantum State. Science, 2003, 299, 867-870.	6.0	194
6	Dioxygen: What Makes This Triplet Diradical Kinetically Persistent?. Journal of the American Chemical Society, 2017, 139, 9010-9018.	6.6	147
7	Annelated Semibullvalenes:Â A Theoretical Study of How They â€œCopeâ€•with Strain. Journal of the American Chemical Society, 1997, 119, 5921-5929.	6.6	121
8	The synergy between qualitative theory, quantitative calculations, and direct experiments in understanding, calculating, and measuring the energy differences between the lowest singlet and triplet states of organic diradicals. Physical Chemistry Chemical Physics, 2011, 13, 11792.	1.3	101
9	Reactions that involve tunneling by carbon and the role that calculations have played in their study. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 20-46.	6.2	93
10	Calculations on Open-Shell Molecules: A Beginner's Guide. Reviews in Computational Chemistry, 2007, , 1-97.	1.5	77
11	Why Are Methylenecyclopropane and 1-Methylcylopropene More â€œStrainedâ€•than Methylcyclopropane?. Journal of the American Chemical Society, 1997, 119, 5930-5933.	6.6	75
12	The Lowest Singlet and Triplet States of the Oxyallyl Diradical. Angewandte Chemie - International Edition, 2009, 48, 8509-8511.	7.2	75
13	Investigation of Cyclopropane Stereomutation by Quasiclassical Trajectories on an Analytical Potential Energy Surface. Journal of the American Chemical Society, 1997, 119, 5253-5254.	6.6	69
14	Ab initio calculations of the relative strengths of the .pi. bonds in acetylene and ethylene and of their effect on the relative energies of .pi.-bond addition reactions. Journal of the American Chemical Society, 1991, 113, 6750-6755.	6.6	68
15	Qualitative Methods for Predicting the Ground States of Non-Kekule Hydrocarbons and the Effects of Heteroatom Substitution on the Ordering of the Electronic States. Molecular Crystals and Liquid Crystals, 1993, 232, 195-218.	0.3	68
16	Ab initio MCSCF and CI calculations of the singlet-triplet energy differences in oxyallyl and in dimethyloxyallyl. Journal of the American Chemical Society, 1990, 112, 1751-1754.	6.6	66
17	Ab initio calculations on m-quinone. The ground state is a triplet. Journal of the American Chemical Society, 1992, 114, 7549-7552.	6.6	65
18	Why Are Nitrenes More Stable than Carbenes? An Ab Initio Study. Journal of the American Chemical Society, 1998, 120, 3499-3503.	6.6	64

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19	Computational Study of Reductive Elimination Reactions to Form Câ^'H Bonds from Platinum(II) and Platinum(IV) Centers with Strongly Coordinating Trimethylphosphine Ligands. Organometallics, 2001, 20, 2669-2678.	1.1	62
20	Potential surface for the methylenecyclopropane rearrangement. Journal of the American Chemical Society, 1982, 104, 967-972.	6.6	60
21	Spectroscopic Characterization, Computational Investigation, and Comparisons of ECX^{â€“} (E = As, P, and N; X = S and O) Anions. Journal of the American Chemical Society, 2017, 139, 8922-8930.	6.6	48
22	Factors Controlling the Barriers to Degenerate Hydrogen Atom Transfers. Journal of the American Chemical Society, 2005, 127, 5794-5795.	6.6	44
23	Photoelectron Spectroscopic Study of the Oxyallyl Diradical. Journal of Physical Chemistry A, 2011, 115, 1634-1649.	1.1	43
24	Calculations on Tunneling in the Reactions of Noradamantyl Carbenes. Journal of the American Chemical Society, 2013, 135, 17274-17277.	6.6	42
25	The Cope Rearrangement of 1,5â€Dimethylsemibullvaleneâ€2(4)â€d₁: Experimental Evidence for Heavyâ€Atom Tunneling. Angewandte Chemie - International Edition, 2017, 56, 10746-10749.	7.2	42
26	A theoretical determination of the electron affinity of methylene. Journal of Chemical Physics, 1982, 77, 6134-6143.	1.2	39
27	Calculation of zero field splitting parameters for trimethylenemethane. Journal of Chemical Physics, 1981, 74, 2256-2259.	1.2	36
28	A theoretical study of paths for decomposition and rearrangement of dihydroxycarbene. Journal of Computational Chemistry, 1980, 1, 158-166.	1.5	31
29	Ab Initio Calculations on the Preferred Mode of Ring Opening in Silacyclopropane. Journal of the American Chemical Society, 1997, 119, 8012-8014.	6.6	30
30	Reinvestigation of the ordering of the low-lying electronic states of cyclobutanetetraone with CASPT2, CCSD(T), G3B3, ccCA, and CBS-QB3 calculations. Molecular Physics, 2009, 107, 863-870.	0.8	28
31	Computational Study of Isomerization Reactions of Silacyclopropene. Journal of Physical Chemistry A, 1999, 103, 4043-4048.	1.1	27
32	The Negative Ion Photoelectron Spectrum of meta-Benzoquinone Radical Anion (MBQ^{â€¢â€“}): A Joint Experimental and Computational Study. Journal of the American Chemical Society, 2014, 136, 3589-3596.	6.6	27
33	Formation of Ground State Triplet Diradicals from Annulated Rosarin Derivatives by Triprotonation. Journal of the American Chemical Society, 2015, 137, 9780-9783.	6.6	25
34	Configuration interaction calculations for 1Eâ€² trimethylenemethane. Journal of Chemical Physics, 1976, 64, 663-666.	1.2	23
35	Ab Initio CI Calculations of the Energy Difference between Trimethylenemethane and Butadiene. Israel Journal of Chemistry, 1983, 23, 105-108.	1.0	22
36	B3LYP calculations on bishomoaromaticity in substituted semibullvalenes*. Journal of Computational Chemistry, 2001, 22, 1565-1573.	1.5	22

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37	Isotope-Controlled Selectivity by Quantum Tunneling: Hydrogen Migration versus Ring Expansion in Cyclopropylmethylcarbenes. Journal of the American Chemical Society, 2017, 139, 9097-9099.	6.6	22
38	CASSCF and CASPT2 Calculations on the Cleavage and Ring Inversion of Bicyclo[2.2.0]hexane Find that These Reactions Involve Formation of a Common Twist-Boat Diradical Intermediate. Journal of the American Chemical Society, 2001, 123, 4069-4072.	6.6	21
39	The Negative Ion Photoelectron Spectrum of Cyclopropane-1,2,3-Trione Radical Anion, (CO)3â€¢â€“ â€” A Joint Experimental and Computational Study. Journal of the American Chemical Society, 2014, 136, 12345-12354.	6.6	21
40	Ring Opening of Bicyclo[n.1.0]alkanones to 2-Cycloalkanone-1,3-diyls. Why Does Oxyallyl Diradical Formation Require Less Energy from Bicyclo[3.1.0]hexan-6-ones than from Bicyclo[1.1.0]butan-2-ones?. Journal of the American Chemical Society, 1996, 118, 4159-4166.	6.6	20
41	Ab Initio and Density Functional Theory Calculations on Heteroatom Analogues of Trimethylenemethane Radical Ions. Can a Quartet Be the Ground State?. Journal of Physical Chemistry A, 2002, 106, 2963-2969.	1.1	19
42	Negative ion photoelectron spectroscopy confirms the prediction that D_{3h} carbon trioxide (CO₃) has a singlet ground state. Chemical Science, 2016, 7, 1142-1150.	3.7	19
43	The Cope Rearrangement of 1,5â€Dimethylsemibullvaleneâ€2(4)â€d₁: Experimental Evidence for Heavyâ€Atom Tunneling. Angewandte Chemie, 2017, 129, 10886-10889.	1.6	18
44	What Accounts for the Remarkable Difference between Silabenzene and Phosphabenzene in Stability toward Dimerization?. Organometallics, 2000, 19, 2208-2214.	1.1	14
45	With a Little Help from My Friends: Forty Years of Fruitful Chemical Collaborations. Journal of Organic Chemistry, 2011, 76, 2943-2964.	1.7	14
46	Negative ion photoelectron spectroscopy of P₂N₃^{â^’}: electron affinity and electronic structures of P₂N₃Ë™. Chemical Science, 2016, 7, 4667-4675.	3.7	14
47	Diradicals â€“ A Fifty Year Fascination. ACS Symposium Series, 2015, , 251-303.	0.5	13
48	Variations in Rotational Barriers of Allyl and Benzyl Cations, Anions, and Radicals. Journal of Organic Chemistry, 2016, 81, 9576-9584.	1.7	13
49	Photoelectron Spectroscopy and Theoretical Studies of PCSe â^’ , AsCS â^’ , AsCSe â^’ , and NCSe â^’ : Insights into the Electronic Structures of the Whole Family of ECX â^’ Anions (E=N, P, As; X=O, S, Se). Angewandte Chemie - International Edition, 2019, 58, 15062-15068.	7.2	13
50	A Simple Mathematical Model for the Cooperative and Competitive Substituent Effects Found in the Cope Rearrangements of Phenyl-Substituted 1,5-Hexadienes. Journal of Chemical Theory and Computation, 2005, 1, 87-94.	2.3	12
51	Why Are Addition Reactions to N₂ Thermodynamically Unfavorable?. Journal of Physical Chemistry A, 2017, 121, 1140-1144.	1.1	12
52	Ab initio calculations find 2,2-disilylcyclopentane-1,3-diyl is a singlet diradical with a high barrier to ring closure. Theoretical Chemistry Accounts, 1999, 102, 207-225.	0.5	11
53	Symmetry breaking, diradicals, and Coping with and Coping without Ernest Davidson. Molecular Physics, 2002, 100, 337-347.	0.8	11
54	Negative Ion Photoelectron Spectroscopy Confirms the Prediction that 1,2,4,5-Tetraoxatetramethylenebenzene Has a Singlet Ground State. Journal of the American Chemical Society, 2015, 137, 9094-9099.	6.6	11

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55	The origin of Felkinâ€“Anh control from an electropositive substituent adjacent to the carbonyl groupâ€Šâ€. Perkin Transactions II RSC, 2001, , 331-338.	1.1	9
56	VIOLATIONS OF HUND'S RULE IN ORGANIC DIRADICALS â€“ WHERE TO LOOK FOR VIOLATIONS AND HOW TO IDENTIFY THEM. , 1997, , 171-195.		8
57	Does Formation of Singlet Propane-1,3-diyl from Propane Deviate from Bond Enthalpy Additivity? Results of Ab Initio Calculations That Bear on the Existence of the Benson Barrier to Diradical Ring Closureâ€. Journal of Physical Chemistry A, 2004, 108, 3024-3029.	1.1	7
58	A Joint Experimental and Computational Study of the Negative Ion Photoelectron Spectroscopy of the 1-Phospha-2,3,4-triazolate Anion, HCPN₃^{â€“}. Journal of Physical Chemistry A, 2016, 120, 6228-6235.	1.1	6
59	Negative Ion Photoelectron Spectroscopy Confirms the Prediction of a Singlet Ground State for the 1,8-Naphthoquinone Diradical. Journal of Physical Chemistry A, 2019, 123, 3142-3148.	1.1	6
60	Experimental and Theoretical Studies of the F^{â€¢} + Hâ€“F Transition-State Region by Photodetachment of [Fâ€“Hâ€“F]^{â¯}. Journal of Physical Chemistry A, 2017, 121, 7895-7902.	1.1	5
61	Negative Ion Photoelectron Spectroscopy Confirms the Prediction of the Relative Energies of the Low-Lying Electronic States of 2,7-Naphthoquinone. Journal of Physical Chemistry A, 2018, 122, 4838-4844.	1.1	5
62	Effects of CF2 group pyramidalization in the 1,1,3,3-tetrafluoropropenyl anion. Journal of Physical Organic Chemistry, 1990, 3, 635-638.	0.9	4
63	The effects of orbital interactions on the geometries of some annelated benzenes. Theoretical Chemistry Accounts, 2011, 130, 261-268.	0.5	4
64	Cooperative and competitive effects associated with Fe(CO)₃binding to annelated benzenes. Chemical Science, 2013, 4, 516-525.	3.7	4
65	H. C. Longuet-Higgins: The Man and His Science. ACS Symposium Series, 2013, , 155-195.	0.5	4
66	Theoretical Analysis of the Fragmentation of (CO)5: A Symmetry-Allowed Highly Exothermic Reaction that Follows a Stepwise Pathway. Journal of Organic Chemistry, 2015, 80, 11788-11793.	1.7	4
67	Calculations of the energies of the lowâ€lying electronic states of dioxatrimethylenemethane (H₂CCO₂) and prediction of the negative ion photoelectron (NIPE) spectrum of its radical anion. Journal of Physical Organic Chemistry, 2017, 30, e3594.	0.9	4
68	Calculations of the relative energies of the lowâ€lying electronic states of 2,7â€naphthoquinodimethane and 2,7â€naphthoquinone. Substitution of oxygen for CH₂ is predicted to increase the singletâ€triplet energy difference (Î”E_{ST}). Journal of Physical Organic Chemistry, 2018, 31, e3824.	0.9	4
69	Calculations on 1,8â€naphthoquinone predict that the ground state of this diradical is a singlet. Journal of Computational Chemistry, 2019, 40, 119-126.	1.5	4
70	Ab initiocoupled-cluster and multi-reference configuration interaction studies of the low-lying electronic states of 1,2,3,4-cyclobutanetetraone. Molecular Physics, 2016, 114, 695-708.	0.8	3
71	Photoelectron Spectroscopy and Theoretical Studies of PCSe â¯ , AsCS â¯ , AsCSe â¯ , and NCSe â¯ : Insights into the Electronic Structures of the Whole Family of ECX â¯ Anions (E=N, P, As; X=O, S, Se). Angewandte Chemie, 2019, 131, 15206-15212.	1.6	3
72	When is H3 stable to asymmetric distortion?. Theoretica Chimica Acta, 1986, 69, 171-174.	0.9	2

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73	The Unpredictability of Research Directions and the Synergy between Theory and Experiment in Physicalâ€Organic Chemistry. Israel Journal of Chemistry, 2016, 56, 16-24.	1.0	2
74	The Partnership between Electronic Structure Calculations and Experiments in the Study of Reactive Intermediates. , 2005, , 961-1004.		1
75	Nucleusâ€independent chemical shift analysis of the electronic states of the (<scp>CO</scp>)₄, (<scp>CS</scp>)₄, and (<scp>CS</scp>e)₄ molecules. Journal of Computational Chemistry, 2016, 37, 46-48.	1.5	0