Thomas C Brunold

List of Publications by Year
in descending order

87 papers	5,074 citations	101543 36 h-index	88630 70 g-index
90 all docs	90 docs citations	90 times ranked	3734 citing authors

#	Article	IF	Citations
1	Spectroscopic and Computational Investigation of the Epoxyqueuosine Reductase QueG Reveals Intriguing Similarities with the Reductive Dehalogenase PceA. Biochemistry, 2022, 61, 195-205.	2.5	5
2	Electronic structure studies of free and enzyme-bound B12 species by magnetic circular dichroism and complementary spectroscopic techniques. Methods in Enzymology, 2022, , .	1.0	0
3	A Spectroscopically Validated Computational Investigation of Viable Reaction Intermediates in the Catalytic Cycle of the Reductive Dehalogenase PceA. Biochemistry, 2021, 60, 2022-2032.	2.5	9
4	Spectroscopic investigation of iron(III) cysteamine dioxygenase in the presence of substrate (analogs): implications for the nature of substrate-bound reaction intermediates. Journal of Biological Inorganic Chemistry, 2021, 26, 947-955.	2.6	2
5	The Crystal Structure of Cysteamine Dioxygenase Reveals the Origin of the Large Substrate Scope of This Vital Mammalian Enzyme. Biochemistry, 2021, 60, 3728-3737.	2.5	10
6	Chlorocob(II)alamin Formation Which Enhances the Thiol Oxidase Activity of the B12-Trafficking Protein CblC. Inorganic Chemistry, 2020, 59, 16065-16072.	4.0	4
7	Spectroscopic Investigation of Cysteamine Dioxygenase. Biochemistry, 2020, 59, 2450-2458.	2.5	10
8	Mutational and Functional Analyses of Substrate Binding and Catalysis of the Listeria monocytogenes EutT ATP:Co(I)rrinoid Adenosyltransferase. Biochemistry, 2020, 59, 1124-1136.	2.5	3
9	The <scp>l</scp>-Thr Kinase/<scp>l</scp>-Thr-Phosphate Decarboxylase (CobD) Enzyme from Methanosarcina mazei GÄ¶1 Contains Metallocenters Needed for Optimal Activity. Biochemistry, 2019, 58, 3260-3279.	2.5	3
10	Spectroscopic and Computational Comparisons of Thiolate-Ligated Ferric Nonheme Complexes to Cysteine Dioxygenase: Second-Sphere Effects on Substrate (Analogue) Positioning. Inorganic Chemistry, 2019, 58, 16487-16499.	4.0	14
11	Sacrificial Cobaltâ€“Carbon Bond Homolysis in Coenzyme B₁₂ as a Cofactor Conservation Strategy. Journal of the American Chemical Society, 2018, 140, 13205-13208.	13.7	24
12	The Role of Mixed Amine/Amide Ligation in Nickel Superoxide Dismutase. Inorganic Chemistry, 2018, 57, 12521-12535.	4.0	10
13	Three Dimensional Triply Resonant Sum Frequency Spectroscopy Revealing Vibronic Coupling in Cobalamins: Toward a Probe of Reaction Coordinates. Journal of Physical Chemistry A, 2018, 122, 9031-9042.	2.5	12
14	Spectroscopic Study of the EutT Adenosyltransferase fromListeria monocytogenes: Evidence for the Formation of a Four-Coordinate Cob(II)alamin Intermediate. Biochemistry, 2018, 57, 5088-5095.	2.5	5
15	Coordination chemistry controls the thiol oxidase activity of the B12-trafficking protein CblC. Journal of Biological Chemistry, 2017, 292, 9733-9744.	3.4	19
16	In-crystal reaction cycle of a toluene-bound diiron hydroxylase. Nature, 2017, 544, 191-195.	27.8	45
17	Spectroscopic Studies of the EutT Adenosyltransferase from Salmonella enterica: Evidence of a Tetrahedrally Coordinated Divalent Transition Metal Cofactor with Cysteine Ligation. Biochemistry, 2017, 56, 364-375.	2.5	6
18	Electronic, Magnetic, and Redox Properties and O₂ Reactivity of Iron(II) and Nickel(II) o-Semiquinonate Complexes of a Tris(thioether) Ligand: Uncovering the Intradiol Cleaving Reactivity of an Iron(II) o-Semiquinonate Complex. Inorganic Chemistry, 2017, 56, 10481-10495.	4.0	10

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19	Electronic Structure of Anilinopyridinate-Supported Ru₂⁵⁺ Paddlewheel Compounds. Inorganic Chemistry, 2017, 56, 14662-14670.	4.0	13
20	Resonance Raman spectroscopic study of the interaction between Co(II)rrinoids and the ATP:corrinoid adenosyltransferase PduO from Lactobacillus reuteri. Journal of Biological Inorganic Chemistry, 2016, 21, 669-681.	2.6	7
21	Synthesis, X-ray Structures, Electronic Properties, and O₂/NO Reactivities of Thiol Dioxygenase Active-Site Models. Inorganic Chemistry, 2016, 55, 11839-11853.	4.0	23
22	Hydrogen Sulfide Oxidation by Myoglobin. Journal of the American Chemical Society, 2016, 138, 8476-8488.	13.7	130
23	Spectroscopic Studies of the EutT Adenosyltransferase from Salmonella enterica: Mechanism of Four-Coordinate Co(II)Cbl Formation. Journal of the American Chemical Society, 2016, 138, 3694-3704.	13.7	11
24	Unprecedented Mechanism Employed by the Salmonella enterica EutT ATP:Co^Irrinoid Adenosyltransferase Precludes Adenosylation of Incomplete Co^{II}rrinoids. Angewandte Chemie, 2015, 127, 7264-7267.	2.0	3
25	Nickel Superoxide Dismutase: Structural and Functional Roles of His1 and Its H-Bonding Network. Biochemistry, 2015, 54, 1016-1027.	2.5	28
26	Spectroscopic and Computational Investigation of the H155A Variant of Cysteine Dioxygenase: Geometric and Electronic Consequences of a Third-Sphere Amino Acid Substitution. Biochemistry, 2015, 54, 2874-2884.	2.5	26
27	Unprecedented Mechanism Employed by the Salmonella enterica EutT ATP:Co^Irrinoid Adenosyltransferase Precludes Adenosylation of Incomplete Co^{II}rrinoids. Angewandte Chemie - International Edition, 2015, 54, 7158-7161.	13.8	13
28	Spectroscopic and Computational Studies of Cobalamin Species with Variable Lower Axial Ligation: Implications for the Mechanism of Coâ€“C Bond Activation by Class I Cobalamin-Dependent Isomerases. Inorganic Chemistry, 2015, 54, 3736-3747.	4.0	21
29	Accessing Ni(III)-Thiolate Versus Ni(II)-Thiyl Bonding in a Family of Niâ€“N₂S₂ Synthetic Models of NiSOD. Inorganic Chemistry, 2015, 54, 3815-3828.	4.0	32
30	Spectroscopic Studies of the Salmonella enterica Adenosyltransferase Enzyme SeCobA: Molecular-Level Insight into the Mechanism of Substrate Cob(II)alamin Activation. Biochemistry, 2014, 53, 7969-7982.	2.5	13
31	Spectroscopic and Computational Investigation of Iron(III) Cysteine Dioxygenase: Implications for the Nature of the Putative Superoxo-Fe(III) Intermediate. Biochemistry, 2014, 53, 5759-5770.	2.5	26
32	Spectral and Electronic Properties of Nitrosylcobalamin. Inorganic Chemistry, 2014, 53, 7676-7691.	4.0	13
33	Structural, Spectroscopic, and Computational Characterization of the Azide Adduct of Fe^{III}(2,6-diacetylpyridinebis(semioxamazide)), a Functional Analogue of Iron Superoxide Dismutase. Inorganic Chemistry, 2013, 52, 8909-8918.	4.0	9
34	Combined Spectroscopic and Computational Analysis of the Vibrational Properties of Vitamin B₁₂ in its Co³⁺, Co²⁺, and Co¹⁺ Oxidation States. Journal of Physical Chemistry B, 2013, 117, 5397-5410.	2.6	23
35	Spectroscopic and Computational Characterization of the NO Adduct of Substrate-Bound Fe(II) Cysteine Dioxygenase: Insights into the Mechanism of O₂ Activation. Biochemistry, 2013, 52, 6040-6051.	2.5	32
36	Combined Spectroscopic/Computational Studies of Vitamin B₁₂ Precursors: Geometric and Electronic Structures of Cobinamides. Inorganic Chemistry, 2012, 51, 2867-2879.	4.0	26

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37	Spectroscopic Characterization of Active-Site Variants of the PduO-type ATP:Corrinoid Adenosyltransferase from Lactobacillus reuteri: Insights into the Mechanism of Four-Coordinate Co(II)corrinoid Formation. Inorganic Chemistry, 2012, 51, 4482-4494.	4.0	12
38	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. Journal of Biological Inorganic Chemistry, 2010, 15, 777-793.	2.6	21
39	Nickel superoxide dismutase: structural and functional roles of Cys2 and Cys6. Journal of Biological Inorganic Chemistry, 2010, 15, 795-807.	2.6	48
40	Spectroscopic insights into axial ligation and active-site H-bonding in substrate-bound human heme oxygenase-2. Journal of Biological Inorganic Chemistry, 2010, 15, 1117-1127.	2.6	12
41	Spectroscopic and Computational Characterization of Substrate-Bound Mouse Cysteine Dioxygenase: Nature of the Ferrous and Ferric Cysteine Adducts and Mechanistic Implications. Biochemistry, 2010, 49, 6033-6041.	2.5	63
42	Spectroscopic and Computational Studies of a Series of High-Spin Ni(II) Thiolate Complexes. Inorganic Chemistry, 2010, 49, 6535-6544.	4.0	9
43	Spectroscopically validated density functional theory studies of the B12 cofactors and their interactions with enzyme active sites. Coordination Chemistry Reviews, 2009, 253, 779-794.	18.8	34
44	Spectroscopic and Computational Characterization of the Base-off Forms of Cob(II)alamin. Journal of Physical Chemistry B, 2009, 113, 5245-5254.	2.6	35
45	Computational studies of bioorganometallic enzymes and cofactors. Metal Ions in Life Sciences, 2009, 6, 417-60.	2.8	0
46	Spectroscopic Study of the Cobalamin-Dependent Methionine Synthase in the Activation Conformation: Effects of the Y1139 Residue and S-Adenosylmethionine on the B12 Cofactor. Journal of the American Chemical Society, 2008, 130, 16374-16381.	13.7	34
47	Spectroscopic and Computational Investigation of Second-Sphere Contributions to Redox Tuning in Escherichia coli Iron Superoxide Dismutase. Inorganic Chemistry, 2008, 47, 3978-3992.	4.0	33
48	Structural Characterization of a Human-Type Corrinoid Adenosyltransferase Confirms That Coenzyme B₁₂ Is Synthesized through a Four-Coordinate Intermediate. Biochemistry, 2008, 47, 5755-5766.	2.5	55
49	Kinetic and Spectroscopic Studies of the ATP:Corrinoid Adenosyltransferase PduO from Lactobacillus reuteri: Substrate Specificity and Insights into the Mechanism of Co(II)corrinoid Reduction. Biochemistry, 2008, 47, 9007-9015.	2.5	36
50	SECOND-SPHERE TUNING OF THE METAL ION REDUCTION POTENTIALS IN IRON AND MANGANESE SUPEROXIDE DISMUTASES. Comments on Inorganic Chemistry, 2008, 29, 134-168.	5.2	38
51	Synthetic iron-oxo â€œdiamond coreâ€•mimics structure of key intermediate in methane monooxygenase catalytic cycle. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 20641-20642.	7.1	13
52	How Can a Single Second Sphere Amino Acid Substitution Cause Reduction Midpoint Potential Changes of Hundreds of Millivolts?. Journal of the American Chemical Society, 2007, 129, 9927-9940.	13.7	44
53	Spectroscopic and Computational Studies of Ni3+ Complexes with Mixed S/N Ligation:â€‰ Implications for the Active Site of Nickel Superoxide Dismutase. Inorganic Chemistry, 2007, 46, 8511-8523.	4.0	22
54	Characterization of the Nitrosyl Adduct of Substrate-Bound Mouse Cysteine Dioxygenase by Electron Paramagnetic Resonance:â€‰ Electronic Structure of the Active Site and Mechanistic Implications. Biochemistry, 2007, 46, 8569-8578.	2.5	99

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55	Probing the Role of the Histidine 759 Ligand in Cobalamin-Dependent Methionine Synthase. Biochemistry, 2007, 46, 8024-8035.	2.5	22
56	Spectroscopic Studies of the Corrinoid/Ironâ^'Sulfur Protein fromMoorella thermoacetica. Journal of the American Chemical Society, 2006, 128, 5010-5020.	13.7	51
57	Spectroscopic and Computational Studies of Reduction of the Metal versus the Tetrapyrrole Ring of Coenzyme F430from Methyl-Coenzyme M Reductaseâ€. Biochemistry, 2006, 45, 11915-11933.	2.5	10
58	Spectroscopic and Computational Studies of Co1+Cobalamin:Â Spectral and Electronic Properties of the â€œSuperreducedâ€•B12Cofactor. Journal of the American Chemical Society, 2006, 128, 9144-9156.	13.7	89
59	Identification of an â€œEnd-onâ€•Nickelâ^'Superoxo Adduct, [Ni(tmc)(O2)]+. Journal of the American Chemical Society, 2006, 128, 14230-14231.	13.7	118
60	Combined Spectroscopic/Computational Study of Binuclear Fe(I)â^'Fe(I) Complexes:Â Implications for the Fully-Reduced Active-Site Cluster of Fe-Only Hydrogenases. Inorganic Chemistry, 2005, 44, 1794-1809.	4.0	40
61	Synthesis, Structure Determination, and Spectroscopic/Computational Characterization of a Series of Fe(II)â^'Thiolate Model Complexes:Â Implications for Feâ^'S Bonding in Superoxide Reductases. Journal of the American Chemical Society, 2005, 127, 1675-1689.	13.7	46
62	Spectroscopic and Computational Studies of the ATP:Corrinoid Adenosyltransferase (CobA) fromSalmonella enterica:Â Insights into the Mechanism of Adenosylcobalamin Biosynthesis. Journal of the American Chemical Society, 2005, 127, 8710-8719.	13.7	90
63	Spectroscopic and Computational Studies of Ni Superoxide Dismutase:Â Electronic Structure Contributions to Enzymatic Function. Journal of the American Chemical Society, 2005, 127, 5449-5462.	13.7	110
64	Coâ^'C Bond Activation in Methylmalonyl-CoA Mutase by Stabilization of the Post-homolysis Product Co2+Cobalamin. Journal of the American Chemical Society, 2005, 127, 16522-16528.	13.7	40
65	Probing the Geometric and Electronic Structures of the Low-Temperature Azide Adduct and the Product-Inhibited Form of Oxidized Manganese Superoxide Dismutase. Biochemistry, 2005, 44, 1504-1520.	2.5	57
66	Spectroscopic Evidence for the Formation of a Four-Coordinate Co2+Cobalamin Species upon Binding to the Human ATP:Cobalamin Adenosyltransferase. Journal of the American Chemical Society, 2005, 127, 7660-7661.	13.7	94
67	Spectroscopic and computational characterization of the nickel-containing F430 cofactor of methyl-coenzyme M reductase. Journal of Biological Inorganic Chemistry, 2004, 9, 77-89.	2.6	26
68	Spectroscopic and computational insights into the geometric and electronic properties of the A-cluster of acetyl-coenzyme A synthase. Journal of Biological Inorganic Chemistry, 2004, 9, 533-541.	2.6	34
69	Combined Spectroscopic/Computational Studies on Fe- and Mn-Dependent Superoxide Dismutases:â€‰ Insights into Second-Sphere Tuning of Active Site Properties. Accounts of Chemical Research, 2004, 37, 461-470.	15.6	105
70	Spectroscopic and Computational Studies of Co2+Corrinoids:Â Spectral and Electronic Properties of the Biologically Relevant Base-On and Base-Off Forms of Co2+Cobalamin. Journal of the American Chemical Society, 2004, 126, 9735-9749.	13.7	120
71	Nickel Oxidation States of F430Cofactor in Methyl-Coenzyme M Reductase. Journal of the American Chemical Society, 2004, 126, 4068-4069.	13.7	53
72	A Monomeric Nickelâ^'Dioxygen Adduct Derived from a Nickel(I) Complex and O2. Inorganic Chemistry, 2004, 43, 3324-3326.	4.0	95

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73	Spectroscopic and Computational Studies of the Azide-Adduct of Manganese Superoxide Dismutase:Â Definitive Assignment of the Ligand Responsible for the Low-Temperature Thermochromism. Journal of the American Chemical Society, 2004, 126, 12477-12491.	13.7	60
74	Definitive Spectroscopic Determination of Zero-Field Splitting in High-Spin Cobalt(II). Journal of the American Chemical Society, 2004, 126, 2148-2155.	13.7	107
75	Computational Studies on the A Cluster of Acetyl-Coenzyme A Synthase:Â Geometric and Electronic Properties of the NiFeC Species and Mechanistic Implications. Journal of the American Chemical Society, 2003, 125, 13962-13963.	13.7	77
76	Spectroscopic and Computational Study of a Non-Heme Iron {Feâ^'NO}7 System:â€‰ Exploring the Geometric and Electronic Structures of the Nitrosyl Adduct of Iron Superoxide Dismutase. Journal of the American Chemical Society, 2003, 125, 8348-8363.	13.7	61
77	Spectroscopic and Computational Studies of Co3+-Corrinoids:Â Spectral and Electronic Properties of the B12Cofactors and Biologically Relevant Precursors. Journal of the American Chemical Society, 2003, 125, 5897-5914.	13.7	122
78	Spectroscopic and Computational Studies of a Ni+â^'CO Model Complex:â€‰ Implications for the Acetyl-CoA Synthase Catalytic Mechanism. Inorganic Chemistry, 2003, 42, 859-867.	4.0	45
79	Second-Sphere Contributions to Substrate-Analogue Binding in Iron(III) Superoxide Dismutase. Journal of the American Chemical Society, 2002, 124, 3769-3774.	13.7	41
80	Spectroscopic and Computational Studies on Iron and Manganese Superoxide Dismutases:â€‰ Nature of the Chemical Events Associated with Active-Site pKs. Journal of the American Chemical Society, 2002, 124, 10833-10845.	13.7	54
81	Hydrogen-Bond-Mediated Tuning of the Redox Potential of the Non-Heme Fe Site of Superoxide Dismutase. Journal of the American Chemical Society, 2002, 124, 3482-3483.	13.7	63
82	Dioxygen Activation by a Nickel Thioether Complex:Â Characterization of a NiIII2(Î¼-O)2Core. Journal of the American Chemical Society, 2001, 123, 9194-9195.	13.7	84
83	Geometric and Electronic Structure/Function Correlations in Non-Heme Iron Enzymes. Chemical Reviews, 2000, 100, 235-350.	47.7	1,594
84	Excited-State Exchange Coupling in Bent Mn(III)â^'Oâ^'Mn(III) Complexes:â€‰ Dominance of the Ï€/Ï*f* Superexchange Pathway and Its Possible Contributions to the Reactivities of Binuclear Metalloproteins. Journal of the American Chemical Society, 2000, 122, 8511-8523.	13.7	70
85	Reversible Dioxygen Binding to Hemerythrin. 2. Mechanism of the Proton-Coupled Two-Electron Transfer to O2at a Single Iron Center. Journal of the American Chemical Society, 1999, 121, 8288-8295.	13.7	64
86	Reversible Dioxygen Binding to Hemerythrin. 1. Electronic Structures of Deoxy- and Oxyhemerythrin. Journal of the American Chemical Society, 1999, 121, 8277-8287.	13.7	65
87	Spectroscopic Study of [Fe2(O2)(OBz)2{HB(pzâ€˜)3}2]:â€‰ Nature of the Î¼-1,2 Peroxideâ^'Fe(III) Bond and Its Possible Relevance to O2 Activation by Non-Heme Iron Enzymes. Journal of the American Chemical Society, 1998, 120, 5674-5690.	13.7	119