Sam P De Visser

List of Publications by Year
in descending order

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276	18,167	10351 72	16605 123
papers	citations	h-index	g-index
292	292	292	8619
all docs	docs citations	times ranked	citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanism of Oxidation Reactions Catalyzed by Cytochrome P450 Enzymes. Chemical Reviews, 2004, 104, 3947-3980.	23.0	2,048
2	Theoretical Perspective on the Structure and Mechanism of Cytochrome P450 Enzymes. Chemical Reviews, 2005, 105, 2279-2328.	23.0	1,127
3	A Model â€œReboundâ€•Mechanism of Hydroxylation by Cytochrome P450:â€‰ Stepwise and Effectively Concerted Pathways, and Their Reactivity Patterns. Journal of the American Chemical Society, 2000, 122, 8977-8989.	6.6	385
4	Two-state reactivity mechanisms of hydroxylation and epoxidation by cytochrome P-450 revealed by theory. Current Opinion in Chemical Biology, 2002, 6, 556-567.	2.8	340
5	A Proton-Shuttle Mechanism Mediated by the Porphyrin in Benzene Hydroxylation by Cytochrome P450 Enzymes. Journal of the American Chemical Society, 2003, 125, 7413-7424.	6.6	324
6	Searching for the Second Oxidant in the Catalytic Cycle of Cytochrome P450:Â A Theoretical Investigation of the Iron(III)-Hydroperoxo Species and Its Epoxidation Pathways. Journal of the American Chemical Society, 2002, 124, 2806-2817.	6.6	295
7	What Factors Affect the Regioselectivity of Oxidation by Cytochrome P450? A DFT Study of Allylic Hydroxylation and Double Bond Epoxidation in a Model Reaction. Journal of the American Chemical Society, 2002, 124, 11809-11826.	6.6	289
8	External Electric Field Will Control the Selectivity of Enzymatic-Like Bond Activations. Journal of the American Chemical Society, 2004, 126, 11746-11749.	6.6	265
9	Photoactivation of the Photoactive Yellow Protein:Â Why Photon Absorption Triggers a Trans-to-Cis Isomerization of the Chromophore in the Protein. Journal of the American Chemical Society, 2004, 126, 4228-4233.	6.6	265
10	A Valence Bond Modeling of Trends in Hydrogen Abstraction Barriers and Transition States of Hydroxylation Reactions Catalyzed by Cytochrome P450 Enzymes. Journal of the American Chemical Society, 2008, 130, 10128-10140.	6.6	232
11	A Predictive Pattern of Computed Barriers for Câˆ’H Hydroxylation by Compound I of Cytochrome P450. Journal of the American Chemical Society, 2004, 126, 8362-8363.	6.6	218
12	Multi-State Epoxidation of Ethene by Cytochrome P450:Â A Quantum Chemical Study. Journal of the American Chemical Society, 2001, 123, 3037-3047.	6.6	213
13	Theoretical Study on the Mechanism of the Oxygen Activation Process in Cysteine Dioxygenase Enzymes. Journal of the American Chemical Society, 2011, 133, 3869-3882.	6.6	197
14	Propene Activation by the Oxo-Iron Active Species of Taurine/Î±-Ketoglutarate Dioxygenase (TauD) Enzyme. How Does the Catalysis Compare to Heme-Enzymes?. Journal of the American Chemical Society, 2006, 128, 9813-9824.	6.6	193
15	Trends in Substrate Hydroxylation Reactions by Heme and Nonheme Iron(IV)-Oxo Oxidants Give Correlations between Intrinsic Properties of the Oxidant with Barrier Height. Journal of the American Chemical Society, 2010, 132, 1087-1097.	6.6	177
16	Combined Experimental and Theoretical Study on Aromatic Hydroxylation by Mononuclear Nonheme Iron(IV)âˆ’Oxo Complexes. Inorganic Chemistry, 2007, 46, 4632-4641.	1.9	174
17	Medium Polarization and Hydrogen Bonding Effects on Compound I of Cytochrome P450:Â What Kind of a Radical Is It Really?. Journal of the American Chemical Society, 2000, 122, 12892-12893.	6.6	171
18	Active Species of Horseradish Peroxidase (HRP) and Cytochrome P450:Â Two Electronic Chameleons. Journal of the American Chemical Society, 2003, 125, 15779-15788.	6.6	168

#	ARTICLE	IF	CITATIONS
19	What Factors Influence the Rate Constant of Substrate Epoxidation by Compound I of Cytochrome P450 and Analogous Iron(IV)-Oxo Oxidants?. Journal of the American Chemical Society, 2010, 132, 7656-7667.	6.6	163
20	Intrinsic properties and reactivities of mononuclear nonheme ironâ€“oxygen complexes bearing the tetramethylcyclam ligand. Coordination Chemistry Reviews, 2013, 257, 381-393.	9.5	157
21	The â€œRebound Controversyâ€: An Overview and Theoretical Modeling of the Rebound Step in Câ˘’H Hydroxylation by Cytochrome P450. European Journal of Inorganic Chemistry, 2004, 2004, 207-226.	1.0	156
22	Radical Clock Substrates, Their Câ˘’H Hydroxylation Mechanism by Cytochrome P450, and Other Reactivity Patterns:Â What Does Theory Reveal about the Clocks' Behavior?. Journal of the American Chemical Society, 2004, 126, 1907-1920.	6.6	156
23	Valence Tautomerism in a High-Valent Manganeseâ€“Oxo Porphyrinoid Complex Induced by a Lewis Acid. Journal of the American Chemical Society, 2012, 134, 10397-10400.	6.6	155
24	The â€˜pushâ€™ effect of the thiolate ligand in cytochrome P450: a theoretical gauging. Journal of Inorganic Biochemistry, 2002, 91, 554-567.	1.5	139
25	What Factors Influence the Ratio of CH Hydroxylation versus CC Epoxidation by a Nonheme Cytochrome P450 Biomimetic?. Journal of the American Chemical Society, 2006, 128, 15809-15818.	6.6	136
26	Quantum Mechanics/Molecular Mechanics Modeling of Enzymatic Processes: Caveats and Breakthroughs. Chemistry - A European Journal, 2016, 22, 2562-2581.	1.7	133
27	The Mechanism of Cysteine Oxygenation by Cysteine Dioxygenase Enzymes. Journal of the American Chemical Society, 2007, 129, 14846-14847.	6.6	129
28	Unprecedented Rate Enhancements of Hydrogenâ€Atom Transfer to a Manganese(V)â€“Oxo Corrolazine Complex. Angewandte Chemie - International Edition, 2010, 49, 5091-5095.	7.2	129
29	Hydrogen Bonding Modulates the Selectivity of Enzymatic Oxidation by P450: Chameleon Oxidant Behavior by Compound I The research was supported in parts by the Israel Science Foundation (ISF), the German Israeli Binational Foundation (GIF), and by the Ministry of Science, Culture, and Sports. F.O. thanks the European community for a Marie Curie Fellowship.. Angewandte Chemie - International Edition, 2002, 41, 1947.	7.2	122
30	Quantum Mechanics/Molecular Mechanics Study on the Oxygen Binding and Substrate Hydroxylation Step in AlkB Repair Enzymes. Chemistry - A European Journal, 2014, 20, 435-446.	1.7	122
31	Can a Single Oxidant with Two Spin States Masquerade as Two Different Oxidants? A Study of the Sulfoxidation Mechanism by Cytochrome P450. Journal of the American Chemical Society, 2003, 125, 8698-8699.	6.6	120
32	Drug Metabolism by Cytochrome P450 Enzymes: What Distinguishes the Pathways Leading to Substrate Hydroxylation Over Desaturation?. Chemistry - A European Journal, 2015, 21, 9083-9092.	1.7	116
33	Structural Characterization and Remarkable Axial Ligand Effect on the Nucleophilic Reactivity of a Nonheme Manganese(III)â€“Peroxo Complex. Angewandte Chemie - International Edition, 2009, 48, 4150-4153.	7.2	115
34	Chameleon States: High-Valent Metal-Oxo Species of Cytochrome P450 and Its Ruthenium Analogue. Angewandte Chemie - International Edition, 2001, 40, 2874-2878.	7.2	114
35	Computational modelling of oxygenation processes in enzymes and biomimetic model complexes. Chemical Communications, 2014, 50, 262-282.	2.2	110
36	Multistate Reactivity in Styrene Epoxidation by Compound I of Cytochrome P450: Mechanisms of Products and Side Products Formation. Chemistry - A European Journal, 2005, 11, 2825-2835.	1.7	108

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37	Long-Range Electron Transfer Triggers Mechanistic Differences between Iron(IV)-Oxo and Iron(IV)-Imido Oxidants. Journal of the American Chemical Society, 2014, 136, 17102-17115.	6.6	106
38	Nature of the Three-Electron Bond in H2Sâˆ´SH2+Ââ€. Journal of Physical Chemistry A, 1998, 102, 9549-9553.	1.1	102
39	Secondary Coordination Sphere Influence on the Reactivity of Nonheme Iron(II) Complexes: An Experimental and DFT Approach. Journal of the American Chemical Society, 2013, 135, 10590-10593.	6.6	102
40	Origin of the Regioselective Fattyâ€•Acid Hydroxylation versus Decarboxylation by a Cytochrome P450 Peroxygenase: What Drives the Reaction to Biofuel Production?. Chemistry - A European Journal, 2016, 22, 5478-5483.	1.7	102
41	Substitution of Hydrogen by Deuterium Changes the Regioselectivity of Ethylbenzene Hydroxylation by an Oxoâ€“Ironâ€“Porphyrin Catalyst. Chemistry - A European Journal, 2006, 12, 8168-8177.	1.7	99
42	Origin of the Correlation of the Rate Constant of Substrate Hydroxylation by Nonheme Iron(IV)â€“oxo Complexes with the Bondâ€•Dissociation Energy of the Cï£¿H Bond of the Substrate. Chemistry - A European Journal, 2009, 15, 6651-6662.	1.7	98
43	Origin of the Enhanced Reactivity of Î¼-Nitrido-Bridged Diiron(IV)-Oxo Porphyrinoid Complexes over Cytochrome P450 Compound I. ACS Catalysis, 2016, 6, 2230-2243.	5.5	98
44	Differences in and Comparison of the Catalytic Properties of Heme and Non-Heme Enzymes with a Central Oxoâ€“Iron Group. Angewandte Chemie - International Edition, 2006, 45, 1790-1793.	7.2	97
45	Sulfoxide Synthase versus Cysteine Dioxygenase Reactivity in a Nonheme Iron Enzyme. Journal of the American Chemical Society, 2017, 139, 9259-9270.	6.6	97
46	A comprehensive test set of epoxidation rate constants for iron(<scp>iv</scp>)â€“oxo porphyrin cation radical complexes. Chemical Science, 2015, 6, 1516-1529.	3.7	96
47	Electrophilic Aromatic Chlorination and Haloperoxidation of Chloride Catalyzed by Polyfluorinated Alcohols:Â A New Manifestation of Template Catalysis. Journal of the American Chemical Society, 2003, 125, 12116-12117.	6.6	94
48	How Does Product Isotope Effect Prove the Operation of a Two-State â€œReboundâ€•Mechanism in Câˆ’H Hydroxylation by Cytochrome P450?. Journal of the American Chemical Society, 2003, 125, 13024-13025.	6.6	93
49	How Does Ethene Inactivate Cytochrome P450 En Route to Its Epoxidation? A Density Functional Study. Angewandte Chemie - International Edition, 2001, 40, 2871-2874.	7.2	89
50	What Is the Difference between the Manganese Porphyrin and Corrole Analogues of Cytochrome P450's Compound I?. Chemistry - A European Journal, 2001, 7, 4954-4960.	1.7	88
51	Comparison of the Reactivity of Nonheme Iron(IV)â€“Oxo versus Iron(IV)â€“Imido Complexes: Which is the Better Oxidant?. Angewandte Chemie - International Edition, 2013, 52, 12288-12292.	7.2	88
52	Singlet versus Triplet Reactivity in an Mn(V)â€“Oxo Species: Testing Theoretical Predictions Against Experimental Evidence. Journal of the American Chemical Society, 2016, 138, 12375-12386.	6.6	88
53	Fluorinated Alcohols Enable Olefin Epoxidation by H2O2:Â Template Catalysis. Journal of Organic Chemistry, 2003, 68, 2903-2912.	1.7	87
54	One oxidant, many pathways: a theoretical perspective of monooxygenation mechanisms by cytochrome P450 enzymes. Journal of Biological Inorganic Chemistry, 2004, 9, 661-668.	1.1	86

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55	Comparative Quantum Mechanics/Molecular Mechanics (QM/MM) and Density Functional Theory Calculations on the Oxoâˆ’Iron Species of Taurine/Î±-Ketoglutarate Dioxygenase. Journal of Physical Chemistry A, 2008, 112, 2464-2468.	1.1	86
56	The Experimentally Elusive Oxidant of Cytochrome P450: A Theoretical â€œTrappingâ€•Defining More Closely the â€œRealâ€•Species. ChemBioChem, 2001, 2, 848.	1.3	85
57	Is the Bound Substrate in Nitric Oxide Synthase Protonated or Neutral and What Is the Active Oxidant that Performs Substrate Hydroxylation?. Journal of the American Chemical Society, 2008, 130, 12961-12974.	6.6	85
58	Hydrogenâ€Bonding Interactions Trigger a Spinâ€Flip in Iron(III) Porphyrin Complexes. Angewandte Chemie - International Edition, 2015, 54, 4796-4800.	7.2	83
59	How Does the Axial Ligand of Cytochrome P450 Biomimetics Influence the Regioselectivity of Aliphatic versus Aromatic Hydroxylation?. Chemistry - A European Journal, 2009, 15, 5577-5587.	1.7	82
60	Effect of the Axial Ligand on Substrate Sulfoxidation Mediated by Iron(IV)â€“Oxo Porphyrin Cation Radical Oxidants. Chemistry - A European Journal, 2011, 17, 6196-6205.	1.7	82
61	Nuclear Quantum Tunneling in the Light-activated Enzyme Protochlorophyllide Oxidoreductase. Journal of Biological Chemistry, 2009, 284, 3762-3767.	1.6	80
62	Substrate Sulfoxidation by an Iron(IV)-Oxo Complex: Benchmarking Computationally Calculated Barrier Heights to Experiment. Journal of Physical Chemistry A, 2016, 120, 9805-9814.	1.1	80
63	Understanding How Prolyl-4-hydroxylase Structure Steers a Ferryl Oxidant toward Scission of a Strong Câ€“H Bond. Journal of the American Chemical Society, 2017, 139, 9855-9866.	6.6	80
64	Oxygen Economy of Cytochrome P450:Â What Is the Origin of the Mixed Functionality as a Dehydrogenaseâˆ’Oxidase Enzyme Compared with Its Normal Function?. Journal of the American Chemical Society, 2004, 126, 5072-5073.	6.6	78
65	Theory Favors a Stepwise Mechanism of Porphyrin Degradation by a Ferric Hydroperoxide Model of the Active Species of Heme Oxygenase. Journal of the American Chemical Society, 2005, 127, 8204-8213.	6.6	78
66	Effect of Porphyrin Ligands on the Regioselective Dehydrogenation versus Epoxidation of Olefins by Oxoiron(IV) Mimics of Cytochrome P450. Journal of Physical Chemistry A, 2009, 113, 11713-11722.	1.1	78
67	How Do Azoles Inhibit Cytochrome P450 Enzymes? A Density Functional Study. Journal of Physical Chemistry A, 2008, 112, 12911-12918.	1.1	76
68	Does Hydrogenâ€Bonding Donation to Manganese(IV)â€“Oxo and Iron(IV)â€“Oxo Oxidants Affect the Oxygenâ€Atom Transfer Ability? A Computational Study. Chemistry - A European Journal, 2013, 19, 4058-4068.	1.7	76
69	Mechanistic Studies of Fatty Acid Activation by CYP152 Peroxygenases Reveal Unexpected Desaturase Activity. ACS Catalysis, 2019, 9, 565-577.	5.5	76
70	Secondâ€Coordination Sphere Effects on Selectivity and Specificity of Heme and Nonheme Iron Enzymes. Chemistry - A European Journal, 2020, 26, 5308-5327.	1.7	75
71	Is the Ruthenium Analogue of Compound I of Cytochrome P450 an Efficient Oxidant? A Theoretical Investigation of the Methane Hydroxylation Reaction. Journal of the American Chemical Society, 2003, 125, 2291-2300.	6.6	74
72	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

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73	A Manganese(V)â€“Oxo Ï€-Cation Radical Complex: Influence of One-Electron Oxidation on Oxygen-Atom Transfer. Journal of the American Chemical Society, 2011, 133, 15874-15877.	6.6	74
74	A Systematic Account on Aromatic Hydroxylation by a Cytochrome P450 Model Compound I: A Lowâ€Pressure Mass Spectrometry and Computational Study. Chemistry - A European Journal, 2016, 22, 18608-18619.	1.7	74
75	Deformylation Reaction by a Nonheme Manganese(III)â€“Peroxo Complex via Initial Hydrogenâ€Atom Abstraction. Angewandte Chemie - International Edition, 2016, 55, 11091-11095.	7.2	73
76	Reactivity Patterns of (Protonated) Compoundâ€…II and Compoundâ€…I of Cytochrome P450: Which is the Better Oxidant?. Chemistry - A European Journal, 2017, 23, 6406-6418.	1.7	71
77	Catalytic Mechanism of Cofactor-Free Dioxygenases and How They Circumvent Spin-Forbidden Oxygenation of Their Substrates. Journal of the American Chemical Society, 2015, 137, 7474-7487.	6.6	70
78	Site-selective formation of an iron(<scp>iv</scp>)â€“oxo species at the more electron-rich iron atom of heteroleptic Î¼-nitrido diiron phthalocyanines. Chemical Science, 2015, 6, 5063-5075.	3.7	70
79	Oxygen-Atom Transfer Reactivity of Axially Ligated Mn(V)â€“Oxo Complexes: Evidence for Enhanced Electrophilic and Nucleophilic Pathways. Journal of the American Chemical Society, 2014, 136, 13845-13852.	6.6	68
80	Computer-Generated High-Valent Iron-Oxo and Manganese-Oxo Species with Polyoxometalate Ligands: How do they Compare with the Iron-Oxo Active Species of Heme Enzymes?. Angewandte Chemie - International Edition, 2004, 43, 5661-5665.	7.2	67
81	Nonheme ferric hydroperoxo intermediates are efficient oxidants of bromide oxidation. Chemical Communications, 2011, 47, 11044.	2.2	67
82	Differences and Comparisons of the Properties and Reactivities of Iron(III)â€“hydroperoxo Complexes with Saturated Coordination Sphere. Chemistry - A European Journal, 2015, 21, 1221-1236.	1.7	67
83	Rationalization of the Barrier Height for <i>p</i>-Z-styrene Epoxidation by Iron(IV)-Oxo Porphyrin Cation Radicals with Variable Axial Ligands. Inorganic Chemistry, 2013, 52, 7968-7979.	1.9	66
84	Direct Observation of a Nonheme Iron(IV)â€“Oxo Complex That Mediates Aromatic Câ€“F Hydroxylation. Journal of the American Chemical Society, 2014, 136, 13542-13545.	6.6	66
85	Ketoâ€“Enol Tautomerization Triggers an Electrophilic Aldehyde Deformylation Reaction by a Nonheme Manganese(III)-Peroxo Complex. Journal of the American Chemical Society, 2017, 139, 18328-18338.	6.6	66
86	Selective Hydrogen Atom Abstraction from Dihydroflavonol by a Nonheme Iron Center Is the Key Step in the Enzymatic Flavonol Synthesis and Avoids Byproducts. Journal of the American Chemical Society, 2019, 141, 20278-20292.	6.6	66
87	Reactivity and Thermochemical Properties of the Water Dimer Radical Cation in the Gas Phase. The Journal of Physical Chemistry, 1995, 99, 15444-15447.	2.9	65
88	How do aldehyde side products occur during alkene epoxidation by cytochrome P450? Theory reveals a state-specific multi-state scenario where the high-spin component leads to all side productsâ˜†. Journal of Inorganic Biochemistry, 2004, 98, 1183-1193.	1.5	65
89	Axial Ligand Effect On The Rate Constant of Aromatic Hydroxylation By Iron(IV)â€“Oxo Complexes Mimicking Cytochrome P450 Enzymes. Journal of Physical Chemistry B, 2012, 116, 718-730.	1.2	64
90	Inversion of Enantioselectivity of a Mononuclear Nonâ€Heme Iron(II)â€dependent Hydroxylase by Tuning the Interplay of Metalâ€Center Geometry and Protein Structure. Angewandte Chemie - International Edition, 2013, 52, 9677-9681.	7.2	62

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91	A Biomimetic Ferric Hydroperoxo Porphyrin Intermediate. Angewandte Chemie - International Edition, 2010, 49, 2099-2101.	7.2	61
92	Porphyrin Traps Its Terminator! Concerted and Stepwise Porphyrin Degradation Mechanisms Induced by Heme-Oxygenase and Cytochrome P450. Angewandte Chemie - International Edition, 2004, 43, 1129-1132.	7.2	60
93	The intrinsic axial ligand effect on propene oxidation by horseradish peroxidase versus cytochrome P450 enzymes. Journal of Biological Inorganic Chemistry, 2005, 10, 181-189.	1.1	60
94	Elucidating enzyme mechanism and intrinsic chemical properties of short-lived intermediates in the catalytic cycles of cysteine dioxygenase and taurine/Î±-ketoglutarate dioxygenase. Coordination Chemistry Reviews, 2009, 253, 754-768.	9.5	58
95	Quantum Mechanics/Molecular Mechanics Studies on the Sulfoxidation of Dimethyl Sulfide by Compound I and Compound 0 of Cytochrome P450: Which Is the Better Oxidant?. Journal of Physical Chemistry A, 2009, 113, 11635-11642.	1.1	56
96	A Non-Heme Diiron Complex for (Electro)catalytic Reduction of Dioxygen: Tuning the Selectivity through Electron Delivery. Journal of the American Chemical Society, 2019, 141, 8244-8253.	6.6	56
97	The axial ligand effect of oxo-iron porphyrin catalysts. How does chloride compare to thiolate?. Journal of Biological Inorganic Chemistry, 2006, 11, 168-178.	1.1	55
98	Can the peroxosuccinate complex in the catalytic cycle of taurine/Î±-ketoglutarate dioxygenase (TauD) act as an alternative oxidant?. Chemical Communications, 2007, , 171-173.	2.2	55
99	Catalytic Mechanism of Aromatic Nitration by Cytochrome P450 TxtE: Involvement of a Ferric-Peroxynitrite Intermediate. Journal of the American Chemical Society, 2020, 142, 15764-15779.	6.6	55
100	Why Do Cysteine Dioxygenase Enzymes Contain a 3-His Ligand Motif Rather than a 2His/1Asp Motif Like Most Nonheme Dioxygenases?. Journal of Physical Chemistry A, 2009, 113, 1835-1846.	1.1	54
101	Generation of a High-Valent Iron Imido Corrolazine Complex and NR Group Transfer Reactivity. Inorganic Chemistry, 2013, 52, 4668-4682.	1.9	54
102	Selective Formation of an Fe^{IV}O or an Fe^{III}OOH Intermediate From Iron(II) and H₂O₂: Controlled Heterolytic versus Homolytic Oxygenâ€"Oxygen Bond Cleavage by the Second Coordination Sphere. Angewandte Chemie - International Edition, 2019, 58, 854-858.	7.2	54
103	Inspiration from Nature: Influence of Engineered Ligand Scaffolds and Auxiliary Factors on the Reactivity of Biomimetic Oxidants. ACS Catalysis, 2021, 11, 9761-9797.	5.5	54
104	What Affects the Quartetâˆ'Doublet Energy Splitting in Peroxidase Enzymes?. Journal of Physical Chemistry A, 2005, 109, 11050-11057.	1.1	53
105	Carbon Dioxide: A Waste Product in the Catalytic Cycle of Î±-Ketoglutarate Dependent Halogenases Prevents the Formation of Hydroxylated By-Products. Journal of Physical Chemistry B, 2009, 113, 12-14.	1.2	53
106	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
107	How Does the Oxidation State of Palladium Surfaces Affect the Reactivity and Selectivity of Direct Synthesis of Hydrogen Peroxide from Hydrogen and Oxygen Gases? A Density Functional Study. Journal of the American Chemical Society, 2019, 141, 901-910.	6.6	52
108	A Comparative Review on the Catalytic Mechanism of Nonheme Iron Hydroxylases and Halogenases. Catalysts, 2018, 8, 314.	1.6	50

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109	Regioâ€•and Enantioâ€selective Chemoâ€enzymatic Câˆ’Hâ€Lactonization of Decanoic Acid to (<i>S</i>)â€Î´â€Decalactone. Angewandte Chemie - International Edition, 2019, 58, 5668-5671.	7.2	50
110	Spin-State Ordering in Hydroxo-Bridged Diiron(III)bisporphyrin Complexes. Inorganic Chemistry, 2015, 54, 1919-1930.	1.9	49
111	Local Charge Distributions, Electric Dipole Moments, and Local Electric Fields Influence Reactivity Patterns and Guide Regioselectivities in Î±-Ketoglutarate-Dependent Non-heme Iron Dioxygenases. Accounts of Chemical Research, 2022, 55, 65-74.	7.6	48
112	REKS calculations on ortho-, meta- and para-benzyne. Physical Chemistry Chemical Physics, 2000, 2, 5046-5048.	1.3	46
113	Mechanistic insight into halide oxidation by non-heme iron complexes. Haloperoxidase versus halogenase activity. Chemical Communications, 2013, 49, 10926.	2.2	45
114	CO₂ Reduction on an Iron-Porphyrin Center: A Computational Study. Journal of Physical Chemistry A, 2019, 123, 6527-6535.	1.1	45
115	The Axial Ligand Effect on Aliphatic and Aromatic Hydroxylation by Nonâ€heme Iron(IV)â€“oxo Biomimetic Complexes. Chemistry - an Asian Journal, 2011, 6, 493-504.	1.7	44
116	Nitrogen Reduction to Ammonia on a Biomimetic Mononuclear Iron Centre: Insights into the Nitrogenase Enzyme. Chemistry - A European Journal, 2018, 24, 5293-5302.	1.7	44
117	Interplay Between Steric and Electronic Effects: A Joint Spectroscopy and Computational Study of Nonheme Iron(IV)â€Oxo Complexes. Chemistry - A European Journal, 2019, 25, 5086-5098.	1.7	44
118	Mechanism of Oxidative Activation of Fluorinated Aromatic Compounds by Nâ€Bridged Diironâ€Phthalocyanine: What Determines the Reactivity?. Chemistry - A European Journal, 2019, 25, 14320-14331.	1.7	43
119	Fe-Catalyzed Aziridination Is Governed by the Electron Affinity of the Active Imido-Iron Species. ACS Catalysis, 2020, 10, 10010-10020.	5.5	42
120	Steric Factors Override Thermodynamic Driving Force in Regioselectivity of Proline Hydroxylation by Prolyl-4-hydroxylase Enzymes. Journal of Physical Chemistry A, 2010, 114, 13234-13243.	1.1	41
121	Negative catalysis / non-Bell-Evans-Polanyi reactivity by metalloenzymes: Examples from mononuclear heme and non-heme iron oxygenases. Coordination Chemistry Reviews, 2021, 439, 213914.	9.5	41
122	Status report on the quantum chemical cluster approach for modeling enzyme reactions. Communications Chemistry, 2022, 5, .	2.0	40
123	Chemical and Thermodynamic Properties of Methyl Chloride Dimer Radical Cations in the Gas Phase. Journal of the American Chemical Society, 1998, 120, 1517-1522.	6.6	39
124	Manganese substituted Compound I of cytochrome P450 biomimetics: A comparative reactivity study of MnV-oxo versus MnIV-oxo species. Archives of Biochemistry and Biophysics, 2011, 507, 4-13.	1.4	39
125	Nonheme iron-oxo and -superoxo reactivities: O2 binding and spin inversion probability matter. Chemical Communications, 2012, 48, 2189.	2.2	39
126	Mechanism of S-Oxygenation by a Cysteine Dioxygenase Model Complex. Journal of Physical Chemistry A, 2012, 116, 582-591.	1.1	38

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127	Identification and Spectroscopic Characterization of Nonheme Iron(III) Hypochlorite Intermediates. Angewandte Chemie - International Edition, 2015, 54, 4357-4361.	7.2	38
128	How does the push/pull effect of the axial ligand influence the catalytic properties of Compound I of catalase and cytochrome P450?. Journal of Inorganic Biochemistry, 2007, 101, 1464-1472.	1.5	37
129	Fundamental Differences of Substrate Hydroxylation by High-Valent Iron(IV)-Oxo Models of Cytochrome P450. Inorganic Chemistry, 2009, 48, 6661-6669.	1.9	37
130	Does Substrate Positioning Affect the Selectivity and Reactivity in the Hectochlorin Biosynthesis Halogenase?. Frontiers in Chemistry, 2018, 6, 513.	1.8	37
131	Hydrogen by Deuterium Substitution in an Aldehyde Tunes the Regioselectivity by a Nonheme Manganese(III)â€“Peroxo Complex. Angewandte Chemie - International Edition, 2019, 58, 10639-10643.	7.2	37
132	Ferromagnetic Bonding:â€‰ Properties of High-Spin Lithium Clusters n+1Lin (n = 2âˆ’12) Devoid of Electron Pairs. Journal of Physical Chemistry A, 2002, 106, 4961-4969.	1.1	36
133	Oxygen Atom Transfer Using an Iron(IV)â€Oxo Embedded in a Tetracyclic Nâ€Heterocyclic Carbene System: How Does the Reactivity Compare to Cytochrome P450 Compoundâ€…I?. Chemistry - A European Journal, 2017, 23, 2935-2944.	1.7	36
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