Stephen Sproules

List of Publications by Year
in descending order

110 papers	3,442 citations	136950 32 h-index	161849 54 g-index
117 all docs	117 docs citations	117 times ranked	4878 citing authors

#	Article	IF	Citations
1	Spectroscopic Studies of the Chanâ€“Lam Amination: A Mechanism-Inspired Solution to Boronic Ester Reactivity. Journal of the American Chemical Society, 2017, 139, 4769-4779.	13.7	264
2	Dithiolene radicals: Sulfur K-edge X-ray absorption spectroscopy and Harry's intuition. Coordination Chemistry Reviews, 2011, 255, 837-860.	18.8	171
3	Electronic and Molecular Structures of the Members of the Electron Transfer Series [Cr(^{<i>t</i>}bpy)₃]^{<i>n</i>} (<i>n</i> = 3+, 2+, 1+, 0): An X-ray Absorption Spectroscopic and Density Functional Theoretical Study. Inorganic Chemistry, 2011, 50, 12446-12462.	4.0	142
4	Oxidative Addition of Aryl Electrophiles to a Prototypical Nickel(0) Complex: Mechanism and Structure/Reactivity Relationships. Organometallics, 2017, 36, 1662-1672.	2.3	135
5	Experimental Fingerprints for Redox-Active Terpyridine in [Cr(tpy)₂](PF₆)_{<i>n</i>} (<i>n</i> = 3â€“0), and the Remarkable Electronic Structure of [Cr(tpy)₂]^{1â€“}. Inorganic Chemistry, 2012, 51, 3718-3732.	4.0	125
6	o-Dithiolene and o-aminothiolate chemistry of iron: Synthesis, structure and reactivity. Coordination Chemistry Reviews, 2010, 254, 1358-1382.	18.8	111
7	Re-evaluating the Cu K pre-edge XAS transition in complexes with covalent metalâ€“ligand interactions. Chemical Science, 2015, 6, 2474-2487.	7.4	110
8	Redoxâ€Switchable Ringâ€Closing Metathesis: Catalyst Design, Synthesis, and Study. Chemistry - A European Journal, 2013, 19, 10866-10875.	3.3	90
9	A Step beyond the Felthamâ€“Enemark Notation: Spectroscopic and Correlated<i>ab Initio</i>Computational Support for an Antiferromagnetically Coupled M(II)â€“(NO)^{âˆ’}Description of Tp*M(NO) (M = Co, Ni). Journal of the American Chemical Society, 2011, 133, 18785-18801.	13.7	89
10	Electronic Structures of the Electron Transfer Series [M(bpy)₃]<i>ⁿ</i>, [M(tpy)₂]<i>ⁿ</i>, and [Fe(^tbpy)₃]<i>ⁿ</i> (M = Fe, Ru; <i>n</i> = 3+, 2+, 1+, 0, 1â€“): A MÃ¶ssbauer Spectroscopic and DFT Study. European Journal of Inorganic Chemistry, 2012, 2012, 4605-4621.	2.0	87
11	Electronic Structure of the [Tris(dithiolene)chromium]^{<i>z</i>}(<i>z</i>= 0, 1âˆ’, 2âˆ’, 3âˆ’) Electron Transfer Series and Their Manganese(IV) Analogues. An X-ray Absorption Spectroscopic and Density Functional Theoretical Study. Inorganic Chemistry, 2009, 48, 5829-5847.	4.0	78
12	Controlled Tuning of the Properties in Optoelectronic Self-Sorted Gels. Journal of the American Chemical Society, 2018, 140, 8667-8670.	13.7	68
13	Inner-sphere vs. outer-sphere reduction of uranyl supported by a redox-active, donor-expanded dipyrrin. Chemical Science, 2017, 8, 108-116.	7.4	64
14	Switchable Interaction in Molecular Double Qubits. CheM, 2016, 1, 727-752.	11.7	60
15	Kinetic Control of Interpenetration in Feâ€“Biphenyl-4,4â€²-dicarboxylate Metalâ€“Organic Frameworks by Coordination and Oxidation Modulation. Journal of the American Chemical Society, 2019, 141, 8346-8357.	13.7	58
16	Six-Membered Electron Transfer Series [V(dithiolene)₃]^{<i>z</i>}(<i>z</i>= 1+, 0,) Tj ETQq0 0 0 rgBT /Overlock Chemistry, 2010, 49, 5241-5261.	4.0	55
17	Monoanionic Molybdenum and Tungsten Tris(dithiolene) Complexes: A Multifrequency EPR Study. Inorganic Chemistry, 2011, 50, 7106-7122.	4.0	55
18	Electronic Structures of Homoleptic [Tris(2,2â€²-bipyridine)M]^{<i>n</i>} Complexes of the Early Transition Metals (M = Sc, Y, Ti, Zr, Hf, V, Nb, Ta; <i>n</i> = 1+, 0, 1â€“, 2â€“, 3âˆ’): An Experimental and Density Functional Theoretical Study. Inorganic Chemistry, 2013, 52, 2242-2256.	4.0	54

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19	Modulation of Magnetic Properties at Room Temperature: Coordinationâ€Induced Valence Tautomerism in a Cobalt Dioxolene Complex. Chemistry - A European Journal, 2014, 20, 11149-11162.	3.3	52
20	Electronic Structures of the [V(^{<i>t</i>}bpy)₃]^{<i>z</i>} (<i>z</i> =) Tj ETQq0 0 0 rgBT /Overlock 1	4.0	50
21	(Î±-Diimine)chromium Complexes: Molecular and Electronic Structures; A Combined Experimental and Density Functional Theoretical Study. Inorganic Chemistry, 2008, 47, 5963-5970.	4.0	49
22	Characterization and Electronic Structures of Five Members of the Electron Transfer Series [Re(benzene-1,2-dithiolato)₃]^{<i>z</i>} (<i>z</i> = 1+, 0, 1âˆ’, 2âˆ’, 3âˆ’): A Spectroscopic and Density Functional Theoretical Study. Inorganic Chemistry, 2009, 48, 10926-10941.	4.0	49
23	Proton-Coupled Electron Transfer Enhances the Electrocatalytic Reduction of Nitrite to NO in a Bioinspired Copper Complex. ACS Catalysis, 2018, 8, 5070-5084.	11.2	46
24	One- and Two-Electron Reduced 1,2-Diketone Ligands in [CrIII(Lâ€¢)3] (S= 0) and Na2(Et2O)2[VIV(LRed)3] (S=1/2). Inorganic Chemistry, 2008, 47, 10935-10944.	4.0	44
25	Outer-Sphere Contributions to the Electronic Structure of Type Zero Copper Proteins. Journal of the American Chemical Society, 2012, 134, 8241-8253.	13.7	42
26	Arene Oxidation with Malonoyl Peroxides. Organic Letters, 2015, 17, 2618-2621.	4.6	41
27	Trivalent Iron and Ruthenium Complexes with a Redox Noninnocent (2-Mercaptophenylimino)-methyl-4,6-di-<i>tert</i>-butylphenolate(2-) Ligand. Inorganic Chemistry, 2009, 48, 3783-3791.	4.0	39
28	Metal-only Lewis pairs between group 10 metals and Tl(<scp>i</scp>) or Ag(<scp>i</scp>): insights into the electronic consequences of Z-type ligand binding. Chemical Science, 2015, 6, 7169-7178.	7.4	39
29	Electronically Stabilized Nonplanar Phenalenyl Radical and Its Planar Isomer. Journal of the American Chemical Society, 2015, 137, 14944-14951.	13.7	38
30	<i>g</i>â€Engineering in Hybrid Rotaxanes To Create AB and AB₂ Electron Spin Systems: EPR Spectroscopic Studies of Weak Interactions between Dissimilar Electron Spin Qubits. Angewandte Chemie - International Edition, 2015, 54, 10858-10861.	13.8	36
31	Controlling Photoconductivity in PBI Films by Supramolecular Assembly. Chemistry - A European Journal, 2018, 24, 4006-4010.	3.3	35
32	Outer-Sphere Effects on Reduction Potentials of Copper Sites in Proteins: The Curious Case of High Potential Type 2 C112D/M121E Pseudomonas aeruginosa Azurin. Journal of the American Chemical Society, 2010, 132, 14590-14595.	13.7	33
33	On the Possibility of Magneto-Structural Correlations: Detailed Studies of Dinickel Carboxylate Complexes. Inorganic Chemistry, 2014, 53, 8464-8472.	4.0	32
34	X-ray Absorption Spectroscopy Systematics at the Tungsten L-Edge. Inorganic Chemistry, 2014, 53, 8230-8241.	4.0	32
35	Molecular and Electronic Structure of the Square Planar Bis(<i>o-</i>amidobenzenethiolato)iron(III) Anion and Its Bis(<i>o-</i>quinoxalinedithiolato)iron(III) Analogue. Inorganic Chemistry, 2008, 47, 10911-10920.	4.0	31
36	Anion directed cation templated synthesis of three ternary copper(II) complexes with a monocondensed N2O donor Schiff base and different pseudohalides. Polyhedron, 2015, 85, 221-231.	2.2	30

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37	Reversible Ligandâ€Centered Reduction in Lowâ€Coordinate Iron Formazanate Complexes. Chemistry - A European Journal, 2018, 24, 9417-9425.	3.3	30
38	Alkali Cation Effects on Redox-Active Formazanate Ligands in Iron Chemistry. Inorganic Chemistry, 2018, 57, 9580-9591.	4.0	30
39	Enhanced Fe-Centered Redox Flexibility in Feâ€"Ti Heterobimetallic Complexes. Inorganic Chemistry, 2019, 58, 6199-6214.	4.0	29
40	Polynuclear Complexes Containing the Redox Noninnocent Schiff Base Ligand 2â€[(<i>E</i>)â€2â€Mercaptophenylimino]methylâ€4,6â€diâ€<i>tert</i>â€butylphenolate(2â€"). European Journal of Inorganic Chemistry, 2009, 2009, 2655-2663.	2.0	28
41	Electronic Structures and Spectroscopy of the Electron Transfer Series [Fe(NO)L₂]^{<i>z</i>} (<i>z</i> = 1+, 0, 1â€", 2â€",3â€"; L = Dithiolene). Inorganic Chemistry, 2011, 50, 12064-12074.	4.0	28
42	EPR/ENDOR, MÃ¶ssbauer, and Quantum-Chemical Investigations of Diiron Complexes Mimicking the Active Oxidized State of [FeFe]Hydrogenase. Inorganic Chemistry, 2012, 51, 8617-8628.	4.0	28
43	The Rhenium Tris(dithiolene) Electron Transfer Series: Calibrating Covalency. Inorganic Chemistry, 2011, 50, 12623-12631.	4.0	26
44	Redox-Controlled Interconversion between Trigonal Prismatic and Octahedral Geometries in a Monodithiolene Tetracarbonyl Complex of Tungsten. Inorganic Chemistry, 2012, 51, 346-361.	4.0	25
45	Ancillary Ligand Effects upon Dithiolene Redox Noninnocence in Tungsten Bis(dithiolene) Complexes. Inorganic Chemistry, 2013, 52, 6743-6751.	4.0	24
46	Long-Range Spin Coupling: A Tetraphosphine-Bridged Palladium Dimer. Inorganic Chemistry, 2011, 50, 2995-3002.	4.0	22
47	Synthesis and molecular structure of a zinc complex of the vitamin K3 analogue phthiocol. Journal of Molecular Structure, 2013, 1048, 223-229.	3.6	22
48	Stabilization of Highâ€Valent Fe^{IV}S₆â€Cores by Dithiocarbamate(1â^') and 1,2â€Dithiolate(2â^') Ligands in Octahedral [Fe^{IV}(Et₂dtc)_{3â^'<i>n</i>}(mnt)_{<i>n</i>}]^{(<i>n</i>â^'1)â^'} Complexes (<i>n</i>=0, 1, 2, 3): A Spectroscopic and Density Functional Theory Computational Study. Chemistry - A European Journal, 2010, 16, 3628-3645.	3.3	21
49	A polynuclear and two dinuclear copper(II) Schiff base complexes: Synthesis, characterization, self-assembly, magnetic property and DFT study. Polyhedron, 2017, 137, 332-346.	2.2	21
50	End-on cyanate or end-to-end thiocyanate bridged dinuclear copper(<scp>ii</scp>) complexes with a tridentate Schiff base blocking ligand: synthesis, structure and magnetic studies. New Journal of Chemistry, 2018, 42, 1634-1641.	2.8	20
51	The molecular and electronic structures of monomeric cobalt complexes containing redox noninnocent o-aminobenzenethiolate ligands. Inorganica Chimica Acta, 2010, 363, 2702-2714.	2.4	19
52	Stable Mixedâ€Valent Radicals from Platinum(II) Complexes of a Bis(dioxolene) Ligand. Chemistry - A European Journal, 2014, 20, 6272-6276.	3.3	19
53	Unexpected Nickel Complex Speciation Unlocks Alternative Pathways for the Reactions of Alkyl Halides with dppf-Nickel(0). ACS Catalysis, 2020, 10, 10717-10725.	11.2	18
54	Syntheses and Electronic Structure of Bimetallic Complexes Containing a Flexible Redox-Active Bridging Ligand. Inorganic Chemistry, 2013, 52, 898-909.	4.0	17

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55	Transparent-to-dark photo- and electrochromic gels. Communications Chemistry, 2018, 1, .	4.5	17
56	The modular synthesis of rare earth-transition metal heterobimetallic complexes utilizing a redox-active ligand. Dalton Transactions, 2018, 47, 10692-10701.	3.3	17
57	A Series of [Co(Mabiq)Cl2â€“n] (n = 0, 1, 2) Compounds and Evidence for the Elusive Bimetallic Form. Inorganic Chemistry, 2015, 54, 5864-5873.	4.0	16
58	Ligand Radicals as Modular Organic Electron Spin Qubits. Chemistry - A European Journal, 2018, 24, 17598-17605.	3.3	15
59	Enabling single qubit addressability in a molecular semiconductor comprising gold-supported organic radicals. Chemical Science, 2019, 10, 1483-1491.	7.4	15
60	Synthesis, structural and physicochemical characterization of a new type Ti₆-oxo cluster protected by a cyclic imide dioxime ligand. Dalton Transactions, 2019, 48, 5551-5559.	3.3	15
61	Molecules as electron spin qubits. Electron Paramagnetic Resonance, 2016, , 61-97.	0.2	15
62	Redox-Active Metallodithiolene Groups Separated by Insulating Tetraphosphinobenzene Spacers. Inorganic Chemistry, 2018, 57, 4023-4038.	4.0	14
63	Heteroleptic Samarium(III) Chalcogenide Complexes: Opportunities for Giant Exchange Coupling in Bridging Ïƒ- and Ï€-Radical Lanthanide Dichalcogenides. Inorganic Chemistry, 2020, 59, 7571-7583.	4.0	14
64	Separation and isolation of tautomers of 2-hydroxy-4-naphthoquinone-1-oxime derivatives by liquid chromatography: Antiproliferative activity and DFT studies. Journal of Chemical Sciences, 2014, 126, 213-225.	1.5	13
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73	Earth-Abundant Mixed-Metal Catalysts for Hydrocarbon Oxygenation. Inorganic Chemistry, 2018, 57, 5915-5928.	4.0	11
74	A macrocyclic â€˜Co0â€™ complex: the relevance of ligand non-innocence to reactivity. Chemical Communications, 2017, 53, 7282-7285.	4.1	10
75	Electrocatalytic hydrogen production by dinuclear cobalt(<scp>ii</scp>) compounds containing redox-active diamidate ligands: a combined experimental and theoretical study. Dalton Transactions, 2020, 49, 15718-15730.	3.3	10
76	An investigation into the unusual linkage isomerization and nitrite reduction activity of a novel tris(2-pyridyl) copper complex. Royal Society Open Science, 2017, 4, 170593.	2.4	9
77	Design and Assembly of Covalently Functionalised Polyoxofluorovanadate Molecular Hybrids. Chemistry - A European Journal, 2018, 24, 3836-3845.	3.3	9
78	A fascinating multifaceted redox-active chelating ligand: introducing the N,Nâ€²-dimethyl-3,3â€²-biquinoxalinium â€œmethylbiquinoxenâ€• platform. Chemical Science, 2016, 7, 3820-3828.	7.4	8
79	Directed Selfâ€Assembly, Symmetry Breaking, and Electronic Modulation of Metal Oxide Clusters by Pyramidal Heteroanions. Chemistry - A European Journal, 2018, 24, 4399-4411.	3.3	8
80	The semiquinone radical anion of 1,10-phenanthroline-5,6-dione: synthesis and rare earth coordination chemistry. Chemical Communications, 2018, 54, 11284-11287.	4.1	8
81	Heteroleptic samarium(<scp>iii</scp>) halide complexes probed by fluorescence-detected L₃-edge X-ray absorption spectroscopy. Dalton Transactions, 2018, 47, 10613-10625.	3.3	8
82	Group 10 Metal Dithiolene Bis(isonitrile) Complexes: Synthesis, Structures, Properties, and Reactivity. Organometallics, 2020, 39, 2854-2870.	2.3	8
83	Molecular and electronic structures of copper-cuprizone and analogues. Inorganica Chimica Acta, 2016, 451, 23-30.	2.4	7
84	Comment on â€œStabilization of Lowâ€Valent Iron(I) in a Highâ€Valent Vanadium(V) Oxide Clusterâ€• Angewandte Chemie - International Edition, 2019, 58, 10043-10047.	13.8	7
85	Mononuclear Sulfido-Tungsten(V) Complexes: Completing the Tp*MEXY (M = Mo, W; E = O, S) Series. Inorganic Chemistry, 2017, 56, 5189-5202.	4.0	6
86	Structural Characterization and Photochemical Properties of Mono- and Bimetallic Cu-Mabiq Complexes. Inorganic Chemistry, 2018, 57, 6401-6409.	4.0	6
87	Molecular and electronic structure of the dithiooxalato radical ligand stabilised by rare earth coordination. Dalton Transactions, 2019, 48, 5491-5495.	3.3	6
88	Evaluating a Dispersion of Sodium in Sodium Chloride for the Synthesis of Lowâ€Valent Nickel Complexes**. European Journal of Inorganic Chemistry, 2022, 2022, .	2.0	6
89	Modulating Iron Spin States with Radical Ligands: A Density Functional Theoretical Study. Asian Journal of Organic Chemistry, 2020, 9, 421-430.	2.7	5
90	Modulating the Magnetic Properties of Copper(II)/Nitroxyl Heterospin Complexes by Suppression of the Jahnâ€“Teller Distortion. Inorganic Chemistry, 2020, 59, 8657-8662.	4.0	5

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91	Triggering Redox Activity in a Thiophene Compound: Radical Stabilization and Coordination Chemistry. Angewandte Chemie, 2017, 129, 8047-8051.	2.0	4
92	Unprecedented Inequivalent Metal Coordination Environments in a Mixedâ€Ligand Dicobalt Complex. European Journal of Inorganic Chemistry, 2017, 2017, 3707-3713.	2.0	4
93	Radical Relatives: Facile Oxidation of Hetero-Diarylmethene Anions to Neutral Radicals. Inorganic Chemistry, 2018, 57, 9592-9600.	4.0	4
94	Rigidification of a macrocyclic tris-catecholate scaffold leads to electronic localisation of its mixed valent redox product. Chemical Communications, 2019, 55, 2281-2284.	4.1	4
95	Exploring the Redox Properties of Bench-Stable Uranyl(VI) Diamidoâ€“Dipyrrin Complexes. Inorganic Chemistry, 2022, 61, 3249-3255.	4.0	4
96	Radicals in carbonaceous residue deposited on mordenite from methanol. Journal of Materials Chemistry A, 2016, 4, 7036-7044.	10.3	3
97	Pâ€Type Lowâ€Molecularâ€Weight Hydrogelators. Macromolecular Rapid Communications, 2018, 39, e1700746.	3.9	3
98	Three Manganese Complexes of Anionic N4-Donor Schiff-Base Macrocycles: Monomeric MnII and MnIII, and dimeric MnIV. Australian Journal of Chemistry, 2019, 72, 805.	0.9	3
99	Oxidative Dehydrogenation of 1-Butene to 1,3-Butadiene Over Metal Ferrite Catalysts. Topics in Catalysis, 2021, 64, 907-915.	2.8	3
100	Open-Ended Metallodithiolene Complexes with the 1,2,4,5-Tetrakis(diphenylphosphino)benzene Ligand: Modular Building Elements for the Synthesis of Multimetal Complexes. Inorganic Chemistry, 2021, 60, 13177-13192.	4.0	3
101	Aggregate dependent electrochromic properties of amino acid appended naphthalene diimides in water. Materials Advances, 2022, 3, 3326-3331.	5.4	3
102	Towards a better understanding of the electrosynthesis of 2,5-dicarboxy-2,5-dihydrofurans: structure, mechanism and influence over stereochemistry. Royal Society Open Science, 2019, 6, 190336.	2.4	2
103	Correction to Oxidative Addition of Aryl Electrophiles to a Prototypical Nickel(0) Complex: Mechanism and Structure/Reactivity Relationships. Organometallics, 2017, 36, 1880-1880.	2.3	1
104	An alternative method to access diverse N,Nâ€²-diquaternised-3,3â€²-biquinoxalinium â€œbiquinoxenâ€• dications. New Journal of Chemistry, 2017, 41, 2949-2954.	2.8	1
105	Using Sugarâ€based Additives to Prolong the Lifetime of Airâ€Stable Radicals in Selfâ€Assembled Perylene Bisimides. ChemNanoMat, 2018, 4, 776-780.	2.8	1
106	Kommentar zu â€œStabilisierung eines niedrigvalenten Eisen(I)â€Ions in einem hochvalenten molekularen Vanadium(V)â€Oxidâ€Clusterâ€• Angewandte Chemie, 2019, 131, 10145-10150.	2.0	1
107	RÃ¼cktitelbild: Large Zero-Field Splittings of the Ground Spin State Arising from Antisymmetric Exchange Effects in Heterometallic Triangles (Angew. Chem. 21/2014). Angewandte Chemie, 2014, 126, 5578-5578.	2.0	0
108	Electronic structure study of divanadium complexes with rigid covalent coordination: potential molecular qubits with slow spin relaxation. Dalton Transactions, 2021, 50, 4778-4782.	3.3	0

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109	Oxo versus Sulfido Coordination at Tungsten: A Spectroscopic and Correlated Ab Initio Electronic Structure Study. Inorganic Chemistry, 2021, 60, 9057-9063.	4.0	0
110	Electronic versatility of vanadium in tris-chelates with redox-active ligands. Dalton Transactions, 2022, , .	3.3	0