Robert D Bach

List of Publications by Year
in descending order

78 papers	3,709 citations	101543 36 h-index	138484 58 g-index
80 all docs	80 docs citations	80 times ranked	3114 citing authors

#	Article	IF	Citations
1	A Reassessment of the Bond Dissociation Energies of Peroxides. Anab InitioStudy. Journal of the American Chemical Society, 1996, 118, 12758-12765.	13.7	262
2	Strain Energy of Small Ring Hydrocarbons. Influence of Câ”H Bond Dissociation Energies. Journal of the American Chemical Society, 2004, 126, 4444-4452.	13.7	228
3	Electronic structure and reactivity of dioxirane and carbonyl oxide. Journal of the American Chemical Society, 1992, 114, 7207-7217.	13.7	165
4	Mechanism of Thiolateâ”Disulfide Interchange Reactions in Biochemistry. Journal of Organic Chemistry, 2008, 73, 12-21.	3.2	124
5	Performance of the B3LYP/ECP DFT Calculations of Iron-Containing Compounds. Journal of Physical Chemistry A, 1997, 101, 316-323.	2.5	123
6	The performance of B3-LYP density functional theory in describing SN2 reactions at saturated carbon. Chemical Physics Letters, 1996, 260, 558-564.	2.6	118
7	The Effect of Carbonyl Substitution on the Strain Energy of Small Ring Compounds and Their Six-Member Ring Reference Compounds. Journal of the American Chemical Society, 2006, 128, 4598-4611.	13.7	106
8	Nature of the Transition Structure for Alkene Epoxidation by Peroxyformic Acid, Dioxirane, and Dimethyldioxirane:Â A Comparison of B3LYP Density Functional Theory with Higher Computational Levels. Journal of Physical Chemistry A, 1997, 101, 6092-6100.	2.5	102
9	Ring Strain Energy in the Cyclooctyl System. The Effect of Strain Energy on [3 + 2] Cycloaddition Reactions with Azides. Journal of the American Chemical Society, 2009, 131, 5233-5243.	13.7	96
10	Oxidation of Amines and Sulfides with Hydrogen Peroxide and Alkyl Hydrogen Peroxide. The Nature of the Oxygen-Transfer Step. Journal of the American Chemical Society, 1994, 116, 5379-5391.	13.7	87
11	The â€œSomersaultâ€•Mechanism for the P-450 Hydroxylation of Hydrocarbons. The Intervention of Transient Inverted Metastable Hydroperoxides. Journal of the American Chemical Society, 2006, 128, 1474-1488.	13.7	81
12	Mechanism of Acid-Catalyzed Epoxidation of Alkenes with Peroxy Acids. Journal of Organic Chemistry, 1997, 62, 5191-5197.	3.2	79
13	Theoretical model for electrophilic oxygen-atom insertion into hydrocarbons. Journal of the American Chemical Society, 1993, 115, 5768-5775.	13.7	70
14	Nature of the transition structure for oxygen atom transfer from a hydroperoxide. Theoretical comparison between water oxide and ammonia oxide. Journal of the American Chemical Society, 1991, 113, 6001-6011.	13.7	69
15	The Effect of Substitutents on the Strain Energies of Small Ring Compounds. Journal of Organic Chemistry, 2002, 67, 2588-2599.	3.2	67
16	Molecular orbital approach to the mechanism of electrophilic additions to olefins. Journal of the American Chemical Society, 1970, 92, 5589-5602.	13.7	66
17	Influence of Electrostatic Effects on Activation Barriers in Enzymatic Reactions:Â Pyridoxal 5â€˜-Phosphate-Dependent Decarboxylation of Î±-Amino Acids. Journal of the American Chemical Society, 1999, 121, 6542-6555.	13.7	66
18	High-Level Computational Study of the Stereoelectronic Effects of Substituents on Alkene Epoxidations with Peroxyformic Acid. Journal of the American Chemical Society, 1998, 120, 9902-9910.	13.7	65

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19	Relative Reactivity of Peracids versus Dioxiranes (DMDO and TFDO) in the Epoxidation of Alkenes. A Combined Experimental and Theoretical Analysis. Journal of the American Chemical Society, 2003, 125, 924-934.	13.7	63
20	The Nature of the Transition Structure for the Oxidation of Alkanes with Dioxiranes. Journal of the American Chemical Society, 1998, 120, 10528-10533.	13.7	60
21	Effect of Geminal Substitution on the Strain Energy of Dioxiranes. Origin of the Low Ring Strain of Dimethyldioxiraneâ€. Journal of Organic Chemistry, 2002, 67, 3884-3896.	3.2	58
22	Oxidation of Alkenes, Sulfides, Amines, and Phosphines with Peroxynitrous Acid:Â Comparison with Other Oxidants Such as Peroxyformic Acid and Dimethyldioxirane. Journal of the American Chemical Society, 1998, 120, 775-783.	13.7	57
23	Thermochemistry of Iron Chlorides and Their Positive and Negative Ions. The Journal of Physical Chemistry, 1996, 100, 8770-8776.	2.9	56
24	Transition structure for the epoxidation of alkenes with peroxy acids. A theoretical study. Journal of the American Chemical Society, 1991, 113, 2338-2339.	13.7	55
25	The Energetics of Valence Isomerization in the Norbornadieneâ"Quadricyclane System. Journal of Organic Chemistry, 1996, 61, 4845-4847.	3.2	54
26	Molecular asymmetry. IX. Partial resolution and asymmetric synthesis of 1,2-cyclononadiene. Journal of the American Chemical Society, 1970, 92, 1243-1247.	13.7	53
27	Electronic Factors Influencing the Decarboxylation of Î²-Keto Acids. A Model Enzyme Study. Journal of Organic Chemistry, 1996, 61, 6346-6353.	3.2	51
28	On the Origin of Substrate Directing Effects in the Epoxidation of Allyl Alcohols with Peroxyformic Acid. Journal of the American Chemical Society, 1998, 120, 680-685.	13.7	50
29	Mechanism of oxygen transfer from oxaziridine to ethylene: the consequences of HOMO-HOMO interactions on frontier orbital narrowing. Journal of the American Chemical Society, 1984, 106, 1410-1415.	13.7	46
30	On the mechanism of metal-catalyzed epoxidation: a model for the bonding in peroxo-metal complexes. Journal of the American Chemical Society, 1984, 106, 6098-6099.	13.7	45
31	Computational Study of the Thermochemistry of C5H5+Isomers:Â Which C5H5+Isomer Is the Most Stable?. The Journal of Physical Chemistry, 1996, 100, 10952-10955.	2.9	42
32	The Transition State for the Hydroxylation of Saturated Hydrocarbons with Hydroperoxonium Ion. Journal of the American Chemical Society, 1994, 116, 10103-10109.	13.7	41
33	Relative Nucleophilicity: The Role of Solvation and Thermodynamics. Journal of the American Chemical Society, 1995, 117, 8586-8593.	13.7	41
34	Theoretical Model for Pyruvoyl-Dependent Enzymatic Decarboxylation of Î±-Amino Acids. Journal of the American Chemical Society, 1997, 119, 11725-11733.	13.7	41
35	Mechanism of oxygen atom transfer from oxaziridine to a lithium enolate. A theoretical study. Journal of Organic Chemistry, 1992, 57, 613-618.	3.2	39
36	Structure and reactivity of diamidoiron(III) hydroperoxide. The mechanism of oxygen-atom transfer to ammonia. Journal of the American Chemical Society, 1993, 115, 8763-8769.	13.7	37

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37	Bond Dissociation Energy of Peroxides Revisited. Journal of Physical Chemistry A, 2020, 124, 4742-4751.	2.5	37
38	Computational study on nature of transition structure for oxygen transfer from dioxirane and carbonyloxide. Journal of Computational Chemistry, 1998, 19, 1353-1369.	3.3	35
39	A Theoretical Study of the Effect of a Tetraalkylammonium Counterion on the Hydrogen Bond Strength inZ-Hydrogen Maleate. Journal of the American Chemical Society, 2001, 123, 7134-7145.	13.7	35
40	Electronic Requirements for Oxygen Atom Transfer from Alkyl Hydroperoxides. Model Studies on Multisubstrate Flavin-Containing Monooxygenases. Journal of Physical Chemistry B, 2003, 107, 12851-12861.	2.6	35
41	Câ^'HÂ·Â·Â·Carboxylate Oxygen Hydrogen Bonding in Substrate Activation by Acyl-CoA Dehydrogenases:Â Synergy between the H-bonds. Journal of Physical Chemistry B, 2002, 106, 4325-4335.	2.6	34
42	Relative oxygen donor potential of dioxirane and carbonyl oxide. A theoretical study. Journal of the American Chemical Society, 1991, 113, 7031-7033.	13.7	33
43	The Curtius Rearrangement of Cyclopropyl and Cyclopropenoyl Azides. A Combined Theoretical and Experimental Mechanistic Study. Journal of Organic Chemistry, 2008, 73, 8189-8197.	3.2	31
44	Mechanism of N-Hydroxylation Catalyzed by Flavin-Dependent Monooxygenases. Journal of Organic Chemistry, 2015, 80, 2139-2147.	3.2	31
45	High-level computational study on the thermochemistry of saturated and unsaturated three- and four-membered nitrogen and phosphorus rings. International Journal of Quantum Chemistry, 1997, 62, 373-384.	2.0	30
46	The Bond Dissociation Energy of the Nâ€“O Bond. Journal of Physical Chemistry A, 2021, 125, 5014-5021.	2.5	30
47	The Role of Acid Catalysis in the Baeyerâ€“Villiger Reaction. A Theoretical Study. Journal of Organic Chemistry, 2012, 77, 6801-6815.	3.2	27
48	Theoretical investigation of the structure and rotational barriers of peroxyformimidic acid. The mechanism of stereomutation at the carbon-nitrogen double bond. Journal of the American Chemical Society, 1981, 103, 3275-3282.	13.7	26
49	Neutral versus Charged Species in Enzyme Catalysis. Classical and Free Energy Barriers for Oxygen Atom Transfer from C4a-Hydroperoxyflavin to Dimethyl Sulfide. Journal of Organic Chemistry, 2002, 67, 8653-8661.	3.2	26
50	Theoretical Analysis of Peroxynitrous Acid:Â Characterization of Its Elusive Biradicaloid (HOÂ·Â·Â·ONO) Singlet States. Journal of the American Chemical Society, 2003, 125, 16204-16205.	13.7	26
51	Chemical Behavior of the Biradicaloid (HOÂ·Â·Â·ONO) Singlet States of Peroxynitrous Acid. The Oxidation of Hydrocarbons, Sulfides, and Selenides. Journal of the American Chemical Society, 2005, 127, 3140-3155.	13.7	26
52	Inductive versus Coulombic Effects on the Barriers to Oxygen Atom Transfer from Alkyl Hydroperoxides. Model Studies on 4.alpha.-Flavin Hydroperoxide. Journal of the American Chemical Society, 1994, 116, 5392-5399.	13.7	25
53	A Computational Study of the Hydroxy-Group Directivity in the Peroxyformic Acid Epoxidation of the Chiral Allylic Alcohol (Z)-3-Methyl-3-penten-2-ol:Â Control of Threo Diastereoselectivity through Allylic Strain and Hydrogen Bonding. Journal of Organic Chemistry, 2000, 65, 6715-6728.	3.2	25
54	Theoretical study of oxygen atom transfer. The role of electron correlation. Journal of the American Chemical Society, 1990, 112, 7065-7067.	13.7	23

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55	Reactivity of Alkyl versus Silyl Peroxides. The Consequences of 1,2-Silicon Bridging on the Epoxidation of Alkenes with Silyl Hydroperoxides and Bis(trialkylsilyl)peroxides. Journal of Organic Chemistry, 2000, 65, 8629-8639.	3.2	21
56	Transient Inverted Metastable Iron Hydroperoxides in Fenton Chemistry. A Nonenzymatic Model for Cytochrome P450 Hydroxylation. Journal of Organic Chemistry, 2010, 75, 3705-3714.	3.2	21
57	The Rate-Limiting Step in P450 Hydroxylation of Hydrocarbons A Direct Comparison of the â€œSomersaultâ€•versus the â€œConsensusâ€•Mechanism Involving Compound I. Journal of Physical Chemistry A, 2010, 114, 9319-9332.	2.5	20
58	Effect of a Charge-Transfer Interaction on the Catalytic Activity of Acyl-CoA Dehydrogenase:Â A Theoretical Study of the Role of Oxidized Flavin. Journal of Physical Chemistry B, 2003, 107, 13229-13236.	2.6	19
59	Reassessment of the Level of Theory Required for the Epoxidation of Ethylene with Dioxiranes. Journal of Physical Chemistry A, 2004, 108, 6886-6892.	2.5	19
60	Spiro versus Planar Transition Structures in the Epoxidation of Simple Alkenes. A Reassessment of the Level of Theory Required. Journal of Physical Chemistry A, 2003, 107, 4300-4306.	2.5	18
61	Role of the Somersault Rearrangement in the Oxidation Step for Flavin Monooxygenases (FMO). A Comparison between FMO and Conventional Xenobiotic Oxidation with Hydroperoxides. Journal of Physical Chemistry A, 2011, 115, 11087-11100.	2.5	18
62	Theoretical model for an alternate mechanism for the cytochrome P-450 hydroxylation of quadricyclane. Journal of the American Chemical Society, 1995, 117, 10121-10122.	13.7	17
63	Catalytic Extraction Processing:Â An Elemental Recycling Technology. Environmental Science & Technology, 1996, 30, 2155-2167.	10.0	15
64	A High-Level Computational Study on the Thermochemistry and Thermal Decomposition of Sulfur Mustard (2,2â€˜-Dichloroethyl Sulfide):â€‰ A Chemical Warfare Agent. Journal of Physical Chemistry A, 1998, 102, 3438-3446.	2.5	14
65	Mechanistic Aspects Regarding the Elimination of H₂O₂ from C(4a)-Hydroperoxyflavin. The Role of a Proton Shuttle Required for H₂O₂ Elimination. Journal of Organic Chemistry, 2013, 78, 8585-8593.	3.2	14
66	A Theoretical Study of the Chorismate Synthase Reaction. Organic Letters, 2001, 3, 4137-4140.	4.6	13
67	The DMDO Hydroxylation of Hydrocarbons via the Oxygen Rebound Mechanism. Journal of Physical Chemistry A, 2016, 120, 840-850.	2.5	13
68	Optical Activity of transâ€Cycloâ€octene. Journal of Chemical Physics, 1970, 52, 6423-6424.	3.0	11
69	Potential for water catalysis in flavin-mediated hydroxylation. A theoretical study. Journal of the American Chemical Society, 1990, 112, 7064-7065.	13.7	11
70	Structure and dynamics of dicyandiamide: A theoretical study. Journal of Physical Organic Chemistry, 1991, 4, 125-134.	1.9	11
71	A model for adhesion-producing interactions of zinc oxide surfaces with alcohols, amines, and alkenes. Journal of Adhesion Science and Technology, 1994, 8, 249-259.	2.6	11
72	Model Studies onp-Hydroxybenzoate Hydroxylase. The Catalytic Role of Arg-214 and Tyr-201 in the Hydroxylation Step. Journal of the American Chemical Society, 2004, 126, 127-142.	13.7	11

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73	Structure and Mechanism for Alkane Oxidation and Alkene Epoxidation with Hydroperoxides, Î±-Hydroxy Hydroperoxides, and Peroxyacids: A Theoretical Study. Journal of Physical Chemistry A, 2019, 123, 9520-9530.	2.5	10
74	The Origin of Alkyl Substituent Effects on the Reactivity and Thermodynamic Stability of Alkenes. A Theoretical Study on Alkene Radical Cations. Israel Journal of Chemistry, 1983, 23, 97-104.	2.3	7
75	A Model for the Free Radical and Electrophilic Hydroxylation of Bicyclo[2.1.0]pentane. Journal of the American Chemical Society, 1994, 116, 3475-3482.	13.7	7
76	Computational insight into the effect of C(19) substituents on [1,7]-hydrogen shift in previtamin D. Theoretical Chemistry Accounts, 2003, 109, 170-175.	1.4	5
77	Mechanism of Orbital Interactions in the Sharpless Epoxidation with Ti(IV) Peroxides: A DFT Study. Journal of Physical Chemistry A, 2021, 125, 10541-10556.	2.5	4
78	Methylmercury(II) Nitrate and Methylmercury (II) Trifluoroacetate. Inorganic Syntheses, 2007, , 143-146.	0.3	1