

Thomas C Brunold

List of Publications by Year in descending order

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87
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5,074
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101543

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90
docs citations

90
times ranked

3734
citing authors

#	ARTICLE	IF	CITATIONS
1	Geometric and Electronic Structure/Function Correlations in Non-Heme Iron Enzymes. <i>Chemical Reviews</i> , 2000, 100, 235-350.	47.7	1,594
2	Hydrogen Sulfide Oxidation by Myoglobin. <i>Journal of the American Chemical Society</i> , 2016, 138, 8476-8488.	13.7	130
3	Spectroscopic and Computational Studies of Co ³⁺ -Corrinoids: Spectral and Electronic Properties of the B ₁₂ Cofactors and Biologically Relevant Precursors. <i>Journal of the American Chemical Society</i> , 2003, 125, 5897-5914.	13.7	122
4	Spectroscopic and Computational Studies of Co ²⁺ -Corrinoids: Spectral and Electronic Properties of the Biologically Relevant Base-On and Base-Off Forms of Co ²⁺ -Cobalamin. <i>Journal of the American Chemical Society</i> , 2004, 126, 9735-9749.	13.7	120
5	Spectroscopic Study of [Fe ₂ (O ₂)(OBz) ₂ {HB(pz ⁻) ₃ } ₂]: Nature of the $\frac{1}{4}$ -1,2 Peroxide-Fe(III) Bond and Its Possible Relevance to O ₂ Activation by Non-Heme Iron Enzymes. <i>Journal of the American Chemical Society</i> , 1998, 120, 5674-5690.	13.7	119
6	Identification of an ϵ -End-on-Nickel ^{II} Superoxo Adduct, [Ni(tmc)(O ₂)] ⁺ . <i>Journal of the American Chemical Society</i> , 2006, 128, 14230-14231.	13.7	118
7	Spectroscopic and Computational Studies of Ni Superoxide Dismutase: Electronic Structure Contributions to Enzymatic Function. <i>Journal of the American Chemical Society</i> , 2005, 127, 5449-5462.	13.7	110
8	Definitive Spectroscopic Determination of Zero-Field Splitting in High-Spin Cobalt(II). <i>Journal of the American Chemical Society</i> , 2004, 126, 2148-2155.	13.7	107
9	Combined Spectroscopic/Computational Studies on Fe- and Mn-Dependent Superoxide Dismutases: Insights into Second-Sphere Tuning of Active Site Properties. <i>Accounts of Chemical Research</i> , 2004, 37, 461-470.	15.6	105
10	Characterization of the Nitrosyl Adduct of Substrate-Bound Mouse Cysteine Dioxygenase by Electron Paramagnetic Resonance: Electronic Structure of the Active Site and Mechanistic Implications. <i>Biochemistry</i> , 2007, 46, 8569-8578.	2.5	99
11	A Monomeric Nickel ^{II} Dioxygen Adduct Derived from a Nickel(I) Complex and O ₂ . <i>Inorganic Chemistry</i> , 2004, 43, 3324-3326.	4.0	95
12	Spectroscopic Evidence for the Formation of a Four-Coordinate Co ²⁺ -Cobalamin Species upon Binding to the Human ATP:Cobalamin Adenosyltransferase. <i>Journal of the American Chemical Society</i> , 2005, 127, 7660-7661.	13.7	94
13	Spectroscopic and Computational Studies of the ATP:Corrinoid Adenosyltransferase (CobA) from <i>Salmonella enterica</i> : Insights into the Mechanism of Adenosylcobalamin Biosynthesis. <i>Journal of the American Chemical Society</i> , 2005, 127, 8710-8719.	13.7	90
14	Spectroscopic and Computational Studies of Co ¹⁺ -Cobalamin: Spectral and Electronic Properties of the ϵ -Superreduced-B ₁₂ Cofactor. <i>Journal of the American Chemical Society</i> , 2006, 128, 9144-9156.	13.7	89
15	Dioxygen Activation by a Nickel Thioether Complex: Characterization of a Ni ^{III} ($\frac{1}{4}$ -O) ₂ Core. <i>Journal of the American Chemical Society</i> , 2001, 123, 9194-9195.	13.7	84
16	Computational Studies on the A Cluster of Acetyl-Coenzyme A Synthase: Geometric and Electronic Properties of the NiFeC Species and Mechanistic Implications. <i>Journal of the American Chemical Society</i> , 2003, 125, 13962-13963.	13.7	77
17	Excited-State Exchange Coupling in Bent Mn(III)-O-Mn(III) Complexes: Dominance of the σ/σ Superexchange Pathway and Its Possible Contributions to the Reactivities of Binuclear Metalloproteins. <i>Journal of the American Chemical Society</i> , 2000, 122, 8511-8523.	13.7	70
18	Reversible Dioxygen Binding to Hemerythrin. 1. Electronic Structures of Deoxy- and Oxyhemerythrin. <i>Journal of the American Chemical Society</i> , 1999, 121, 8277-8287.	13.7	65

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19	Reversible Dioxygen Binding to Hemerythrin. 2. Mechanism of the Proton-Coupled Two-Electron Transfer to O ₂ at a Single Iron Center. <i>Journal of the American Chemical Society</i> , 1999, 121, 8288-8295.	13.7	64
20	Hydrogen-Bond-Mediated Tuning of the Redox Potential of the Non-Heme Fe Site of Superoxide Dismutase. <i>Journal of the American Chemical Society</i> , 2002, 124, 3482-3483.	13.7	63
21	Spectroscopic and Computational Characterization of Substrate-Bound Mouse Cysteine Dioxygenase: Nature of the Ferrous and Ferric Cysteine Adducts and Mechanistic Implications. <i>Biochemistry</i> , 2010, 49, 6033-6041.	2.5	63
22	Spectroscopic and Computational Study of a Non-Heme Iron {Fe ^{II} NO} ₇ System: Exploring the Geometric and Electronic Structures of the Nitrosyl Adduct of Iron Superoxide Dismutase. <i>Journal of the American Chemical Society</i> , 2003, 125, 8348-8363.	13.7	61
23	Spectroscopic and Computational Studies of the Azide-Adduct of Manganese Superoxide Dismutase: Definitive Assignment of the Ligand Responsible for the Low-Temperature Thermochromism. <i>Journal of the American Chemical Society</i> , 2004, 126, 12477-12491.	13.7	60
24	Probing the Geometric and Electronic Structures of the Low-Temperature Azide Adduct and the Product-Inhibited Form of Oxidized Manganese Superoxide Dismutase. <i>Biochemistry</i> , 2005, 44, 1504-1520.	2.5	57
25	Structural Characterization of a Human-Type Corrinoid Adenosyltransferase Confirms That Coenzyme B ₁₂ Is Synthesized through a Four-Coordinate Intermediate. <i>Biochemistry</i> , 2008, 47, 5755-5766.	2.5	55
26	Spectroscopic and Computational Studies on Iron and Manganese Superoxide Dismutases: Nature of the Chemical Events Associated with Active-Site pKs. <i>Journal of the American Chemical Society</i> , 2002, 124, 10833-10845.	13.7	54
27	Nickel Oxidation States of F430 Cofactor in Methyl-Coenzyme M Reductase. <i>Journal of the American Chemical Society</i> , 2004, 126, 4068-4069.	13.7	53
28	Spectroscopic Studies of the Corrinoid/Iron-Sulfur Protein from <i>Moorella thermoacetica</i> . <i>Journal of the American Chemical Society</i> , 2006, 128, 5010-5020.	13.7	51
29	Nickel superoxide dismutase: structural and functional roles of Cys2 and Cys6. <i>Journal of Biological Inorganic Chemistry</i> , 2010, 15, 795-807.	2.6	48
30	Synthesis, Structure Determination, and Spectroscopic/Computational Characterization of a Series of Fe(II)-Thiolate Model Complexes: Implications for Fe-S Bonding in Superoxide Reductases. <i>Journal of the American Chemical Society</i> , 2005, 127, 1675-1689.	13.7	46
31	Spectroscopic and Computational Studies of a Ni-CO Model Complex: Implications for the Acetyl-CoA Synthase Catalytic Mechanism. <i>Inorganic Chemistry</i> , 2003, 42, 859-867.	4.0	45
32	In-crystal reaction cycle of a toluene-bound diiron hydroxylase. <i>Nature</i> , 2017, 544, 191-195.	27.8	45
33	How Can a Single Second Sphere Amino Acid Substitution Cause Reduction Midpoint Potential Changes of Hundreds of Millivolts?. <i>Journal of the American Chemical Society</i> , 2007, 129, 9927-9940.	13.7	44
34	Second-Sphere Contributions to Substrate-Analogue Binding in Iron(III) Superoxide Dismutase. <i>Journal of the American Chemical Society</i> , 2002, 124, 3769-3774.	13.7	41
35	Combined Spectroscopic/Computational Study of Binuclear Fe(I)-Fe(I) Complexes: Implications for the Fully-Reduced Active-Site Cluster of Fe-Only Hydrogenases. <i>Inorganic Chemistry</i> , 2005, 44, 1794-1809.	4.0	40
36	Co-C Bond Activation in Methylmalonyl-CoA Mutase by Stabilization of the Post-homolysis Product Co ₂ +Cobalamin. <i>Journal of the American Chemical Society</i> , 2005, 127, 16522-16528.	13.7	40

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37	SECOND-SPHERE TUNING OF THE METAL ION REDUCTION POTENTIALS IN IRON AND MANGANESE SUPEROXIDE DISMUTASES. <i>Comments on Inorganic Chemistry</i> , 2008, 29, 134-168.	5.2	38
38	Kinetic and Spectroscopic Studies of the ATP:Corrinoid Adenosyltransferase PduO from <i>Lactobacillus reuteri</i> : Substrate Specificity and Insights into the Mechanism of Co(II)corrinoid Reduction. <i>Biochemistry</i> , 2008, 47, 9007-9015.	2.5	36
39	Spectroscopic and Computational Characterization of the Base-off Forms of Cob(II)alamin. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5245-5254.	2.6	35
40	Spectroscopic and computational insights into the geometric and electronic properties of the A-cluster of acetyl-coenzyme A synthase. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 533-541.	2.6	34
41	Spectroscopic Study of the Cobalamin-Dependent Methionine Synthase in the Activation Conformation: Effects of the Y1139 Residue and S-Adenosylmethionine on the B12 Cofactor. <i>Journal of the American Chemical Society</i> , 2008, 130, 16374-16381.	13.7	34
42	Spectroscopically validated density functional theory studies of the B12 cofactors and their interactions with enzyme active sites. <i>Coordination Chemistry Reviews</i> , 2009, 253, 779-794.	18.8	34
43	Spectroscopic and Computational Investigation of Second-Sphere Contributions to Redox Tuning in <i>Escherichia coli</i> Iron Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2008, 47, 3978-3992.	4.0	33
44	Spectroscopic and Computational Characterization of the NO Adduct of Substrate-Bound Fe(II) Cysteine Dioxygenase: Insights into the Mechanism of O ₂ Activation. <i>Biochemistry</i> , 2013, 52, 6040-6051.	2.5	32
45	Accessing Ni(III)-Thiolate Versus Ni(II)-Thiyl Bonding in a Family of Ni ^{II} N ₂ S ₂ Synthetic Models of NiSOD. <i>Inorganic Chemistry</i> , 2015, 54, 3815-3828.	4.0	32
46	Nickel Superoxide Dismutase: Structural and Functional Roles of His1 and Its H-Bonding Network. <i>Biochemistry</i> , 2015, 54, 1016-1027.	2.5	28
47	Spectroscopic and computational characterization of the nickel-containing F430 cofactor of methyl-coenzyme M reductase. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 77-89.	2.6	26
48	Combined Spectroscopic/Computational Studies of Vitamin B ₁₂ Precursors: Geometric and Electronic Structures of Cobinamides. <i>Inorganic Chemistry</i> , 2012, 51, 2867-2879.	4.0	26
49	Spectroscopic and Computational Investigation of Iron(III) Cysteine Dioxygenase: Implications for the Nature of the Putative Superoxo-Fe(III) Intermediate. <i>Biochemistry</i> , 2014, 53, 5759-5770.	2.5	26
50	Spectroscopic and Computational Investigation of the H155A Variant of Cysteine Dioxygenase: Geometric and Electronic Consequences of a Third-Sphere Amino Acid Substitution. <i>Biochemistry</i> , 2015, 54, 2874-2884.	2.5	26
51	Sacrificial Cobalt-Carbon Bond Homolysis in Coenzyme B ₁₂ as a Cofactor Conservation Strategy. <i>Journal of the American Chemical Society</i> , 2018, 140, 13205-13208.	13.7	24
52	Combined Spectroscopic and Computational Analysis of the Vibrational Properties of Vitamin B ₁₂ in its Co ³⁺ , Co ²⁺ , and Co ¹⁺ Oxidation States. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5397-5410.	2.6	23
53	Synthesis, X-ray Structures, Electronic Properties, and O ₂ /NO Reactivities of Thiol Dioxygenase Active-Site Models. <i>Inorganic Chemistry</i> , 2016, 55, 11839-11853.	4.0	23
54	Spectroscopic and Computational Studies of Ni ³⁺ Complexes with Mixed S/N Ligation: Implications for the Active Site of Nickel Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2007, 46, 8511-8523.	4.0	22

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55	Probing the Role of the Histidine 759 Ligand in Cobalamin-Dependent Methionine Synthase. <i>Biochemistry</i> , 2007, 46, 8024-8035.	2.5	22
56	Spectroscopic and computational investigation of three Cys-to-Ser mutants of nickel superoxide dismutase: insight into the roles played by the Cys2 and Cys6 active-site residues. <i>Journal of Biological Inorganic Chemistry</i> , 2010, 15, 777-793.	2.6	21
57	Spectroscopic and Computational Studies of Cobalamin Species with Variable Lower Axial Ligation: Implications for the Mechanism of Co ^{II} -C Bond Activation by Class I Cobalamin-Dependent Isomerases. <i>Inorganic Chemistry</i> , 2015, 54, 3736-3747.	4.0	21
58	Coordination chemistry controls the thiol oxidase activity of the B12-trafficking protein CblC. <i>Journal of Biological Chemistry</i> , 2017, 292, 9733-9744.	3.4	19
59	Spectroscopic and Computational Comparisons of Thiolate-Ligated Ferric Nonheme Complexes to Cysteine Dioxygenase: Second-Sphere Effects on Substrate (Analogue) Positioning. <i>Inorganic Chemistry</i> , 2019, 58, 16487-16499.	4.0	14
60	Synthetic iron-oxo σ -diamond core ⁺ -mimics structure of key intermediate in methane monooxygenase catalytic cycle. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 20641-20642.	7.1	13
61	Spectroscopic Studies of the <i>Salmonella enterica</i> Adenosyltransferase Enzyme <i>SeCobA</i> : Molecular-Level Insight into the Mechanism of Substrate Cob(II)alamin Activation. <i>Biochemistry</i> , 2014, 53, 7969-7982.	2.5	13
62	Spectral and Electronic Properties of Nitrosylcobalamin. <i>Inorganic Chemistry</i> , 2014, 53, 7676-7691.	4.0	13
63	Unprecedented Mechanism Employed by the <i>Salmonella enterica</i> EutT ATP:Co ^I rrinoid Adenosyltransferase Precludes Adenylation of Incomplete Co ^{II} rrinoids. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 7158-7161.	13.8	13
64	Electronic Structure of Anilinopyridinate-Supported Ru ₂ ⁵⁺ Paddlewheel Compounds. <i>Inorganic Chemistry</i> , 2017, 56, 14662-14670.	4.0	13
65	Spectroscopic insights into axial ligation and active-site H-bonding in substrate-bound human heme oxygenase-2. <i>Journal of Biological Inorganic Chemistry</i> , 2010, 15, 1117-1127.	2.6	12
66	Spectroscopic Characterization of Active-Site Variants of the PduO-type ATP:Corrinoid Adenosyltransferase from <i>Lactobacillus reuteri</i> : Insights into the Mechanism of Four-Coordinate Co(II)corrinoid Formation. <i>Inorganic Chemistry</i> , 2012, 51, 4482-4494.	4.0	12
67	Three Dimensional Triply Resonant Sum Frequency Spectroscopy Revealing Vibronic Coupling in Cobalamins: Toward a Probe of Reaction Coordinates. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9031-9042.	2.5	12
68	Spectroscopic Studies of the EutT Adenosyltransferase from <i>Salmonella enterica</i> : Mechanism of Four-Coordinate Co(II)Cbl Formation. <i>Journal of the American Chemical Society</i> , 2016, 138, 3694-3704.	13.7	11
69	Spectroscopic and Computational Studies of Reduction of the Metal versus the Tetrapyrrole Ring of Coenzyme F430 from Methyl-Coenzyme M Reductase. <i>Biochemistry</i> , 2006, 45, 11915-11933.	2.5	10
70	Electronic, Magnetic, and Redox Properties and O ₂ Reactivity of Iron(II) and Nickel(II) <i>o</i> -Semiquinone Complexes of a Tris(thioether) Ligand: Uncovering the Intradiol Cleaving Reactivity of an Iron(II) <i>o</i> -Semiquinone Complex. <i>Inorganic Chemistry</i> , 2017, 56, 10481-10495.	4.0	10
71	The Role of Mixed Amine/Amide Ligation in Nickel Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2018, 57, 12521-12535.	4.0	10
72	Spectroscopic Investigation of Cysteamine Dioxygenase. <i>Biochemistry</i> , 2020, 59, 2450-2458.	2.5	10

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73	The Crystal Structure of Cysteamine Dioxygenase Reveals the Origin of the Large Substrate Scope of This Vital Mammalian Enzyme. <i>Biochemistry</i> , 2021, 60, 3728-3737.	2.5	10
74	Spectroscopic and Computational Studies of a Series of High-Spin Ni(II) Thiolate Complexes. <i>Inorganic Chemistry</i> , 2010, 49, 6535-6544.	4.0	9
75	Structural, Spectroscopic, and Computational Characterization of the Azide Adduct of Fe ^{III} (2,6-diacetylpyridinebis(semioxamazide)), a Functional Analogue of Iron Superoxide Dismutase. <i>Inorganic Chemistry</i> , 2013, 52, 8909-8918.	4.0	9
76	A Spectroscopically Validated Computational Investigation of Viable Reaction Intermediates in the Catalytic Cycle of the Reductive Dehalogenase PceA. <i>Biochemistry</i> , 2021, 60, 2022-2032.	2.5	9
77	Resonance Raman spectroscopic study of the interaction between Co(II)rrinoids and the ATP:corrinoid adenosyltransferase PduO from <i>Lactobacillus reuteri</i> . <i>Journal of Biological Inorganic Chemistry</i> , 2016, 21, 669-681.	2.6	7
78	Spectroscopic Studies of the EutT Adenosyltransferase from <i>Salmonella enterica</i> : Evidence of a Tetrahedrally Coordinated Divalent Transition Metal Cofactor with Cysteine Ligation. <i>Biochemistry</i> , 2017, 56, 364-375.	2.5	6
79	Spectroscopic Study of the EutT Adenosyltransferase from <i>Listeria monocytogenes</i> : Evidence for the Formation of a Four-Coordinate Cob(II)alamin Intermediate. <i>Biochemistry</i> , 2018, 57, 5088-5095.	2.5	5
80	Spectroscopic and Computational Investigation of the Epoxyqueuosine Reductase QueG Reveals Intriguing Similarities with the Reductive Dehalogenase PceA. <i>Biochemistry</i> , 2022, 61, 195-205.	2.5	5
81	Chlorocob(II)alamin Formation Which Enhances the Thiol Oxidase Activity of the B12-Trafficking Protein CblC. <i>Inorganic Chemistry</i> , 2020, 59, 16065-16072.	4.0	4
82	Unprecedented Mechanism Employed by the <i>Salmonella enterica</i> EutT ATP:Co ^I rrinoid Adenosyltransferase Precludes Adenylation of Incomplete Co ^{II} rrinoids. <i>Angewandte Chemie</i> , 2015, 127, 7264-7267.	2.0	3
83	The <i>l</i> -Thr Kinase- <i>l</i> -Thr-Phosphate Decarboxylase (CobD) Enzyme from <i>Methanosarcina mazei</i> GÅ¶1 Contains Metalcenters Needed for Optimal Activity. <i>Biochemistry</i> , 2019, 58, 3260-3279.	2.5	3
84	Mutational and Functional Analyses of Substrate Binding and Catalysis of the <i>Listeria monocytogenes</i> EutT ATP:Co(I)rrinoid Adenosyltransferase. <i>Biochemistry</i> , 2020, 59, 1124-1136.	2.5	3
85	Spectroscopic investigation of iron(III) cysteamine dioxygenase in the presence of substrate (analog): implications for the nature of substrate-bound reaction intermediates. <i>Journal of Biological Inorganic Chemistry</i> , 2021, 26, 947-955.	2.6	2
86	Electronic structure studies of free and enzyme-bound B12 species by magnetic circular dichroism and complementary spectroscopic techniques. <i>Methods in Enzymology</i> , 2022, , .	1.0	0
87	Computational studies of bioorganometallic enzymes and cofactors. <i>Metal Ions in Life Sciences</i> , 2009, 6, 417-60.	2.8	0