Hajime Hirao

List of Publications by Year
in descending order

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178	9,953	30551	51423
papers	citations	56 h-index	90 g-index

208	208	208	10599
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Energy Decomposition Analysis of the Nature of Coordination Bonding at the Heme Iron Center in Cytochrome P450 Inhibition. Chemistry - an Asian Journal, 2022, 17, .	1.7	4
2	Controllable multiple-step configuration transformations in a thermal/photoinduced reaction. Nature Communications, 2022, 13, .	5.8	32
3	Energy Decomposition Analysis of the Nature of Coordination Bonding at the Heme Iron Center in Cytochrome P450 Inhibition. Chemistry - an Asian Journal, 2022, 17, .	1.7	3
4	An intramolecular photoswitch can significantly promote photoactivation of Pt(<scp>iv</scp>) prodrugs. Chemical Science, 2021, 12, 6536-6542.	3.7	31
5	Copper-Catalyzed Meta-Selective Arylation of Phenol Derivatives: An Easy Access to m-Aryl Phenols. ACS Catalysis, 2021, 11, 2302-2309.	5.5	14
6	Theoretical Study on the Aliphatic Câ”€H Bond Activation by a Mononuclear Manganese(III) Iodosylbenzene Complex. Bulletin of the Korean Chemical Society, 2021, 42, 1033-1036.	1.0	5
7	Intramolecular Alkeneâ€“Alkene Coupling via Rh(III)-Catalyzed Alkenyl sp² Câ€“H Functionalization: Divergent Pathways to Indene or Î±-Naphthol Derivatives. ACS Catalysis, 2021, 11, 11494-11500.	5.5	6
8	Mechanistic insight into hydroxamate transfer reaction mimicking the inhibition of zinc-containing enzymes. Chemical Science, 2020, 11, 9017-9021.	3.7	2
9	Titelbild: Direct Atomicâ€Level Imaging of Zeolites: Oxygen, Sodium in Naâ€LTA and Iron in Feâ€MFI (Angew.) Tj ETQq1 1 0.784314 rgB	1.6	0
10	Câ€“H oxidation enhancement on a gold nanoisland by atomic-undercoordination induced polarization. Physical Chemistry Chemical Physics, 2020, 22, 14458-14464.	1.3	4
11	Direct Atomicâ€Level Imaging of Zeolites: Oxygen, Sodium in Naâ€LTA and Iron in Feâ€MFI. Angewandte Chemie - International Edition, 2020, 59, 19510-19517.	7.2	28
12	Ultrafast Luminescent Light-Up Guest Detection Based on the Lock of the Host Molecular Vibration. Journal of the American Chemical Society, 2020, 142, 6690-6697.	6.6	185
13	Direct Atomicâ€Level Imaging of Zeolites: Oxygen, Sodium in Naâ€LTA and Iron in Feâ€MFI. Angewandte Chemie, 2020, 132, 19678-19685.	1.6	2
14	Chiral Monolayers with Achiral Tetrapod Molecules on Highly Oriented Pyrolytic Graphite. Journal of Physical Chemistry C, 2020, 124, 7760-7767.	1.5	12
15	Fluoresceinâ€Containing Superoxide Probes with a Modular Copperâ€Based Trigger. ChemPlusChem, 2020, 85, 653-658.	1.3	5
16	Phorbiplatin, a Highly Potent Pt(IV) Antitumor Prodrug That Can Be Controllably Activated by Red Light. CheM, 2019, 5, 3151-3165.	5.8	107
17	Molecular weight fractionation by confinement of polymer in one-dimensional pillar[5]arene channels. Nature Communications, 2019, 10, 479.	5.8	38
18	Hostâ€“Guest Complexation Using Pillar[5]arene Crystals: Crystalâ€Structure Dependent Uptake, Release, and Molecular Dynamics of an Alkane Guest. Chemistry - A European Journal, 2019, 25, 2497-2502.	1.7	14

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19	Hostâ€“Guest Complexation Using Pillar[5]arene Crystals: Crystalâ€Structure Dependent Uptake, Release, and Molecular Dynamics of an Alkane Guest. Chemistry - A European Journal, 2019, 25, 2378-2378.	1.7	0
20	Applications of Computational Chemistry to Selected Problems of Transition-Metal Catalysis in Biological and Nonbiological Systems. Challenges and Advances in Computational Chemistry and Physics, 2019, , 463-486.	0.6	1
21	Copperâ€Catalyzed Asymmetric Arylation of N â€Heteroaryl Aldimines: Elementary Step of a 1,4â€Insertion. Angewandte Chemie, 2019, 131, 2731-2735.	1.6	2
22	Copperâ€Catalyzed Asymmetric Arylation of Nâ€Heteroaryl Aldimines: Elementary Step of a 1,4â€Insertion. Angewandte Chemie - International Edition, 2019, 58, 2705-2709.	7.2	15
23	Palladiumâ€Catalyzed paraâ€Selective Alkylation of Electronâ€Deficient Arenes. Angewandte Chemie - International Edition, 2018, 57, 6294-6298.	7.2	59
24	Analytical hessian fitting schemes for efficient determination of forceâ€constant parameters in molecular mechanics. Journal of Computational Chemistry, 2018, 39, 307-318.	1.5	8
25	Separation of Linear and Branched Alkanes Using Hostâ€“Guest Complexation of Cyclic and Branched Alkane Vapors by Crystal State Pillar[6]arene. Angewandte Chemie, 2018, 130, 1608-1611.	1.6	30
26	Separation of Linear and Branched Alkanes Using Hostâ€“Guest Complexation of Cyclic and Branched Alkane Vapors by Crystal State Pillar[6]arene. Angewandte Chemie - International Edition, 2018, 57, 1592-1595.	7.2	101
27	How Does CO₂ React with Styrene Oxide in Co-MOF-74 and Mg-MOF-74? Catalytic Mechanisms Proposed by QM/MM Calculations. Journal of Physical Chemistry C, 2018, 122, 503-514.	1.5	25
28	Ferrihydrite Particle Encapsulated within a Molecular Organic Cage. Journal of the American Chemical Society, 2018, 140, 17753-17759.	6.6	48
29	Facile Activation of Homoatomic Ïƒ Bonds in White Phosphorus and Diborane by a Diboraallene. Angewandte Chemie, 2018, 130, 15917-15921.	1.6	12
30	Facile Activation of Homoatomic Ïƒ Bonds in White Phosphorus and Diborane by a Diboraallene. Angewandte Chemie - International Edition, 2018, 57, 15691-15695.	7.2	30
31	Zwitterionic Inorganic Benzene Valence Isomer with Ïƒ-Bonding between Two Ï€-Orbitals. Journal of the American Chemical Society, 2018, 140, 11921-11925.	6.6	14
32	Revisiting the catalytic mechanism of Moâ€“Cu carbon monoxide dehydrogenase using QM/MM and DFT calculations. Physical Chemistry Chemical Physics, 2018, 20, 18938-18948.	1.3	19
33	Hydrodehalogenation of Haloarenes by a Sodium Hydrideâ€“Iodide Composite. Angewandte Chemie - International Edition, 2017, 56, 1840-1844.	7.2	81
34	Selective and Catalyst-free Oxidation of D-Glucose to D-Glucuronic acid induced by High-Frequency Ultrasound. Scientific Reports, 2017, 7, 40650.	1.6	46
35	The mechanism of an asymmetric ring-opening reaction of epoxide with amine catalyzed by a metalâ€“organic framework: insights from combined quantum mechanics and molecular mechanics calculations. Dalton Transactions, 2017, 46, 3470-3481.	1.6	35
36	Hybrid computational approaches for deriving quantum mechanical insights into metalâ€“organic frameworks. Tetrahedron Letters, 2017, 58, 2309-2317.	0.7	15

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37	Kinetics and DFT Studies of Photoredox Carbonâ€“Carbon Bond Cleavage Reactions by Molecular Vanadium Catalysts under Ambient Conditions. ACS Catalysis, 2017, 7, 4682-4691.	5.5	74
38	A reaction mode of carbene-catalysed aryl aldehyde activation and induced phenol OH functionalization. Nature Communications, 2017, 8, 15598.	5.8	55
39	Using Voltammetry to Measure the Relative Hydrogenâ€Bonding Strengths of Pyridine and Its Derivatives in Acetonitrile. ChemPhysChem, 2017, 18, 2250-2257.	1.0	6
40	Hydrodehalogenation of Haloarenes by a Sodium Hydrideâ€“Iodide Composite. Angewandte Chemie, 2017, 129, 1866-1870.	1.6	22
41	Pdâ€Catalyzed, Ligandâ€Enabled Stereoselective 1,2â€Iodine(III) Shift/1,1â€Carboxyalkynylation of Alkynylbenziodoxoles. Chemistry - A European Journal, 2017, 23, 1521-1525.	1.7	35
42	Al₂O₃ Surface Complexation for Photocatalytic Organic Transformations. Journal of the American Chemical Society, 2017, 139, 269-276.	6.6	64
43	Infrared Investigation of Dynamic Behavior of BrÃ¸nsted Acid Sites on Zeolites at High Temperatures. Journal of Physical Chemistry C, 2017, 121, 25411-25420.	1.5	35
44	The Dual Roles of Phenylenediamines: Using their Voltammetric Behavior to Measure the Hydrogen Donor and Acceptor Abilities of Alcohols in Acetonitrile. ChemPhysChem, 2017, 18, 3562-3569.	1.0	2
45	Highly Selective and Efficient Ring Hydroxylation of Alkylbenzenes with Hydrogen Peroxide and an Osmium(VI) Nitrido Catalyst. Angewandte Chemie, 2017, 129, 12428-12431.	1.6	0
46	Gold(I)/Gold(III)-Catalyzed Selective Synthesis of N-Sulfonyl Enaminone Isomers from Sulfonamides and Ynones via Two Distinct Reaction Pathways. Organic Letters, 2017, 19, 4734-4737.	2.4	32
47	Front Cover Picture: Acceptorless and Baseâ€free Dehydrogenation of Cyanohydrin with (Î·⁶â€Arene)halide(Bidentate Phosphine)ruthenium(II) Complex (Adv. Synth. Catal. 19/2017). Advanced Synthesis and Catalysis, 2017, 359, 3273-3273.	2.1	0
48	Lewis Acid-Catalyzed Selective [2 + 2]-Cycloaddition and Dearomatizing Cascade Reaction of Aryl Alkynes with Acrylates. Journal of the American Chemical Society, 2017, 139, 13570-13578.	6.6	65
49	Electrostatic Catalyst Generated from Diazadiborinine for Carbonyl Reduction. CheM, 2017, 3, 134-151.	5.8	34
50	Highly Selective and Efficient Ring Hydroxylation of Alkylbenzenes with Hydrogen Peroxide and an Osmium(VI) Nitrido Catalyst. Angewandte Chemie - International Edition, 2017, 56, 12260-12263.	7.2	21
51	Alkane-length sorting using activated pillar[5]arene crystals. Chemical Communications, 2017, 53, 8577-8580.	2.2	44
52	Acceptorless and Baseâ€free Dehydrogenation of Cyanohydrin with (Î·⁶â€Arene)halide(Bidentate Phosphine)ruthenium(II) Complex. Advanced Synthesis and Catalysis, 2017, 359, 3292-3298.	2.1	3
53	Enhanced selectivity in mixed matrix membranes for CO2 capture through efficient dispersion of amine-functionalized MOF nanoparticles. Nature Energy, 2017, 2, .	19.8	428
54	Understanding the Origins of Nucleophilic Hydride Reactivity of a Sodium Hydrideâ€“Iodide Composite. Chemistry - A European Journal, 2016, 22, 7108-7114.	1.7	44

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55	Enantioselective Sulfoxidation Catalyzed by a Bisguanidinium Diphosphatobisperoxotungstate Ion Pair. Angewandte Chemie - International Edition, 2016, 55, 7101-7105.	7.2	52
56	Integrated Experimental and Theoretical Study of Shape-Controlled Catalytic Oxidative Coupling of Aromatic Amines over CuO Nanostructures. ACS Omega, 2016, 1, 1121-1138.	1.6	39
57	Hydride Reduction by a Sodium Hydrideâ€“Iodide Composite. Angewandte Chemie, 2016, 128, 3783-3787.	1.6	29
58	Nickelâ€Catalyzed Enantioselective Reductive Amination of Ketones with Both Arylamines and Benzhydrazide. Angewandte Chemie, 2016, 128, 12262-12266.	1.6	30
59	Partial hessian fitting for determining force constant parameters in molecular mechanics. Journal of Computational Chemistry, 2016, 37, 2349-2359.	1.5	19
60	Nickelâ€Catalyzed Enantioselective Reductive Amination of Ketones with Both Arylamines and Benzhydrazide. Angewandte Chemie - International Edition, 2016, 55, 12083-12087.	7.2	110
61	The First Synthesis of the Sterically Encumbered Adamantoid Phosphazane P₄(N^tBu)₆: Enabled by Mechanochemistry. Angewandte Chemie, 2016, 128, 12928-12932.	1.6	30
62	The First Synthesis of the Sterically Encumbered Adamantoid Phosphazane P₄(N^tBu)₆: Enabled by Mechanochemistry. Angewandte Chemie - International Edition, 2016, 55, 12736-12740.	7.2	98
63	Ambiphilic boron in 1,4,2,5-diazadiborinine. Nature Communications, 2016, 7, 11871.	5.8	84
64	Bisguanidinium dinuclear oxodiperoxomolybdosulfate ion pair-catalyzed enantioselective sulfoxidation. Nature Communications, 2016, 7, 13455.	5.8	48
65	Pd-Catalyzed Conversion of Alkynyl-Î»³-iodanes to Alkenyl-Î»³-iodanes via Stereoselective 1,2-Iodine(III) Shift/1,1-Hydrocarboxylation. Journal of the American Chemical Society, 2016, 138, 9105-9108.	6.6	61
66	Dioxygen binding to Fe-MOF-74: microscopic insights from periodic QM/MM calculations. Canadian Journal of Chemistry, 2016, 94, 1144-1150.	0.6	21
67	Fluorescent Porous Organic Frameworks Containing Molecular Rotors for Size-Selective Recognition. Chemistry of Materials, 2016, 28, 7889-7897.	3.2	101
68	Size-Dependent Catalytic Activity of Palladium Nanoparticles Fabricated in Porous Organic Polymers for Alkene Hydrogenation at Room Temperature. ACS Applied Materials & Interfaces, 2016, 8, 15307-15319.	4.0	109
69	Asymmetric Conjugate Addition of Organoboron Reagents to Common Enones Using Copper Catalysts. Journal of the American Chemical Society, 2016, 138, 742-745.	6.6	77
70	Hydride Reduction by a Sodium Hydrideâ€“Iodide Composite. Angewandte Chemie - International Edition, 2016, 55, 3719-3723.	7.2	78
71	Hydroamination of alkenyl N-arylhydrazones mediated by t-BuOK for the synthesis of nitrogen heterocycles. Organic Chemistry Frontiers, 2016, 3, 609-613.	2.3	12
72	To rebound or dissociate? This is the mechanistic question in Câ€“H hydroxylation by heme and nonheme metalâ€“oxo complexes. Chemical Society Reviews, 2016, 45, 1197-1210.	18.7	167

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73	Chapter 8. Key Concepts and Applications of ONIOM Methods. RSC Theoretical and Computational Chemistry Series, 2016, , 245-293.	0.7	4
74	Fabrication of Ruthenium Nanoparticles in Porous Organic Polymers: Towards Advanced Heterogeneous Catalytic Nanoreactors. Chemistry - A European Journal, 2015, 21, 19016-19027.	1.7	81
75	Diastereoâ€Divergent Synthesis of Saturated Azaheterocycles Enabled by tBuOKâ€Mediated Hydroamination of Alkenyl Hydrazones. Chemistry - A European Journal, 2015, 21, 19112-19118.	1.7	17
76	Insight into Enzymatic Nitrile Reduction: QM/MM Study of the Catalytic Mechanism of QueF Nitrile Reductase. ACS Catalysis, 2015, 5, 3740-3751.	5.5	28
77	An attempt to evaluate the effect of proton-coupled electron transfer on the H-abstraction step of the reaction between 1,1-dimethylhydrazine and cytochrome P450 compound I. Chemical Physics Letters, 2015, 621, 188-192.	1.2	11
78	Mechanistic Insights into Bicyclic Guanidine-Catalyzed Reactions from Microscopic and Macroscopic Perspectives. Journal of Organic Chemistry, 2015, 80, 5745-5752.	1.7	63
79	Electronic and magnetic properties of C60â€“Fenâ€“graphene intercalating nanostructures (n=1â€“6) predicted from first-principles calculations. Chemical Physics Letters, 2015, 618, 127-131.	1.2	1
80	Nickelâ€Catalyzed Asymmetric Transfer Hydrogenation of Hydrazones and Other Ketimines. Angewandte Chemie - International Edition, 2015, 54, 5112-5116.	7.2	138
81	Na, K-ATPase Î±3 is a death target of Alzheimer patient amyloid-Î² assembly. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E4465-74.	3.3	112
82	Estrogen Formation via H-Abstraction from the Oâ€“H Bond of gem-Diol by Compound I in the Reaction of CYP19A1: Mechanistic Scenario Derived from Multiscale QM/MM Calculations. ACS Catalysis, 2015, 5, 4175-4179.	5.5	22
83	Benzyne Formation in the Mechanism-Based Inactivation of Cytochrome P450 by 1-Aminobenzotriazole and N-Benzyl-1-Aminobenzotriazole: Computational Insights. ACS Catalysis, 2015, 5, 2952-2960.	5.5	17
84	Multiscale Model for a Metalâ€“Organic Framework: High-Spin Rebound Mechanism in the Reaction of the Oxoiron(IV) Species of Fe-MOF-74. ACS Catalysis, 2015, 5, 3287-3291.	5.5	50
85	Palladiumâ€Catalyzed Asymmetric Reductive Heck Reaction of Aryl Halides. Angewandte Chemie - International Edition, 2015, 54, 6531-6535.	7.2	148
86	Optimizing the lifetimes of phenoxonium cations derived from vitamin E via structural modifications. Organic and Biomolecular Chemistry, 2015, 13, 11732-11739.	1.5	8
87	Selective photocatalytic Câ€“C bond cleavage under ambient conditions with earth abundant vanadium complexes. Chemical Science, 2015, 6, 7130-7142.	3.7	142
88	Reversible [4 + 2] cycloaddition reaction of 1,3,2,5-diazadiborinine with ethylene. Chemical Science, 2015, 6, 7150-7155.	3.7	52
89	Measuring the Relative Hydrogenâ€Bonding Strengths of Alcohols in Aprotic Organic Solvents. ChemPhysChem, 2015, 16, 160-168.	1.0	20
90	Metalâ€Free Ïƒâ€Bond Metathesis in 1,3,2â€Diazaphospholeneâ€Catalyzed Hydroboration of Carbonyl Compounds. Angewandte Chemie - International Edition, 2015, 54, 190-194.	7.2	167

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91	Applications of density functional theory to iron-containing molecules of bioinorganic interest. Frontiers in Chemistry, 2014, 2, 14.	1.8	27
92	Metal-Free Ïƒ-Bond Metathesis in Ammonia Activation by a Diazadiphosphapentalene. Journal of the American Chemical Society, 2014, 136, 16764-16767.	6.6	75
93	Inorganicâ€Baseâ€Mediated Hydroamination of Alkenyl Oximes for the Synthesis of Cyclic Nitrones. Angewandte Chemie - International Edition, 2014, 53, 1959-1962.	7.2	47
94	CHâ€“Ïâ€ and CFâ€“Ïâ€ Interactions Lead to Structural Changes of Nâ€Heterocyclic Carbene Palladium Complexes. Angewandte Chemie - International Edition, 2014, 53, 1283-1287.	7.2	29
95	A Concerted Transfer Hydrogenolysis: 1,3,2â€Diazaphospholeneâ€Catalyzed Hydrogenation of Nï£¾N Bond with Ammoniaâ€“Borane. Angewandte Chemie - International Edition, 2014, 53, 3342-3346.	7.2	131
96	Tandem Insertionâ€“Cyclization Reaction of Isocyanides in the Synthesis of 1,4-Diaryl-1H-imidazoles: Presence of N-Arylformimidate Intermediate. Journal of Organic Chemistry, 2014, 79, 9231-9245.	1.7	64
97	Nanostructures of C₆₀â€“Metalâ€“Graphene (Metal = Ti, Cr, Mn, Fe, or Ni): A Spin-Polarized Density Functional Theory Study. Journal of Physical Chemistry C, 2014, 118, 21057-21065.	1.5	14
98	Stereoelectronic and Catalytic Properties of Chiral Cyclometalated Phospha-palladium and -platinum Complexes. Organometallics, 2014, 33, 6053-6058.	1.1	22
99	A General Palladiumâ€Catalyzed Method for Alkylation of Heteroarenes Using Secondary and Tertiary Alkyl Halides. Angewandte Chemie - International Edition, 2014, 53, 13573-13577.	7.2	127
100	A total synthesis of (+)-negamycin through isoxazolidine allylation. Organic and Biomolecular Chemistry, 2014, 12, 4879.	1.5	19
101	Effect of Protein Environment within Cytochrome P450cam Evaluated Using a Polarizable-Embedding QM/MM Method. Journal of Physical Chemistry B, 2014, 118, 2084-2092.	1.2	21
102	Regioselective Heck reaction of aliphatic olefins and aryl halides. Chemical Communications, 2013, 49, 10236.	2.2	42
103	Zwitterionic Baseâ€Stabilized Digermadistannacyclobutadiene and Tetragermacyclobutadiene. Chemistry - A European Journal, 2013, 19, 14726-14731.	1.7	25
104	First-principles modeling of C60â€“Crâ€“graphene nanostructures for supporting metal clusters. Physical Chemistry Chemical Physics, 2013, 15, 19395.	1.3	7
105	1â€(2â€²â€Anilinyl)propâ€2â€ynâ€1â€ol Rearrangement for Oxindole Synthesis. Chemistry - A European Journal, 2013, 19, 1978-1985.	1.7	19
106	Guanine binding to gold nanoparticles through nonbonding interactions. Physical Chemistry Chemical Physics, 2013, 15, 19284-19292.	1.3	29
107	ONIOM (DFT:MM) Study of the Catalytic Mechanism of myo-Inositol Monophosphatase: Essential Role of Water in Enzyme Catalysis in the Two-Metal Mechanism. Journal of Physical Chemistry B, 2013, 117, 833-842.	1.2	8
108	Electrochemical Properties of Phenols and Quinones in Organic Solvents are Strongly Influenced by Hydrogen-Bonding with Water. Journal of Physical Chemistry C, 2013, 117, 1081-1090.	1.5	60

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109	Abnormal N-Heterocyclic Carbene Gold(I) Complexes: Synthesis, Structure, and Catalysis in Hydration of Alkynes. Organometallics, 2013, 32, 164-171.	1.1	59
110	Comparative computational analysis of binding energies between several divalent first-row transition metals (Cr2+, Mn2+, Fe2+, Co2+, Ni2+, and Cu2+) and ligands (porphine, corrin, and TMC). Polyhedron, 2013, 52, 96-101.	1.0	23
111	Gold-Catalyzed Cycloisomerization of 1,6-Diyne Carbonates and Esters to 2,4a-Dihydro-1H-fluorenes. Journal of the American Chemical Society, 2013, 135, 7926-7932.	6.6	122
112	Water Complexes of Cytochrome P450: Insights from Energy Decomposition Analysis. Molecules, 2013, 18, 6782-6791.	1.7	42
113	Weak Arene Cï£¿Hâ‹…â‹…â‹…O Hydrogen Bonding in Palladiumâ€Catalyzed Arylation and Vinylation of Lactones. Angewandte Chemie - International Edition, 2013, 52, 5807-5812.	7.2	86
114	Palladiumâ€Catalyzed Asymmetric Intermolecular Cyclization. Angewandte Chemie - International Edition, 2013, 52, 8676-8680.	7.2	82
115	How Is a Metabolic Intermediate Formed in the Mechanismâ€Based Inactivation of Cytochrome P450 by Using 1,1â€Dimethylhydrazine: Hydrogen Abstraction or Nitrogen Oxidation?. Chemistry - A European Journal, 2013, 19, 7361-7369.	1.7	38
116	Achieving Vinylic Selectivity in Mizorokiâ€“Heck Reaction of Cyclic Olefins. Chemistry - A European Journal, 2013, 19, 6014-6020.	1.7	18
117	QM/MM Modeling of Environmental Effects on Electronic Transitions of the FMO Complex. Journal of Physical Chemistry B, 2013, 117, 3488-3495.	1.2	52
118	Importance of H-Abstraction in the Final Step of Nitrosoalkane Formation in the Mechanism-Based Inactivation of Cytochrome P450 by Amine-Containing Drugs. International Journal of Molecular Sciences, 2013, 14, 24692-24705.	1.8	21
119	Co²⁺/Co⁺ Redox Tuning in Methyltransferases Induced by a Conformational Change at the Axial Ligand. Inorganic Chemistry, 2012, 51, 5533-5538.	1.9	15
120	Co+â€“H interaction inspired alternate coordination geometries of biologically important cob(I)alamin: possible structural and mechanistic consequences for methyltransferases. Journal of Biological Inorganic Chemistry, 2012, 17, 1107-1121.	1.1	15
121	The ONIOM method: its foundation and applications to metalloenzymes and photobiology. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 327-350.	6.2	173
122	Pivotal Role of Water in Terminating Enzymatic Function: A Density Functional Theory Study of the Mechanism-Based Inactivation of Cytochromes P450. Journal of Physical Chemistry B, 2012, 116, 7787-7794.	1.2	20
123	Characteristic vibration patterns of odor compounds from bread-baking volatiles upon protein binding: density functional and ONIOM study and principal component analysis. Journal of Molecular Modeling, 2012, 18, 2227-2240.	0.8	7
124	The Effects of Protein Environment and Dispersion on the Formation of Ferric-Superoxide Species in myo-Inositol Oxygenase (MIOX): A Combined ONIOM(DFT:MM) and Energy Decomposition Analysis. Journal of Physical Chemistry B, 2011, 115, 11278-11285.	1.2	27
125	Disilylfluoronium Ionsâ€”Synthesis, Structure, and Bonding. Organometallics, 2011, 30, 4087-4096.	1.1	46
126	Theoretical Study of the Mechanism of Oxoiron(IV) Formation from H₂O₂ and a Nonheme Iron(II) Complex: Oâ€“O Cleavage Involving Proton-Coupled Electron Transfer. Inorganic Chemistry, 2011, 50, 6637-6648.	1.9	65

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127	Comparative Reactivity of Ferric-Superoxo and Ferryl-Oxo Species in Heme and Non-Heme Complexes. Journal of the American Chemical Society, 2011, 133, 20076-20079.	6.6	52
128	Computational Studies of Bacterial Resistance to Î²-Lactam Antibiotics: Mechanism of Covalent Inhibition of the Penicillin-Binding Protein 2a (PBP2a). Journal of Chemical Information and Modeling, 2011, 51, 3226-3234.	2.5	10
129	ONIOM(DFT:MM) Study of 2-Hydroxyethylphosphonate Dioxygenase: What Determines the Destinies of Different Substrates?. Journal of the American Chemical Society, 2011, 133, 14550-14553.	6.6	42
130	Which DFT Functional Performs Well in the Calculation of Methylcobalamin? Comparison of the B3LYP and BP86 Functionals and Evaluation of the Impact of Empirical Dispersion Correction. Journal of Physical Chemistry A, 2011, 115, 9308-9313.	1.1	91
131	Energy Decomposition Analysis of the Protein Environmental Effect: The Case of Cytochrome P450cam Compound I. Chemistry Letters, 2011, 40, 1179-1181.	0.7	14
132	Correlation diagram approach as a tool for interpreting chemistry: an introductory overview. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 337-349.	6.2	3
133	Ferric Superoxide and Ferric Hydroxide Are Used in the Catalytic Mechanism of Hydroxyethylphosphonate Dioxygenase: A Density Functional Theory Investigation. Journal of the American Chemical Society, 2010, 132, 17901-17909.	6.6	75
134	What is the Real Nature of Ferrous Soybean Lipoxygenase-1? A New Two-Conformation Model Based on Combined ONIOM(DFT:MM) and Multireference Configuration Interaction Characterization. Journal of Physical Chemistry Letters, 2010, 1, 901-906.	2.1	24
135	A Twoâ€State Reactivity Model Explains Unusual Kinetic Isotope Effect Patterns in Cï£¿H Bond Cleavage by Nonheme Oxoiron(IV) Complexes. Angewandte Chemie - International Edition, 2009, 48, 1291-1295.	7.2	111
136	Insights into the (Superoxo)Fe(III)Fe(III) Intermediate and Reaction Mechanism of myo-Inositol Oxygenase: DFT and ONIOM(DFT:MM) Study. Journal of the American Chemical Society, 2009, 131, 17206-17214.	6.6	60
137	QM/MM theoretical study of the pentacoordinate Mn(III) and resting states of manganese-reconstituted cytochrome P450cam. Journal of Biological Inorganic Chemistry, 2008, 13, 521-530.	1.1	10
138	A Twoâ€State Reactivity Rationale for Counterintuitive Axial Ligand Effects on the Cï£¿H Activation Reactivity of Nonheme Fe^{IV}ï£¾O Oxidants. Chemistry - A European Journal, 2008, 14, 1740-1756.	1.7	198
139	A reactive bond orbital investigation of the Dielsâ€Alder reaction between 1,3â€butadiene and ethylene: Energy decomposition, state correlation diagram, and electron density analyses. Journal of Computational Chemistry, 2008, 29, 1399-1407.	1.5	8
140	Experiment and Theory Reveal the Fundamental Difference between Twoâ€State and Singleâ€State Reactivity Patterns in Nonheme Fe^{IV}ï£¾O versus Ru^{IV}ï£¾O Oxidants. Angewandte Chemie - International Edition, 2008, 47, 3356-3359.	7.2	74
141	Which Oxidant is Really Responsible for Sulfur Oxidation by Cytochrome P450?. Angewandte Chemie - International Edition, 2008, 47, 8148-8148.	7.2	4
142	Which Oxidant is Really Responsible for Sulfur Oxidation by Cytochrome P450?. Angewandte Chemie, 2008, 120, 8267-8267.	1.6	0
143	Discovery of selective and nonpeptidic cathepsin S inhibitors. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 3959-3962.	1.0	23
144	4-Amino-2-cyanopyrimidines: Novel scaffold for nonpeptidic cathepsin S inhibitors. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 4642-4646.	1.0	20

#	Article	IF	Citations
145	Overcoming hERG issues for brain-penetrating cathepsin S inhibitors: 2-Cyanopyrimidines. Part 2. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 5280-5284.	1.0	25
146	Theoretical study of formic acid: A new look at the origin of the planar Z conformation and Câ€“O rotational barrier. Chemical Physics, 2008, 344, 213-220.	0.9	14
147	Effect of External Electric Fields on the Câˆ’H Bond Activation Reactivity of Nonheme Ironâˆ’Oxo Reagents. Journal of the American Chemical Society, 2008, 130, 3319-3327.	6.6	97
148	Electron Transfer Activation of Chromopyrrolic Acid by Cytochrome P450 En Route to the Formation of an Antitumor Indolocarbazole Derivative: Theory Supports Experiment. Journal of the American Chemical Society, 2008, 130, 7170-7171.	6.6	49
149	Compound I in Heme Thiolate Enzymes: A Comparative QM/MM Study. Journal of Physical Chemistry A, 2008, 112, 13128-13138.	1.1	32
150	Quantum Mechanical/Molecular Mechanical Study on the Mechanisms of Compound I Formation in the Catalytic Cycle of Chloroperoxidase: An Overview on Heme Enzymes. Journal of Physical Chemistry B, 2008, 112, 9490-9500.	1.2	60
151	Discovery of Orally Bioavailable Cathepsin S Inhibitors for the Reversal of Neuropathic Pain. Journal of Medicinal Chemistry, 2008, 51, 5502-5505.	2.9	36
152	Axial ligand tuning of a nonheme iron(IV)â€“oxo unit for hydrogen atom abstraction. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 19181-19186.	3.3	376
153	Reactivity patterns of cytochrome P450 enzymes: multifunctionality of the active species, and the two statesâ€“two oxidants conundrum. Natural Product Reports, 2007, 24, 533-552.	5.2	109
154	QM/MM Study of the Active Species of the Human Cytochrome P450 3A4, and the Influence Thereof of the Multiple Substrate Binding. Journal of Physical Chemistry B, 2007, 111, 13822-13832.	1.2	36
155	The Electronic Structure of Reduced Phosphovanadomolybdates and the Implications on Their Use in Catalytic Oxidation Initiated by Electron Transfer. Journal of Physical Chemistry C, 2007, 111, 7711-7719.	1.5	20
156	NR Transfer Reactivity of Azo-Compound I of P450. How Does the Nitrogen Substituent Tune the Reactivity of the Species toward CH and CC Activation?. Journal of Physical Chemistry B, 2007, 111, 10288-10299.	1.2	66
157	Reactivity of High-Valent Ironâ€“Oxo Species in Enzymes and Synthetic Reagents: A Tale of Many States. Accounts of Chemical Research, 2007, 40, 532-542.	7.6	507
158	Which Oxidant Is Really Responsible for Sulfur Oxidation by Cytochrome P450?. Angewandte Chemie - International Edition, 2007, 46, 8168-8170.	7.2	70
159	Reactive bond orbitals: A localized resonance-structure approach to charge transfer. Chemical Physics Letters, 2007, 443, 141-146.	1.2	21
160	Gauging the Relative Oxidative Powers of Compound I, Ferric-Hydroperoxide, and the Ferric-Hydrogen Peroxide Species of Cytochrome P450 Toward Câˆ’H Hydroxylation of a Radical Clock Substrate. Journal of the American Chemical Society, 2006, 128, 473-484.	6.6	66
161	Theoretical Analysis of the Structural and Electronic Properties of Metalloporphyrin Ï€-Cation Radicals. Journal of Physical Chemistry A, 2006, 110, 6091-6099.	1.1	32
162	Proton-Shuffle Mechanism of Oâˆ’O Activation for Formation of a High-Valent Oxoâˆ’Iron Species of Bleomycin. Journal of the American Chemical Society, 2006, 128, 16148-16158.	6.6	42

#	Article	IF	Citations
163	Two-State Reactivity in Alkane Hydroxylation by Non-Heme Ironâ”Oxo Complexes. Journal of the American Chemical Society, 2006, 128, 8590-8606.	6.6	331
164	On the identity and reactivity patterns of the â€œsecond oxidantâ€•of the T252A mutant of cytochrome P450cam in the oxidation of 5-methylenenylcamphor. Journal of Inorganic Biochemistry, 2006, 100, 2054-2068.	1.5	27
165	New Features in the Catalytic Cycle of Cytochrome P450 during the Formation of Compound I from Compound 0. Journal of Physical Chemistry B, 2005, 109, 19946-19951.	1.2	52
166	Sulfoxidation Mechanisms Catalyzed by Cytochrome P450 and Horseradish Peroxidase Models:â€‰ Spin Selection Induced by the Ligand,. Biochemistry, 2005, 44, 8148-8158.	1.2	74
167	Theoretical Investigation of Câ”H Hydroxylation by (N4Py)FeIVO2+:Â An Oxidant More Powerful than P450?. Journal of the American Chemical Society, 2005, 127, 8026-8027.	6.6	185
168	Theoretical Revisit of Regioselectivities of Dielsâ”Alder Reactions:Â Orbital-Based Reevaluation of Multicentered Reactivity in Terms of Reactive Hybrid Orbitals. Journal of Physical Chemistry A, 2005, 109, 816-824.	1.1	31
169	Generation of Orbitals that Control Molecular Reactivity:Â Projected Reactive Orbital Approach. Journal of Physical Chemistry A, 2005, 109, 7642-7647.	1.1	4
170	Two States and Two More in the Mechanisms of Hydroxylation and Epoxidation by Cytochrome P450. Journal of the American Chemical Society, 2005, 127, 13007-13018.	6.6	162
171	Theoretical Analysis of Lewis Basicity Based on Local Electron-Donating Ability. Origin of Basic Strength of Cyclic Amines. Journal of Organic Chemistry, 2004, 69, 7486-7494.	1.7	61
172	Rationale for the Acidity of Meldrum's Acid. Consistent Relation of Câ”H Acidities to the Properties of Localized Reactive Orbital. Journal of Organic Chemistry, 2004, 69, 4309-4316.	1.7	66
173	Theoretical Study of Reactivities in Electrophilic Aromatic Substitution Reactions:â€‰ Reactive Hybrid Orbital Analysis. Journal of Physical Chemistry A, 2003, 107, 2875-2881.	1.1	44
174	Transition-state optimization by the free energy gradient method: Application to aqueous-phase Menshutkin reaction between ammonia and methyl chloride. Chemical Physics Letters, 2001, 348, 350-356.	1.2	74
175	Theoretical Study of the Anomeric Effect in CH2ClOH. Journal of Physical Chemistry A, 2000, 104, 6499-6504.	1.1	27
176	Theoretical Study of Substituent Effects on the Lewis Acidâ”Base Property of Aminoboranes. Journal of Physical Chemistry A, 2000, 104, 6649-6655.	1.1	13
177	Theoretical Study ofEndoSelectivity in the Dielsâ”Alder Reactions between Butadienes and Cyclopropene. Journal of Organic Chemistry, 1999, 64, 6697-6701.	1.7	24
178	Lewis Acidity of Boron Trihalides. Journal of Physical Chemistry A, 1999, 103, 5807-5811.	1.1	64