# Julie A Kovacs

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | Richard Hadley Holm: A Remembrance and A Tribute. Comments on Inorganic Chemistry, 2022, 42, 61-108. | 5.2 | 2 |
| 2 | 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 |
| 3 | 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 |
| 4 | Superoxide Oxidation by a Thiolate-Ligated Iron Complex and Anion Inhibition. Inorganic Chemistry, 2021, 60, 7250-7261. | 4.0 | 4 |
| 5 | Increasing reactivity by incorporating Ï€-acceptor ligands into coordinatively unsaturated thiolate-ligated iron(II) complexes. Inorganica Chimica Acta, 2021, 524, 120422. | 2.4 | 1 |
| 6 | Comparison of two Mn<sup>IV</sup>Mn<sup>IV</sup>-bis-Î¼-oxo complexes {[Mn<sup>IV</sup>(N<sub>4</sub>(6-Me-DPEN))]<sub>2</sub>(Î¼-O)<sub>2</sub>}<sup>2+</sup> and {[Mn<sup>IV</sup>(N<sub>4</sub>(6-Me-DPPN))]<sub>2</sub>(Î¼-O)<sub>2</sub>}<sup>2+</sup>. Acta Crystallographica Section E: Crystallographic Communications, 2020, 76, 1042-1046. | 0.5 | 1 |
| 7 | 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 |
| 8 | 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 |
| 9 | Formation of a Reactive, Alkyl Thiolate-Ligated Fe<sup>III</sup>-Superoxo Intermediate Derived from Dioxygen. Journal of the American Chemical Society, 2019, 141, 1867-1870. | 13.7 | 38 |
| 10 | 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 |
| 11 | Comparative electronic structures of nitrogenase FeMoco and FeVco. Dalton Transactions, 2017, 46, 2445-2455. | 3.3 | 65 |
| 12 | Metal-Assisted Oxo Atom Addition to an Fe(III) Thiolate. Journal of the American Chemical Society, 2017, 139, 119-129. | 13.7 | 25 |
| 13 | Iron L<sub>2,3</sub>-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 |
| 14 | X-ray Absorption and Emission Study of Dioxygen Activation by a Small-Molecule Manganese Complex. Inorganic Chemistry, 2015, 54, 6410-6422. | 4.0 | 49 |
| 15 | Water-Soluble Fe(II)â€“H<sub>2</sub>O 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 |
| 16 | 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 |
| 17 | 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 |
| 18 | Isolation and Characterization of a Dihydroxo-Bridged Iron(III,III)(Î¼-OH)<sub>2</sub> Diamond Core Derived from Dioxygen. Inorganic Chemistry, 2013, 52, 13325-13331. | 4.0 | 12 |

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| 19 | 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 |
| 20 | 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 |
| 21 | 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 |
| 22 | 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 |
| 23 | Investigation of the Mechanism of Formation of a Thiolate-Ligated Fe(III)-OOH. Inorganic Chemistry, 2011, 50, 1592-1602. | 4.0 | 37 |
| 24 | Influence of Thiolate Ligands on Reductive Nâˆ’O Bond Activation. Probing the O<sub>2</sub><sup>â"</sup> 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 |
| 25 | S K-Edge X-Ray Absorption Spectroscopy and Density Functional Theory Studies of High and Low Spin {FeNO}<sup>7</sup> Thiolate Complexes: Exchange Stabilization of Electron Delocalization in {FeNO}<sup>7</sup> and {FeO<sub>2</sub>}<sup>8</sup>. Inorganic Chemistry, 2011, 50, 427-436. | 4.0 | 38 |
| 26 | 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 |
| 27 | 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 |
| 28 | Properties of Square-Pyramidal Alkylâˆ’Thiolate Fe<sup>III</sup> Complexes, Including an Analogue of the Unmodified Form of Nitrile Hydratase. Inorganic Chemistry, 2008, 47, 11228-11236. | 4.0 | 27 |
| 29 | 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 |
| 30 | Understanding the Mechanism of Superoxide Reductase Promoted Reduction of Superoxide. European Journal of Inorganic Chemistry, 2007, 2007, 29-38. | 2.0 | 22 |
| 31 | Periodic Trends within a Series of Five-Coordinate Thiolate-Ligated [MII(SMe2N4(tren))]+ (M = Mn, Fe,) Tj ETQq1 1 0.784314 rgBT /Ov 2007, 46, 9267-9277. | 4.0 | 39 |
| 32 | 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 |
| 33 | How Does Single Oxygen Atom Addition Affect the Properties of an Feâˆ'Nitrile Hydratase Analogue? The Compensatory Role of the Unmodified Thiolate. Journal of the American Chemical Society, 2006, 128, 11211-11221. | 13.7 | 93 |
| 34 | 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 |
| 35 | 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 |
| 36 | Role of Protons in Superoxide Reduction by a Superoxide Reductase Analogue. Inorganic Chemistry, 2005, 44, 1169-1171. | 4.0 | 18 |

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| 37 | Synthetic Analogues of Cysteinate-Ligated Non-Heme Iron and Non-Corrinoid Cobalt Enzymes. ChemInform, 2004, 35, no. | 0.0 | 0 |
| 38 | Ligand Oxidations in High-Spin Nickel Thiolate Complexes and Zinc Analogues. Inorganic Chemistry, 2004, 43, 7726-7734. | 4.0 | 23 |
| 39 | Synthetic Analogues of Cysteinate-Ligated Non-Heme Iron and Non-Corrinoid Cobalt Enzymes. Chemical Reviews, 2004, 104, 825-848. | 47.7 | 260 |
| 40 | 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 |
| 41 | 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 |
| 42 | 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 |
| 43 | 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 |
| 44 | BIOCHEMISTRY: How Iron Activates O2. Science, 2003, 299, 1024-1025. | 12.6 | 66 |
| 45 | 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 |
| 46 | 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 |
| 47 | Enhancing Reactivity via Structural Distortion. Inorganic Chemistry, 2002, 41, 3128-3136. | 4.0 | 26 |
| 48 | 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 |
| 49 | Modeling the Reactivity of Superoxide Reducing Metalloenzymes with a Nitrogen and Sulfur Coordinated Iron Complex. Inorganic Chemistry, 2001, 40, 5483-5484. | 4.0 | 37 |
| 50 | 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 |
| 51 | 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 |
| 52 | 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 |
| 53 | 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 |
| 54 | 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 |

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| 55 | 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 |
| 56 | A Synthetic Model for the NO-Inactivated Form of Nitrile Hydratase. Journal of the American Chemical Society, 1998, 120, 10996-10997. | 13.7 | 52 |
| 57 | 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 |
| 58 | 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 |
| 59 | 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 |
| 60 | A model for the interaction of alcohol with the zinc thiolate site of alcohol dehydrogenase. Inorganic Chemistry, 1995, 34, 5933-5934. | 4.0 | 21 |
| 61 | A Model for the Low-Spin, Non-Heme, Thiolate-Ligated Iron Site of Nitrile Hydratase. Inorganic Chemistry, 1995, 34, 4517-4518. | 4.0 | 48 |
| 62 | Metal-Carbon Bonds in Nature. Science, 1995, 270, 587-588. | 12.6 | 13 |
| 63 | Synthesis and structure of a water-soluble five-coordinate nickel alkanethiolate complex. Inorganic Chemistry, 1994, 33, 7-8. | 4.0 | 39 |
| 64 | 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 |
| 65 | Probing the influence of local coordination environment on ligand binding in nickel hydrogenase model complexes. Inorganic Chemistry, 1993, 32, 5868-5877. | 4.0 | 30 |
| 66 | 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 |
| 67 | Reactivities and biological functions of iron-sulfur clusters. Journal of Cluster Science, 1990, 1, 29-73. | 3.3 | 30 |
| 68 | 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 |
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| 70 | 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 |
| 71 | Structural chemistry of vanadium-iron-sulfur clusters containing the cubane-type [VFe3S4]2+ core. Inorganic Chemistry, 1987, 26, 711-718. | 4.0 | 58 |
| 72 | [Fe2S2(CO)6]2â˘’ as a cluster precursor: synthesis and structure of [MoFe3S6(CO)6]2â˘’ and oxidative decarbonylation to a persulfide-bridged MoFe3S4 double cubane. Polyhedron, 1987, 6, 1445-1456. | 2.2 | 13 |

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| 73 | 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 |
| 74 | Synthesis of a new class of Mo-Fe-S clusters containing the MoS2Fe2 unit. Polyhedron, 1986, 5, 393-398. | 2.2 | 27 |
| 75 | 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 |