David A Shultz

List of Publications by Year
in descending order

105	3,426	134610	198040
papers	citations	34 h-index	52 g-index

111	111	111	3228
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Excited State Exchange Control of Photoinduced Electron Spin Polarization in Electronic Ground States. Journal of Physical Chemistry Letters, 2022, 13, 872-878.	2.1	13
2	Excited State Magneto-Structural Correlations Related to Photoinduced Electron Spin Polarization. Journal of the American Chemical Society, 2022, 144, 12781-12788.	6.6	9
3	Chromophore-radical excited state antiferromagnetic exchange controls the sign of photoinduced ground state spin polarization. Chemical Science, 2021, 12, 13704-13710.	3.7	21
4	Controlled Light and Temperature Induced Valence Tautomerism in a Cobalt-o-Dioxolene Complex. Inorganic Chemistry, 2021, 60, 8665-8671.	1.9	5
5	Metal Ion Control of Photoinduced Electron Spin Polarization in Electronic Ground States. Journal of the American Chemical Society, 2021, 143, 10519-10523.	6.6	18
6	Magnetic Exchange Coupling through the Nonalternant Cyclopentadienyl Ï€-System of Ferrocene. Organic Letters, 2021, 23, 8235-8239.	2.4	1
7	Rules for Magnetic Exchange in Azulene-Bridged Biradicals: Quo Vadis?. Journal of Organic Chemistry, 2021, 86, 15577-15587.	1.7	7
8	Spectroscopic Signatures of Resonance Inhibition Reveal Differences in Donorâ€“Bridge and Bridgeâ€“Acceptor Couplings. Journal of the American Chemical Society, 2020, 142, 4916-4924.	6.6	20
9	In Search of Stable, High-Spin Polymers. Applied Magnetic Resonance, 2020, 51, 1331-1341.	0.6	1
10	Exploiting chemistry and molecular systems for quantum information science. Nature Reviews Chemistry, 2020, 4, 490-504.	13.8	247
11	Transferrable property relationships between magnetic exchange coupling and molecular conductance. Chemical Science, 2020, 11, 11425-11434.	3.7	8
12	Wave Function Control of Charge-Separated Excited-State Lifetimes. Journal of the American Chemical Society, 2019, 141, 3986-3992.	6.6	20
13	Long-range spin dependent delocalization promoted by the pseudo Jahn-Teller effect. Journal of Chemical Physics, 2019, 151, 201103.	1.2	7
14	Excited State Magnetic Exchange Interactions Enable Large Spin Polarization Effects. Journal of the American Chemical Society, 2018, 140, 2221-2228.	6.6	33
15	Ground State Nuclear Magnetic Resonance Chemical Shifts Predict Charge-Separated Excited State Lifetimes. Inorganic Chemistry, 2018, 57, 13470-13476.	1.9	14
16	Heterospin biradicals provide insight into molecular conductance and rectification. Chemical Science, 2017, 8, 5408-5415.	3.7	11
17	Influence of Radical Bridges on Electron Spin Coupling. Journal of Physical Chemistry A, 2017, 121, 216-225.	1.1	14
18	Hard X-ray-Induced Valence Tautomeric Interconversion in Cobalt-o-Dioxolene Complexes. Journal of Physical Chemistry Letters, 2017, 8, 4774-4778.	2.1	20

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19	Toward Controlling the Solid State Valence Tautomeric Interconversion Character by Solvation. Crystal Growth and Design, 2016, 16, 2385-2393.	1.4	18
20	Determining the Conformational Landscape of Ïƒ and Ï€ Coupling Using para-Phenylene and â€œAviramâ€“Ratnerâ€•Bridges. Journal of the American Chemical Society, 2015, 137, 9222-9225.	6.6	30
21	Synthesis, Characterization, and Photophysical Studies of an Iron(III) Catecholateâ€“Nitronylnitroxide Spin-Crossover Complex. Inorganic Chemistry, 2015, 54, 4466-4474.	1.9	29
22	Ligand Control of Donorâ€“Acceptor Excited-State Lifetimes. Inorganic Chemistry, 2014, 53, 4791-4793.	1.9	41
23	Molecular spintronics: a web themed issue. Chemical Communications, 2014, 50, 7401.	2.2	12
24	Correction to â€œElectronic and Exchange Coupling in a Cross-Conjugated Dâ€“Bâ€“A Biradical: Mechanistic Implications for Quantum Interference Effectsâ€• Journal of the American Chemical Society, 2014, 136, 4090-4090.	6.6	1
25	Towards Controlling the Valance Tautomer Interconversion Character by Solvation. Acta Crystallographica Section A: Foundations and Advances, 2014, 70, C1252-C1252.	0.0	0
26	Superexchange Contributions to Distance Dependence of Electron Transfer/Transport: Exchange and Electronic Coupling in Oligo(para-Phenylene)- and Oligo(2,5-Thiophene)-Bridged Donorâ€“Bridgeâ€“Acceptor Biradical Complexes. Journal of the American Chemical Society, 2013, 135, 17144-17154.	6.6	61
27	Electronic and Exchange Coupling in a Cross-Conjugated Dâ€“Bâ€“A Biradical: Mechanistic Implications for Quantum Interference Effects. Journal of the American Chemical Society, 2013, 135, 14713-14725.	6.6	53
28	Iron(ii) spin crossover films on Au(111): scanning probe microscopy and photoelectron spectroscopy. Chemical Communications, 2013, 49, 10446.	2.2	69
29	Transition metal complexes of donorâ€“acceptor biradicals. Coordination Chemistry Reviews, 2013, 257, 218-233.	9.5	61
30	Modification of Molecular Spin Crossover in Ultrathin Films. Nano Letters, 2013, 13, 1429-1434.	4.5	83
31	Complex Materials for Molecular Spintronics Applications: Cobalt Bis(dioxolene) Valence Tautomers, from Molecules to Polymers. Journal of Physical Chemistry B, 2012, 116, 13141-13148.	1.2	42
32	Spectroscopic Studies of Bridge Contributions to Electronic Coupling in a Donor-Bridge-Acceptor Biradical System. Journal of the American Chemical Society, 2012, 134, 7812-7819.	6.6	22
33	Linear freeâ€•energy relationships in semiquinone species and their Mn(II) and Cu(II) complexes. Journal of Physical Organic Chemistry, 2012, 25, 101-109.	0.9	0
34	Synthesis of and structureâ€“property relationships in zinc complexes of bisâ€•metaphenylene semiquinone biradical species. Journal of Physical Organic Chemistry, 2012, 25, 314-321.	0.9	7
35	Nitronyl Nitroxide Radicals as Organic Memory Elements with Both nâ€•and pâ€•Type Properties. Angewandte Chemie - International Edition, 2011, 50, 4414-4418.	7.2	103
36	Magnetic Bistability in a Cobalt Bis(dioxolene) Complex: Long-Lived Photoinduced Valence Tautomerism. Inorganic Chemistry, 2010, 49, 3162-3168.	1.9	38

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37	Goldilocks Effect in Magnetic Bistability: Remote Substituent Modulation and Lattice Control of Photoinduced Valence Tautomerism and Light-Induced Thermal Hysteresis. Journal of the American Chemical Society, 2010, 132, 6261-6273.	6.6	81
38	Hyperfine Interaction, Spin Polarization, and Spin Delocalization as Probes of Donorâ^'Bridgeâ^'Acceptor Interactions in Exchange-Coupled Biradicals. Journal of Physical Chemistry B, 2010, 114, 14712-14716.	1.2	20
39	Ferromagnetic Nanoscale Electron Correlation Promoted by Organic Spin-Dependent Delocalization. Journal of the American Chemical Society, 2009, 131, 18304-18313.	6.6	29
40	Donorâ^'Acceptor Biradicals as Ground State Analogues of Photoinduced Charge Separated States. Journal of the American Chemical Society, 2007, 129, 1937-1943.	6.6	42
41	Influence of Ligand Geometry in Bimetallic Ytterbocene Complexes of Bridging Bis(bipyridyl) Ligands. Organometallics, 2007, 26, 4234-4242.	1.1	14
42	Substituent Effects on Exchange Coupling:Â 5-Aryl-Substituted Semiquinones and Their Complexes with MnIIand CuII. Inorganic Chemistry, 2007, 46, 273-277.	1.9	7
43	Electron Spinâ^'Spin Exchange Coupling Mediated by the Porphyrin Ï€ System. Inorganic Chemistry, 2006, 45, 5752-5759.	1.9	22
44	Testing Bridge-Mediated Differences in Dinuclear Valence Tautomeric Behavior. Inorganic Chemistry, 2006, 45, 4461-4467.	1.9	47
45	Ligand design modulates photoinduced properties of cobalt-dioxolene valence tautomers. Chemical Physics Letters, 2006, 428, 400-404.	1.2	36
46	Design, Synthesis, and Properties of Conformationally Fixed Semiquinone Monoradical Species. Journal of Organic Chemistry, 2006, 71, 9104-9113.	1.7	30
47	Valence tautomerization and exchange coupling in a cobaltâ€"nitronylnitroxideâ€"semiquinone complex. Polyhedron, 2005, 24, 2876-2879.	1.0	21
48	Beyond the active-electron approximation: Origin of ferromagnetic exchange in donorâ€"acceptor heterospin biradicals. Polyhedron, 2005, 24, 2880-2884.	1.0	21
49	Supramolecular Control of Valence-Tautomeric Equilibrium on Nanometer-Scale Gold Clusters. Journal of the American Chemical Society, 2005, 127, 5328-5329.	6.6	30
50	Polyoxolenes May Provide a Tool for Designing Paramagnetic Molecules with Predetermined Spin Topologies. ChemInform, 2004, 35, no.	0.1	0
51	The donorâ€"acceptor contributions to ferromagnetic exchange coupling in heterospin biradicals. Polyhedron, 2003, 22, 2423-2426.	1.0	7
52	Polyoxolenes may provide a tool for designing paramagnetic molecules with predetermined spin topologies. Comptes Rendus Chimie, 2003, 6, 663-676.	0.2	15
53	New Paradigm for Design of High-Spin Organic Molecules:Â The Mechanism of Spin-Dependent Delocalization in Exchange-Coupled, Mixed-Valent Organic Species. Journal of Physical Chemistry A, 2003, 107, 4292-4299.	1.1	6
54	Trends in Metalâ^'Biradical Exchange Interaction for First-Row MII(Nitronyl Nitroxide-Semiquinone) Complexes. Journal of the American Chemical Society, 2003, 125, 1607-1617.	6.6	74

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55	Trends in Exchange Coupling for Trimethylenemethane-Type Bis(semiquinone) Biradicals and Correlation of Magnetic Exchange with Mixed Valency for Cross-Conjugated Systems. Journal of the American Chemical Society, 2003, 125, 11761-11771.	6.6	77
56	Mechanisms of Exchange Modulation in Trimethylenemethane-type Biradicals:â€‰ The Roles of Conformation and Spin Density. Journal of the American Chemical Society, 2003, 125, 15426-15432.	6.6	62
57	Structure-Property Relationships in New Semiquinone-Type Ligands: Past, Present, and Future Research Efforts. Comments on Inorganic Chemistry, 2002, 23, 1-21.	3.0	32
58	High-Spin Metal Complexes Containing a Ferromagnetically Coupled Tris(semiquinone) Ligand. Inorganic Chemistry, 2002, 41, 1086-1092.	1.9	39
59	Singletâ^'Triplet Gap in Triplet Ground-State Biradicals Is Modulated by Substituent Effects. Journal of the American Chemical Society, 2002, 124, 10054-10061.	6.6	49
60	Charge Distribution in Bis-Dioxolene Radical Metal Complexes. Synthesis and DFT Characterization of Dinuclear Co(III) and Cr(III) Complexes with a Mixed-Valent,S=1/2Semiquinone-Catecholate Ligand. Inorganic Chemistry, 2001, 40, 1582-1590.	1.9	58
61	Structureâ€“property relationships in building blocks for open-shell molecules and materials. Synthetic Metals, 2001, 122, 495-500.	2.1	4
62	A bis-bidentate dioxolene ligand induces thermal hysteresis in valence tautomerism interconversion processes. Chemical Communications, 2001, , 2150-2151.	2.2	54
63	Molecular structure of and exchange coupling in a bis(semiquinone) complex. Chemical Communications, 2001, , 93-94.	2.2	8
64	Observation of a Hysteretic Phase Transition in a Crystalline Dinitroxide Biradical That Leads to Magnetic Bistability. Journal of the American Chemical Society, 2001, 123, 10403-10404.	6.6	30
65	Molecular Structures of Carbonyl-Linked Bis(dioxolene) Complexes:Â Can a Carbonyl Group Act as an Effective Ferromagnetic Coupler?. Inorganic Chemistry, 2001, 40, 546-549.	1.9	15
66	Spin Robustness of a New Hybrid Inorganicâ^'Organic High-Spin Molecule. Journal of the American Chemical Society, 2001, 123, 3133-3134.	6.6	22
67	Ferromagnetically Coupled Bis(semiquinone) Ligand Enforces High-Spin Ground States in Bis-metal Complexes. Inorganic Chemistry, 2001, 40, 408-411.	1.9	60
68	One-Electron Reduction of an Antiferromagnetically Coupled Triradical Yields a Mixed-Valent Biradical with Enhanced Ferromagnetic Coupling. Journal of the American Chemical Society, 2001, 123, 6431-6432.	6.6	21
69	Structureâ€“property relationships in cross-conjugated, high-spin, dinuclear ligands: building blocks for open-shell molecules and materials. Polyhedron, 2001, 20, 1627-1631.	1.0	16
70	Synthesis of nanometer-sized hollow polymer capsules from alkanethiol-coated gold particles. Chemical Communications, 2000, , 775-776.	2.2	46
71	Preparation and EPR Spectroscopic Investigation of Conjugated Oligomers Containing Semiquinone Repeat Units. Chemistry of Materials, 2000, 12, 580-585.	3.2	20
72	Synthesis and Structure of a Complex Having a Quartet Ground State with Three Entirely Different Spin Carriers:Â Nitronyl Nitroxide,o-Semiquinone, and CuII. Inorganic Chemistry, 2000, 39, 6091-6093.	1.9	51

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73	Synthesis and characterization of a planarized, trimethylenemethane-type bis(semiquinone) biradical. Tetrahedron, 1999, 55, 12079-12086.	1.0	17
74	Gold Nanoparticles as Templates for the Synthesis of Hollow Nanometer-Sized Conductive Polymer Capsules. Advanced Materials, 1999, 11, 34-37.	11.1	142
75	Semiempirical computational assessment of porphyrins as building blocks for molecule-based magnets: spin-spin coupling in radical-substituted metalloporphyrins. Journal of Physical Organic Chemistry, 1999, 12, 10-18.	0.9	9
76	Paramagnetic Zinc(II) Complexes of a Bis(catechol):â€‰ Dependence of Product Spin State on Tautomerization of the Bis(catechol) Ligand. Inorganic Chemistry, 1999, 38, 591-594.	1.9	35
77	Cross-Conjugated Bis(porphryin)s:Â Synthesis, Electrochemical Behavior, Mixed Valency, and Biradical Dication Formation. Journal of Organic Chemistry, 1999, 64, 9124-9136.	1.7	45
78	Structureâ^'Property Relationships in Trimethylenemethane-Type Biradicals. 2. Synthesis and EPR Spectral Characterization of Dinitroxide Biradicalsâ€. Journal of Organic Chemistry, 1999, 64, 4386-4396.	1.7	39
79	Electronic Properties of Bisporphyrin Biradical Dications. Molecular Crystals and Liquid Crystals, 1999, 334, 459-467.	0.3	3
80	Both an Oxidation/Reduction Sequence and Deprotonation of a Unique Paramagnetic Ligand Lead to a Mixed-Valent Complex. Journal of the American Chemical Society, 1999, 121, 10664-10665.	6.6	31
81	Improved method for estimating the ZFS parameterD for delocalized biradicals. Journal of Physical Organic Chemistry, 1998, 11, 819-824.	0.9	6
82	A Modified Procedure for Sonogashira Couplings:â€‰ Synthesis and Characterization of a Bisporphyrin, 1,1-Bis[zinc(II) 5â€˜-ethynyl-10â€˜,15â€˜,20â€˜-trimesitylporphyrinyl]methylenecyclohexane. Journal of Organic Chemistry, 1998, 63, 4034-4038.	1.7	71
83	pH-Gated Single-Electron Tunneling in Chemically Modified Gold Nanoclusters. Journal of the American Chemical Society, 1998, 120, 7645-7646.	6.6	87
84	Oxidation of a Bis[Zn(II) porphyrin] Yields a Nondisjoint, Exchange-Coupled Ï€ Dication-Biradical. Journal of Organic Chemistry, 1998, 63, 7584-7585.	1.7	20
85	Effect of Aliphatic Amine Bases on the Aggregation of Alkali Metal Salts of 3,5-Di-tert-butylsemiquinone (3,5-DBSQ). Inorganic Chemistry, 1998, 37, 1540-1543.	1.9	17
86	Synthesis of Bis(semiquinone)s and Their Electrochemical and Electron Paramagnetic Resonance Spectral Characterization. Journal of Organic Chemistry, 1998, 63, 9462-9469.	1.7	47
87	Synthesis and Characterization of a Nitroxideâ^'Semiquinone Biradical. Journal of Organic Chemistry, 1998, 63, 6254-6257.	1.7	38
88	Synthesis and Characterization of Phenylnitroxide-Substituted Zinc(II) Porphyrins. Journal of Organic Chemistry, 1998, 63, 769-774.	1.7	47
89	Electrochemical and Spectroelectrochemical Study of a Bis(arylgalvinol)-Substituted Alkyl Disulfide Monolayer and Mixed Monolayers on Polycrystalline Gold. Langmuir, 1998, 14, 3682-3690.	1.6	11
90	Preparation of Paramagnetic Ligands for Coordination-Complexes and Networks with Interesting Magnetic Properties. Molecular Crystals and Liquid Crystals, 1997, 305, 303-310.	0.3	25

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91	Attempted Synthesis of a Stable, Quintet, Tetraphenoxyl Tetraradical:Â Facile Rearrangement of a Substituted Bicyclobutane. Journal of Organic Chemistry, 1997, 62, 7575-7584.	1.7	9
92	The Biradical, Bis(3,5-di-tert-butyl-4-phenoxyl)methyleneadamantane, Exhibits Matrix-Dependent EPR Spectra Suggesting Rotamer Bistability with Differential Exchange Coupling. Journal of the American Chemical Society, 1997, 119, 3846-3847.	6.6	43
93	Preparation and characterization of a bis-galvinoxyl-disulfide. Tetrahedron Letters, 1996, 37, 8837-8840.	0.7	2
94	Nitroxyl-Galvinoxyl â€“ A New Biradical. Molecular Crystals and Liquid Crystals, 1995, 272, 75-79.	0.3	7
95	Preparation and Characterization of a Bis-Semiquinone: a Bidentate Dianion Biradical. Journal of Organic Chemistry, 1995, 60, 3578-3579.	1.7	34
96	Comparative stability of fluoroketone hemi-thio acetals, ketals and hydrates. Tetrahedron Letters, 1994, 35, 6437-6440.	0.7	9
97	Electrochemical Oxidation of a Galvinol-Substituted Alkanethiol Monolayer. Journal of Organic Chemistry, 1994, 59, 6159-6160.	1.7	12
98	Preparation of meso-tetra(4-galvinolphenyl)porphyrinâ€”A building block for molecular magnetic materials. Tetrahedron Letters, 1993, 34, 3975-3978.	0.7	7
99	Evaluation of potential ferromagnetic coupling units: the bis(TMM) [bis(trimethylenemethane)] approach to high-spin organic molecules. Journal of the American Chemical Society, 1993, 115, 1744-1753.	6.6	82
100	New Organic Polymers And Molecules With Very High Spin States. Molecular Crystals and Liquid Crystals, 1993, 232, 289-304.	0.3	14
101	Structural effects on the disproportionation equilibrium of tethered tetraphenylethylene radical anions. Journal of Organic Chemistry, 1990, 55, 1047-1051.	1.7	7
102	Effect of phenyl ring torsional rigidity on the photophysical behavior of tetraphenylethylenes. Journal of the American Chemical Society, 1989, 111, 6311-6320.	6.6	97
103	Spectroscopic properties of [n.1]-Metacyclophanenylidenes. Tetrahedron Letters, 1988, 29, 4377-4380.	0.7	20
104	Twisting in the tetraphenylethylene dianion. Journal of Organic Chemistry, 1988, 53, 4386-4390.	1.7	14
105	Valence Tautomerism in Dioxolene Complexes of Cobalt. , 0, , 281-306.		49