Julie A Kovacs

List of Publications by Year
in descending order

75 papers	3,054 citations	109321 35 h-index	168389 53 g-index
78 all docs	78 docs citations	78 times ranked	2319 citing authors

#	Article	IF	Citations
1	Synthetic Analogues of Cysteinate-Ligated Non-Heme Iron and Non-Corrinoid Cobalt Enzymes. Chemical Reviews, 2004, 104, 825-848.	47.7	260
2	Nickel L-Edge Soft X-ray Spectroscopy of Nickelâ˘'Iron Hydrogenases and Model CompoundsEvidence for High-Spin Nickel(II) in the Active Enzyme. Journal of the American Chemical Society, 2000, 122, 10544-10552.	13.7	140
3	How Does Single Oxygen Atom Addition Affect the Properties of an Feâ˘'Nitrile Hydratase Analogue? The Compensatory Role of the Unmodified Thiolate. Journal of the American Chemical Society, 2006, 128, 11211-11221.	13.7	93
4	Sulfur K-Edge XAS and DFT Calculations on Nitrile Hydratase:Â Geometric and Electronic Structure of the Non-heme Iron Active Site. Journal of the American Chemical Society, 2006, 128, 533-541.	13.7	91
5	Understanding How the Thiolate Sulfur Contributes to the Function of the Non-Heme Iron Enzyme Superoxide Reductase. Accounts of Chemical Research, 2007, 40, 501-509.	15.6	91
6	Synthetic Models for the Cysteinate-Ligated Non-Heme Iron Enzyme Superoxide Reductase:â€‰ Observation and Structural Characterization by XAS of an FeIIIâ˘'OOH Intermediate. Journal of the American Chemical Society, 2002, 124, 11709-11717.	13.7	89
7	Characterization of Metastable Intermediates Formed in the Reaction between a Mn(II) Complex and Dioxygen, Including a Crystallographic Structure of a Binuclear Mn(III)â€"Peroxo Species. Journal of the American Chemical Society, 2013, 135, 5631-5640.	13.7	80
8	Assembly of vanadium-iron-sulfur cubane clusters from mononuclear and linear trinuclear reactants. Journal of the American Chemical Society, 1986, 108, 340-341.	13.7	75
9	Correlation Between Structural, Spectroscopic, and Reactivity Properties Within a Series of Structurally Analogous Metastable Manganese(III)â€"Alkylperoxo Complexes. Journal of the American Chemical Society, 2013, 135, 4260-4272.	13.7	67
10	Reactivity of Five-Coordinate Models for the Thiolate-Ligated Fe Site of Nitrile Hydratase. Journal of the American Chemical Society, 1998, 120, 5691-5700.	13.7	66
11	Why Is There an â€œInertâ€•Metal Center in the Active Site of Nitrile Hydratase? Reactivity and Ligand Dissociation from a Five-Coordinate Co(III) Nitrile Hydratase Model. Journal of the American Chemical Society, 2001, 123, 463-468.	13.7	66
12	BIOCHEMISTRY: How Iron Activates O2. Science, 2003, 299, 1024-1025.	12.6	66
13	How Do Oxidized Thiolate Ligands Affect the Electronic and Reactivity Properties of a Nitrile Hydratase Model Compound?. Journal of the American Chemical Society, 2000, 122, 8299-8300.	13.7	65
14	A Functional Model for the Cysteinate-Ligated Non-Heme Iron Enzyme Superoxide Reductase (SOR). Journal of the American Chemical Society, 2006, 128, 14448-14449.	13.7	65
15	Comparative electronic structures of nitrogenase FeMoco and FeVco. Dalton Transactions, 2017, 46, 2445-2455.	3.3	65
16	Structural chemistry of vanadium-iron-sulfur clusters containing the cubane-type [VFe3S4]2+ core. Inorganic Chemistry, 1987, 26, 711-718.	4.0	58
17	Structural and Spectroscopic Characterization of Metastable Thiolate-Ligated Manganese(III)â€"Alkylperoxo Species. Journal of the American Chemical Society, 2011, 133, 12470-12473.	13.7	58
18	Heterometallic clusters: synthesis and reactions of vanadium-iron-sulfur single- and double-cubane clusters and the structure of [V2Fe6S8Cl4(C2H4S2)2]4-. Inorganic Chemistry, 1987, 26, 702-711.	4.0	56

#	Article	IF	Citations
19	A Synthetic Model for the NO-Inactivated Form of Nitrile Hydratase. Journal of the American Chemical Society, 1998, 120, 10996-10997.	13.7	52
20	Comparative electronic properties of vanadium-iron-sulfur and molybdenum-iron-sulfur clusters containing isoelectronic cubane-type [VFe3S4]2+ and [MoFe3S4]3+ cores. Inorganic Chemistry, 1987, 26, 719-724.	4.0	51
21	X-ray Spectroscopy of Nitric Oxide Binding to Iron in Inactive Nitrile Hydratase and a Synthetic Model Compound. Journal of the American Chemical Society, 1998, 120, 9237-9245.	13.7	51
22	The First Example of a Nitrile Hydratase Model Complex that Reversibly Binds Nitriles. Journal of the American Chemical Society, 2002, 124, 11417-11428.	13.7	51
23	Persulfide-bridged iron-molybdenum-sulfur clusters of biological relevance: two synthetic routes and the structures of intermediate and product clusters. Journal of the American Chemical Society, 1985, 107, 1784-1786.	13.7	50
24	Tuning the Relative Stability and Reactivity of Manganese Dioxygen and Peroxo Intermediates via Systematic Ligand Modification. Accounts of Chemical Research, 2015, 48, 2744-2753.	15.6	50
25	X-ray Absorption and Emission Study of Dioxygen Activation by a Small-Molecule Manganese Complex. Inorganic Chemistry, 2015, 54, 6410-6422.	4.0	49
26	A Model for the Low-Spin, Non-Heme, Thiolate-Ligated Iron Site of Nitrile Hydratase. Inorganic Chemistry, 1995, 34, 4517-4518.	4.0	48
27	Nitrile Hydration by Thiolate- and Alkoxide-Ligated Co-NHase Analogues. Isolation of Co(III)-Amidate and Co(III)-Iminol Intermediates. Journal of the American Chemical Society, 2011, 133, 3954-3963.	13.7	48
28	Synthesis and Structural Characterization of a Series of MnIIIOR Complexes, Including a Water-Soluble MnIIIOH That Promotes Aerobic Hydrogen-Atom Transfer. Inorganic Chemistry, 2013, 52, 12383-12393.	4.0	44
29	Steric and Electronic Control over the Reactivity of a Thiolate-Ligated Fe(II) Complex with Dioxygen and Superoxide:Â Reversible Î¼-Oxo Dimer Formation. Inorganic Chemistry, 2004, 43, 7682-7690.	4.0	41
30	Synthesis and structure of a water-soluble five-coordinate nickel alkanethiolate complex. Inorganic Chemistry, 1994, 33, 7-8.	4.0	39
31	Periodic Trends within a Series of Five-Coordinate Thiolate-Ligated [MII(SMe2N4(tren))]+ (M = Mn, Fe,) Tj ETQq1 1 0.784314 rgBT /Ove 2007, 46, 9267-9277.	4.0	39
32	S K-Edge X-Ray Absorption Spectroscopy and Density Functional Theory Studies of High and Low Spin {FeNO}⁷ Thiolate Complexes: Exchange Stabilization of Electron Delocalization in {FeNO}⁷ and {FeO₂}⁸. Inorganic Chemistry, 2011, 50, 427-436.	4.0	38
33	Formation of a Reactive, Alkyl Thiolate-Ligated Fe^{III}-Superoxo Intermediate Derived from Dioxygen. Journal of the American Chemical Society, 2019, 141, 1867-1870.	13.7	38
34	Modeling the Reactivity of Superoxide Reducing Metalloenzymes with a Nitrogen and Sulfur Coordinated Iron Complex. Inorganic Chemistry, 2001, 40, 5483-5484.	4.0	37
35	Investigation of the Mechanism of Formation of a Thiolate-Ligated Fe(III)-OOH. Inorganic Chemistry, 2011, 50, 1592-1602.	4.0	37
36	Influence of Thiolate Ligands on Reductive Nâˆ'O Bond Activation. Probing the O₂^{âˆ'} Binding Site of a Biomimetic Superoxide Reductase Analogue and Examining the Proton-Dependent Reduction of Nitrite. Journal of the American Chemical Society, 2011, 133, 1419-1427.	13.7	37

#	Article	IF	Citations
37	Iron L_{2,3}-Edge X-ray Absorption and X-ray Magnetic Circular Dichroism Studies of Molecular Iron Complexes with Relevance to the FeMoco and FeVco Active Sites of Nitrogenase. Inorganic Chemistry, 2017, 56, 8147-8158.	4.0	37
38	How does cyanide inhibit superoxide reductase? Insight from synthetic FeIIIN4S model complexes. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 3671-3676.	7.1	36
39	Spectroscopy of Non-Heme Iron Thiolate Complexes:Â Insight into the Electronic Structure of the Low-Spin Active Site of Nitrile Hydratase. Inorganic Chemistry, 2005, 44, 1826-1836.	4.0	36
40	Probing the Influence of Local Coordination Environment on the Properties of Fe-Type Nitrile Hydratase Model Complexes. Inorganic Chemistry, 2001, 40, 1646-1653.	4.0	35
41	Characterization and Dioxygen Reactivity of a New Series of Coordinatively Unsaturated Thiolate-Ligated Manganese(II) Complexes. Inorganic Chemistry, 2012, 51, 6633-6644.	4.0	35
42	Nickel-promoted reductive carbon-sulfur bond cleavage: a model for the first step in the reaction promoted by methyl coenzyme M reductase. Inorganic Chemistry, 1993, 32, 1860-1863.	4.0	32
43	Synthesis and reactivity of the first structurally characterized heterobimetallic complex containing an unsupported bridging sulfur atom. Journal of the American Chemical Society, 1989, 111, 1131-1133.	13.7	30
44	Reactivities and biological functions of iron-sulfur clusters. Journal of Cluster Science, 1990, 1, 29-73.	3.3	30
45	Probing the influence of local coordination environment on ligand binding in nickel hydrogenase model complexes. Inorganic Chemistry, 1993, 32, 5868-5877.	4.0	30
46	Synthesis of a new class of Mo-Fe-S clusters containing the MoS2Fe2 unit. Polyhedron, 1986, 5, 393-398.	2.2	27
47	Properties of Square-Pyramidal Alkylâˆ’Thiolate Fe^{III} Complexes, Including an Analogue of the Unmodified Form of Nitrile Hydratase. Inorganic Chemistry, 2008, 47, 11228-11236.	4.0	27
48	Enhancing Reactivity via Structural Distortion. Inorganic Chemistry, 2002, 41, 3128-3136.	4.0	26
49	Water-Soluble Fe(II)â€“H₂O Complex with a Weak Oâ€“H Bond Transfers a Hydrogen Atom via an Observable Monomeric Fe(III)â€“OH. Journal of the American Chemical Society, 2015, 137, 2253-2264.	13.7	25
50	Metal-Assisted Oxo Atom Addition to an Fe(III) Thiolate. Journal of the American Chemical Society, 2017, 139, 119-129.	13.7	25
51	Structural Comparison of Five-Coordinate Thiolate-Ligated MII= FeII, CoII, NiII, and ZnIIIons Wrapped in a Chiral Helical Ligand. Inorganic Chemistry, 1998, 37, 5721-5726.	4.0	23
52	Ligand Oxidations in High-Spin Nickel Thiolate Complexes and Zinc Analogues. Inorganic Chemistry, 2004, 43, 7726-7734.	4.0	23
53	Understanding the Mechanism of Superoxide Reductase Promoted Reduction of Superoxide. European Journal of Inorganic Chemistry, 2007, 2007, 29-38.	2.0	22
54	The Structure of a Toroidal, Neutral, Homoleptic Ni(II) Complex with a Chelate Dithiolate Ligand, [Ni6(SCH2CH2CH2S)6].. Acta Chemica Scandinavica, 1994, 48, 929-932.	0.7	22

#	Article	IF	Citations
55	A model for the interaction of alcohol with the zinc thiolate site of alcohol dehydrogenase. Inorganic Chemistry, 1995, 34, 5933-5934.	4.0	21
56	Comparison of structurally-related alkoxide, amine, and thiolate-ligated MII (M=Fe, Co) complexes: The influence of thiolates on the properties of biologically relevant metal complexes. Inorganica Chimica Acta, 2008, 361, 1070-1078.	2.4	21
57	Role of Protons in Superoxide Reduction by a Superoxide Reductase Analogue. Inorganic Chemistry, 2005, 44, 1169-1171.	4.0	18
58	Synthesis and structure of a thiolate-ligated Ni cluster which contains an unusual thiolate bridging mode and an exposed Ni site. Inorganica Chimica Acta, 1997, 263, 153-159.	2.4	17
59	A Co(III) Complex in a Mixed Sulfur/Nitrogen Ligand Environment:Â Modeling the Substrate- and Product-Bound Forms of the Metalloenzyme Thiocyanate Hydrolase. Inorganic Chemistry, 2000, 39, 4998-4999.	4.0	15
60	How Metal Ion Lewis Acidity and Steric Properties Influence the Barrier to Dioxygen Binding, Peroxo Oâ€“O Bond Cleavage, and Reactivity. Journal of the American Chemical Society, 2019, 141, 15046-15057.	13.7	15
61	[Fe2S2(CO)6]2âˆ’ as a cluster precursor: synthesis and structure of [MoFe3S6(CO)6]2âˆ’ and oxidative decarbonylation to a persulfide-bridged MoFe3S4 double cubane. Polyhedron, 1987, 6, 1445-1456.	2.2	13
62	Metal-Carbon Bonds in Nature. Science, 1995, 270, 587-588.	12.6	13
63	Isolation and Characterization of a Dihydroxo-Bridged Iron(III,III)(Î¼-OH)₂ Diamond Core Derived from Dioxygen. Inorganic Chemistry, 2013, 52, 13325-13331.	4.0	12
64	Influence of Thiolate versus Alkoxide Ligands on the Stability of Crystallographically Characterized Mn(III)-Alkylperoxo Complexes. Journal of the American Chemical Society, 2021, 143, 6104-6113.	13.7	9
65	How Do Ring Size and Ï€-Donating Thiolate Ligands Affect Redox-Active, Î±-Imino-<i>N</i>-heterocycle Ligand Activation?. Inorganic Chemistry, 2018, 57, 1935-1949.	4.0	7
66	Geometric and electronic structure of a crystallographically characterized thiolate-ligated binuclear peroxo-bridged cobalt(III) complex. Journal of Biological Inorganic Chemistry, 2019, 24, 919-926.	2.6	5
67	Electronic Structure and Reactivity of Dioxygen-Derived Aliphatic Thiolate-Ligated Fe-Peroxo and Fe(IV) Oxo Compounds. Journal of the American Chemical Society, 2022, 144, 8515-8528.	13.7	5
68	Superoxide Oxidation by a Thiolate-Ligated Iron Complex and Anion Inhibition. Inorganic Chemistry, 2021, 60, 7250-7261.	4.0	4
69	Richard Hadley Holm: A Remembrance and A Tribute. Comments on Inorganic Chemistry, 2022, 42, 61-108.	5.2	2
70	Preparation and properties of [NiII(BEES)(Cl)](BPh4): a NiII complex in a mixed nitrogen/thioether coordination environment. Inorganica Chimica Acta, 2002, 336, 61-64.	2.4	1
71	A chloride ion contained in a cobalt `claw': [Co3(DADIT)3]Cl(PF6)2. Acta Crystallographica Section C: Crystal Structure Communications, 2003, 59, m379-m380.	0.4	1
72	Increasing reactivity by incorporating Ï€-acceptor ligands into coordinatively unsaturated thiolate-ligated iron(II) complexes. Inorganica Chimica Acta, 2021, 524, 120422.	2.4	1

#	Article	IF	Citations
73	Comparison of two Mn^{IV}Mn^{IV}-bis-Î¼-oxo complexes {[Mn^{IV}(N₄(6-Me-DPEN))]₂(Î¼-O)₂}²⁺ and {[Mn^{IV}(N₄(6-Me-DPPN))]₂(Î¼-O)₂}²⁺. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1042-1046.	0.5	1
74	Understanding the mechanism of superoxide reduction by the non-heme iron enzyme superoxide reductase (SOR) using a synthetic analogue approach. Journal of Inorganic Biochemistry, 2003, 96, 20.	3.5	0
75	Synthetic Analogues of Cysteinate-Ligated Non-Heme Iron and Non-Corrinoid Cobalt Enzymes. ChemInform, 2004, 35, no.	0.0	0