Charles Edwin Webster

List of Publications by Year
in descending order

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104	3,858	117625	133252
papers	citations	34 h-index	59 g-index

109	109	109	4264
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Sensitized and Selfâ€Sensitized Photocatalytic Carbon Dioxide Reduction Under Visible Light with Ruthenium Catalysts Shows Enhancements with More Conjugated Pincer Ligands. European Journal of Inorganic Chemistry, 2022, 2022, .	2.0	5
2	Triphenylene containing blue-light emitting semi-fluorinated aryl ether polymers with excellent thermal and photostability. Materials Chemistry Frontiers, 2022, 6, 1391-1404.	5.9	3
3	Mechanistic Studies of Oxygen-Atom Transfer (OAT) in the Homogeneous Conversion of N2O by Ru Pincer Complexes. Inorganics, 2022, 10, 69.	2.7	5
4	Low-Valent Cobalt(I) CNC Pincer Complexes as Catalysts for Light-Driven Carbon Dioxide Reduction. ACS Catalysis, 2022, 12, 8718-8728.	11.2	8
5	Predicting Absorption and Emission Maxima of Polycyclic Aromatic Azaborines: Reliable Transition Energies and Character. Journal of Physical Chemistry A, 2021, 125, 3-12.	2.5	1
6	Singlet Oxygen Formation vs Photodissociation for Light-Responsive Protic Ruthenium Anticancer Compounds: The Oxygenated Substituent Determines Which Pathway Dominates. Inorganic Chemistry, 2021, 60, 2138-2148.	4.0	20
7	Benchmarking the Fluxional Processes of Organometallic Piano-Stool Complexes. Molecules, 2021, 26, 2310.	3.8	3
8	Lightâ€responsive and Protic Ruthenium Compounds Bearing Bathophenanthroline and Dihydroxybipyridine Ligands Achieve Nanomolar Toxicity towards Breast Cancer Cells. Photochemistry and Photobiology, 2021, , .	2.5	6
9	The curious case of DMSO: A CCSD(T)/CBS(aQ56+d) benchmark and DFT study. Journal of Chemical Physics, 2021, 155, 114304.	3.0	2
10	Cheminformatic quantum mechanical enzyme model design: A catechol-O-methyltransferase case study. Biophysical Journal, 2021, 120, 3577-3587.	0.5	7
11	Structureâ€Functional Analysis of Hydrogen Production Catalyzed by Molecular Cobalt Complexes with Pentadentate Ligands in Aqueous Solutions. European Journal of Inorganic Chemistry, 2020, 2020, 3534-3547.	2.0	9
12	Tris(carbene) Stabilization of Monomeric Magnesium Cations: A Neutral, Nontethered Ligand Approach. Organometallics, 2020, 39, 4329-4339.	2.3	12
13	Planar, Stairâ€Stepped, and Twisted: Modulating Structure and Photophysics in Pyreneâ€and Benzeneâ€Fused Nâ€Heterocyclic Boranes. Chemistry - A European Journal, 2020, 26, 10072-10082.	3.3	6
14	Impact of the Dissolved Anion on the Electrocatalytic Reduction of CO 2 to CO with Ruthenium CNC Pincer Complexes. ChemCatChem, 2020, 12, 4879-4885.	3.7	7
15	Structure Function Relationships in Ruthenium Carbon Dioxide Reduction Catalysts with CNC Pincers Containing Donor Groups. European Journal of Inorganic Chemistry, 2020, 2020, 2709-2717.	2.0	10
16	Enhanced Hydrogen Evolution in Neutral Water Catalyzed by a Cobalt Complex with a Softer Polypyridyl Ligand. Angewandte Chemie, 2020, 132, 12794-12797.	2.0	3
17	Enhanced Hydrogen Evolution in Neutral Water Catalyzed by a Cobalt Complex with a Softer Polypyridyl Ligand. Angewandte Chemie - International Edition, 2020, 59, 12694-12697.	13.8	25
18	Two Carbenes versus One in Magnesium Chemistry: Synthesis of Terminal Dihalide, Dialkyl, and Grignard Reagents. Organometallics, 2019, 38, 688-696.	2.3	24

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19	Highly Active Ruthenium CNC Pincer Photocatalysts for Visible-Light-Driven Carbon Dioxide Reduction. Inorganic Chemistry, 2019, 58, 8012-8020.	4.0	49
20	Catalytic H₂ Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand. European Journal of Inorganic Chemistry, 2019, 2019, 2134-2139.	2.0	14
21	Photocatalytic H₂-Evolution by Homogeneous Molybdenum Sulfide Clusters Supported by Dithiocarbamate Ligands. Inorganic Chemistry, 2019, 58, 16458-16474.	4.0	11
22	Extremely twisted and bent pyrene-fused N-heterocyclic germylenes. Chemical Communications, 2019, 55, 14954-14957.	4.1	5
23	The missing agostomer in the fluxionality of cyclohexenylmanganese tricarbonyl. Journal of Organometallic Chemistry, 2018, 864, 128-135.	1.8	4
24	A Mononuclear Tungsten Photocatalyst for H₂ Production. ACS Catalysis, 2018, 8, 4838-4847.	11.2	21
25	Nickel(<scp>ii</scp>) pincer complexes demonstrate that the remote substituent controls catalytic carbon dioxide reduction. Chemical Communications, 2018, 54, 3819-3822.	4.1	39
26	Free methylidyne? CCC-NHC tantalum bis(imido) reactivity: protonation, rearrangement to a mixed unsymmetrical CCC-N-heterocyclic carbene/N-heterocyclic dicarbene (CCC-NHC/NHDC) pincer tantalum bis(imido) complex. Inorganica Chimica Acta, 2018, 469, 164-172.	2.4	10
27	Investigation of metallation/transmetallation reactions to synthesize a series of CCCâ€“NHC Co pincer complexes and their X-ray structures. Polyhedron, 2018, 151, 568-574.	2.2	10
28	Computational Analysis of the Intramolecular Oxidative Amination of an Alkene Catalyzed by the Extreme Ï€-Loading N-Heterocyclic Carbene Pincer Tantalum(V) Bis(imido) Complex. Organometallics, 2018, 37, 1671-1681.	2.3	11
29	Electronic and Steric Tuning of Catalytic H₂ Evolution by Cobalt Complexes with Pentadentate Polypyridyl-Amine Ligands. Journal of the American Chemical Society, 2018, 140, 9219-9229.	13.7	88
30	Controlling Photoisomerization Reactivity Through Single Functional Group Substitutions in Ruthenium Phosphine Sulfoxide Complexes. Journal of the American Chemical Society, 2018, 140, 9819-9822.	13.7	8
31	Synthesis of C-Unsubstituted 1,2-Diazetidines and Their Ring-Opening Reactions via Selective Nâ€“N Bond Cleavage. Journal of Organic Chemistry, 2018, 83, 9497-9503.	3.2	12
32	Iridium and Ruthenium Complexes of N-Heterocyclic Carbene- and Pyridinol-Derived Chelates as Catalysts for Aqueous Carbon Dioxide Hydrogenation and Formic Acid Dehydrogenation: The Role of the Alkali Metal. Organometallics, 2017, 36, 1091-1106.	2.3	94
33	Synthesis, characterization, photophysics, and a ligand rearrangement of CCC-NHC pincer nickel complexes: Colors, polymorphs, emission, and Raman spectra. Journal of Organometallic Chemistry, 2017, 845, 258-265.	1.8	17
34	Phosphoramidate hydrolysis catalyzed by human histidine triad nucleotide binding protein 1 (hHint1): a cluster-model DFT computational study. Organic and Biomolecular Chemistry, 2017, 15, 8661-8668.	2.8	7
35	Electrocatalytic reduction of CO₂ with CCC-NHC pincer nickel complexes. Chemical Communications, 2017, 53, 9442-9445.	4.1	53
36	Prediction of the reduction potential in transitionâ€metal containing complexes: How expensive? For what accuracy?. Journal of Computational Chemistry, 2017, 38, 2430-2438.	3.3	23

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37	Synthesis, computational, and spectroscopic analysis of tunable highly fluorescent BN-1,2-azaborine derivatives containing the N-BOH moiety. Organic and Biomolecular Chemistry, 2017, 15, 10172-10183.	2.8	9
38	Calibrating Reaction Enthalpies: Use of Density Functional Theory and the Correlation Consistent Composite Approach in the Design of Photochromic Materials. Journal of Physical Chemistry A, 2016, 120, 9982-9997.	2.5	6
39	Experimental and Computational Studies of the Mechanisms of Hydroamination/Cyclisation of Unactivated Î±,Ï‰-Amino-alkenes with CCC-NHC Pincer Zr Complexes. Australian Journal of Chemistry, 2016, 69, 573.	0.9	10
40	The Synthesis and Characterization of Highly Fluorescent Polycyclic Azaborine Chromophores. Journal of Organic Chemistry, 2016, 81, 10955-10963.	3.2	17
41	Extreme Ï€-Loading as a Design Element for Accessing Imido Ligand Reactivity. A CCC-NHC Pincer Tantalum Bis(imido) Complex: Synthesis, Characterization, and Catalytic Oxidative Amination of Alkenes. Organometallics, 2016, 35, 3452-3460.	2.3	31
42	Transmetallation from CCC-NHC pincer Zr complexes in the synthesis of air-stable CCC-NHC pincer Co(<scp>iii</scp>) complexes and initial hydroboration trials. Dalton Transactions, 2016, 45, 2823-2828.	3.3	68
43	Î²-Boration of Î±,Î²-unsaturated carbonyl compounds in ethanol and methanol catalyzed by CCC-NHC pincer Rh complexes. Journal of Organometallic Chemistry, 2016, 802, 32-38.	1.8	27
44	The transâ€“cis isomerization of Ni(Î·2-TEMPO)2: Interconnections and conformational complexity. Inorganica Chimica Acta, 2015, 436, 220-229.	2.4	2
45	A Theoretical Study of Phosphoryl Transfers of Tyrosyl-DNA Phosphodiesterase I (Tdp1) and the Possibility of a â€œDead-Endâ€•Phosphohistidine Intermediate. Biochemistry, 2015, 54, 4236-4247.	2.5	20
46	Synthesis, characterization, photophysical properties, and catalytic activity of an SCS bis(N-heterocyclic thione) (SCS-NHT) Pd pincer complex. Dalton Transactions, 2015, 44, 14475-14482.	3.3	41
47	Water Oxidation by Mononuclear Ruthenium Complex with a Pentadentate Isoquinoline-Bipyridyl Ligand. European Journal of Inorganic Chemistry, 2014, 2014, 715-721.	2.0	9
48	Degenerate Pathways for Metallacycle Ring Inversions: A Common Phenomenon Consistent with the Principle of Microscopic Reversibility. Organometallics, 2014, 33, 5928-5931.	2.3	10
49	Theoretical studies of cyclic adenosine monophosphate dependent protein kinase: native enzyme and ground-state and transition-state analogues. Dalton Transactions, 2014, 43, 3039-3043.	3.3	5
50	Synthesis, Characterization, and X-ray Molecular Structure of Tantalum CCC-N-Heterocyclic Carbene (CCC-NHC) Pincer Complexes with Imidazole- and Triazole-Based Ligands. Organometallics, 2014, 33, 952-958.	2.3	30
51	Electronic Effects on a Mononuclear Co Complex with a Pentadentate Ligand for Catalytic H₂ Evolution. Inorganic Chemistry, 2014, 53, 10094-10100.	4.0	79
52	Organometallics Roundtable 2013â€“2014. Organometallics, 2014, 33, 1505-1527.	2.3	24
53	Photochemistry of Chromium Arene Tricarbonyl Complexes with Tethered Pyridinyl and Propenyl Groups: Investigations of the Effect of Ring Size on Chelate Formation, Structure, and Linkage Isomerization. Organometallics, 2014, 33, 485-497.	2.3	14
54	Phosphoryl Transfers of the Phospholipase D Superfamily: A Quantum Mechanical Theoretical Study. Journal of the American Chemical Society, 2013, 135, 13764-13774.	13.7	26

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55	Metalâ€“Ligand Synergistic Effects in the Complex Ni(Î·²-TEMPO)₂: Synthesis, Structures, and Reactivity. Inorganic Chemistry, 2013, 52, 13882-13893.	4.0	13
56	Platinum CCC-NHC benzimidazolyl pincer complexes: synthesis, characterization, photostability, and theoretical investigation of a blue-green emitter. Dalton Transactions, 2013, 42, 8820.	3.3	33
57	Time-Resolved Infrared Studies of a Trimethylphosphine Model Derivative of [FeFe]-Hydrogenase. Journal of Physical Chemistry B, 2013, 117, 15792-15803.	2.6	19
58	Near attack conformers dominate Î²-phosphoglucomutase complexes where geometry and charge distribution reflect those of substrate. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 6910-6915.	7.1	47
59	Time-Resolved Vibrational Spectroscopy of [FeFe]-Hydrogenase Model Compounds. Journal of Physical Chemistry A, 2012, 116, 7261-7271.	2.5	36
60	Synthesis, Air Stability, Photobleaching, and DFT Modeling of Blue Light Emitting Platinum CCC-N-Heterocyclic Carbene Pincer Complexes. Organometallics, 2012, 31, 1664-1672.	2.3	104
61	Computational Investigation of the Mechanism for the Activation of CO by Oxorhenium Complexes. Organometallics, 2012, 31, 4055-4062.	2.3	19
62	Electrocatalytic and Photocatalytic Hydrogen Production in Aqueous Solution by a Molecular Cobalt Complex. Angewandte Chemie - International Edition, 2012, 51, 5941-5944.	13.8	280
63	Engineering Femtosecond Organometallic Chemistry: Photochemistry and Dynamics of Ultrafast Chelation of Cyclopentadienylmanganese Tricarbonyl Derivatives with Pendant Benzenecarbonyl and Pyridinecarbonyl Groups. Organometallics, 2011, 30, 5611-5619.	2.3	26
64	Water Oxidation by Mononuclear Ruthenium Complexes with TPA-Based Ligands. Inorganic Chemistry, 2011, 50, 10564-10571.	4.0	80
65	Ligand Displacement from TpMn(CO)₂L Complexes: A Large Rate Enhancement in Comparison to the CpMn(CO)₂L Analogues. Organometallics, 2011, 30, 3054-3063.	2.3	13
66	Bond Energies, Reaction Volumes, and Kinetics for Ïƒ- and Ï€-Complexes of Mo(CO)5L. Journal of Physical Chemistry A, 2011, 115, 9004-9013.	2.5	6
67	Time-resolved IR Studies on the Mechanism for the Functionalization of Primary Cî—¸H Bonds by Photoactivated Cp*W(CO)₃(Bpin). Journal of the American Chemical Society, 2010, 132, 1848-1859.	13.7	41
68	Development of Ultrafast Photochromic Organometallics and Photoinduced Linkage Isomerization of Arene Chromium Carbonyl Derivatives. Journal of Physical Chemistry A, 2009, 113, 2666-2676.	2.5	48
69	Theoretical study of the biologically important dioxo diiron diamond core structures. Theoretical Chemistry Accounts, 2008, 120, 467-478.	1.4	2
70	Disulfido ironâ€“manganese carbonyl cluster complexes: Synthesis, structure, bonding and properties of the radical CpFeMn2(CO)7(Î¼3-S2)2. Journal of Organometallic Chemistry, 2008, 693, 2732-2738.	1.8	10
71	Linkage Isomerization as a Mechanism for Photochromic Materials: Cyclopentadienylmanganese Tricarbonyl Derivatives with Chelatable Functional Groups. Organometallics, 2008, 27, 289-296.	2.3	52
72	Probing the Mechanism of Carbonî—¸Hydrogen Bond Activation by Photochemically Generated Hydridotris(pyrazolyl)borato Carbonyl Rhodium Complexes: New Experimental and Theoretical Investigations. Organometallics, 2008, 27, 189-201.	2.3	29

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73	Carbonâ^'Hydrogen Bond Activation in Hydridotris(pyrazolyl)borate Platinum(IV) Complexes:â€‰Comparison of Density Functionals, Basis Sets, and Bonding Patterns. Journal of Chemical Theory and Computation, 2007, 3, 2268-2281.	5.3	14
74	Computational Insights into Degenerate Ethylene Exchange with a Grubbs-Type Catalyst. Journal of the American Chemical Society, 2007, 129, 7490-7491.	13.7	44
75	Forty years of Fenske-Hall molecular orbital theory. , 2005, , 1143-1165.		13
76	Electronic and Steric Effects on Molecular Dihydrogen Activation in [Cp*OsH4(L)]+(L = PPh3, AsPh3,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	13.7	33
77	Urea decomposition facilitated by a urease model complex: a theoretical investigation. Dalton Transactions, 2005, , 3542.	3.3	17
78	Rhodium Boryl Complexes in the Catalytic, Terminal Functionalization of Alkanes. Journal of the American Chemical Society, 2005, 127, 2538-2552.	13.7	317
79	High Nuclearity Iridiumâ^'Platinum Clusters:Â Synthesis, Structures, Bonding, and Reactivity. Journal of the American Chemical Society, 2005, 127, 1007-1014.	13.7	34
80	Rhodium Silyl Boryl Hydride Complexes: Comparison of Bonding and the Rates of Elimination of Borane, Silane, and Dihydrogen. Angewandte Chemie - International Edition, 2004, 43, 5474-5477.	13.8	41
81	Quantum Mechanical Models of the Resting State of the Vanadium-Dependent Haloperoxidase. Inorganic Chemistry, 2004, 43, 4127-4136.	4.0	58
82	Structures and Energetics of Models for the Active Site of Acetyl-Coenzyme A Synthase:Â Role of Distal and Proximal Metals in Catalysis. Journal of the American Chemical Society, 2004, 126, 3410-3411.	13.7	59
83	Reaction of the 1,8-Bis(diphenylmethylium)naphthalenediyl Dication with Fluoride:â€‰Formation of a Cation Containing a Câ^'Fâ†'C Bridge. Journal of the American Chemical Society, 2004, 126, 8189-8196.	13.7	43
84	Dinuclear Ruthenium and Iron Complexes Containing Palladium and Platinum with Tri-tert-Butylphosphine Ligands:Â Synthesis, Structures, and Bonding. Inorganic Chemistry, 2004, 43, 3921-3929.	4.0	30
85	Superloading of Tin Ligands into Rhodium and Iridium Carbonyl Cluster Complexes. Inorganic Chemistry, 2004, 43, 7576-7578.	4.0	66
86	Bimetallic Cluster Complexes:Â The Synthesis, Structures, and Bonding of Ruthenium Carbonyl Cluster Complexes Containing Palladium and Platinum with the Bulky Tri-tert-butyl-phosphine Ligand. Journal of the American Chemical Society, 2004, 126, 5253-5267.	13.7	64
87	Nickelâ^'Manganese Sulfido Carbonyl Cluster Complexes. Synthesis, Structure, and Properties of the Unusual Paramagnetic Complexes Cp2Ni2Mn(CO)3(Î¼3-E)2, E = S, Se. Inorganic Chemistry, 2004, 43, 2515-2525.	4.0	32
88	High-Energy Intermediate or Stable Transition State Analogue:â€‰Theoretical Perspective of the Active Site and Mechanism of Î²-Phosphoglucomutase. Journal of the American Chemical Society, 2004, 126, 6840-6841.	13.7	41
89	De Novo design in organometallic chemistry: stabilizing iridium(V). Coordination Chemistry Reviews, 2003, 238-239, 315-331.	18.8	28
90	Experimental and Computational Evidence for a Boron-Assisted, Ïƒ-Bond Metathesis Pathway for Alkane Borylation. Journal of the American Chemical Society, 2003, 125, 858-859.	13.7	177

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91	The role of triplet states in the long wavelength absorption region of bromine nitrate. Journal of Chemical Physics, 2003, 119, 7864-7870.	3.0	5
92	Factors affecting the structure of substituted tris(pyrazolyl)borate rhodium dicarbonyl complexes. Inorganica Chimica Acta, 2002, 330, 268-282.	2.4	21
93	The vibrational spectrum of Tp3,5-MeRhH2(H2): a computational and inelastic neutron scattering study. Inorganica Chimica Acta, 2002, 330, 240-249.	2.4	9
94	The Theoretical Transition State Structure of a Model Complex Bears a Striking Resemblance to the Active Site Structure of DMSO Reductase. Journal of the American Chemical Society, 2001, 123, 5820-5821.	13.7	81
95	Minimum Energy Structure of Hydridotris(pyrazolyl)borato Iridium(V) Tetrahydride Is Not aC3vCapped Octahedron. Journal of the American Chemical Society, 2001, 123, 9822-9829.	13.7	20
96	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 20. Carbonâ^'Hydrogen and Carbonâ^'Carbon Bond Activation of Cyclopropane by Cationic Iridium(III) and Neutral Rhodium(I) and Iridium(I) Complexes. Organometallics, 2001, 20, 5606-5613.	2.3	27
97	A thermodynamic analysis of the Calâ€“Ad method with respect to gasâ€“solid calorimetry. Microporous and Mesoporous Materials, 1999, 31, 205-209.	4.4	5
98	The multiple equilibrium analysis quantitative prediction of single and multi-component adsorption isotherms on carbonaceous and zeolitic solids. Microporous and Mesoporous Materials, 1999, 33, 291-306.	4.4	19
99	Extension of the electrostatic-covalent model to 2:1 adducts. Polyhedron, 1999, 18, 1097-1106.	2.2	4
100	Multiple Equilibrium Analysis Description of Adsorption on Naâ^'Mordenite and Hâ^'Mordenite. Journal of the American Chemical Society, 1999, 121, 12127-12139.	13.7	59
101	A Method for Characterizing Effective Pore Sizes of Catalysts. Journal of Physical Chemistry B, 1999, 103, 1242-1249.	2.6	65
102	Exploring Surfaces and Cavities in Lipoxygenase and Other Proteins by Hyperpolarized Xenon-129 NMR. Journal of the American Chemical Society, 1999, 121, 9370-9377.	13.7	54
103	A Multiple-Process Equilibrium Analysis of Silica Gel and HZSM-5. Journal of the American Chemical Society, 1998, 120, 538-547.	13.7	37
104	Molecular Dimensions for Adsorptives. Journal of the American Chemical Society, 1998, 120, 5509-5516.	13.7	353