Charles Edwin Webster

List of Publications by Year
in descending order

104	3,858	117453	138251
papers	citations	34 h-index	58 g-index

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

#	Article	IF	Citations
1	Molecular Dimensions for Adsorptives. Journal of the American Chemical Society, 1998, 120, 5509-5516.	6.6	353
2	Rhodium Boryl Complexes in the Catalytic, Terminal Functionalization of Alkanes. Journal of the American Chemical Society, 2005, 127, 2538-2552.	6.6	317
3	Electrocatalytic and Photocatalytic Hydrogen Production in Aqueous Solution by a Molecular Cobalt Complex. Angewandte Chemie - International Edition, 2012, 51, 5941-5944.	7.2	280
4	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.	6.6	177
5	Synthesis, Air Stability, Photobleaching, and DFT Modeling of Blue Light Emitting Platinum CCC-N-Heterocyclic Carbene Pincer Complexes. Organometallics, 2012, 31, 1664-1672.	1.1	104
6	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.	1.1	94
7	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.	6.6	88
8	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.	6.6	81
9	Water Oxidation by Mononuclear Ruthenium Complexes with TPA-Based Ligands. Inorganic Chemistry, 2011, 50, 10564-10571.	1.9	80
10	Electronic Effects on a Mononuclear Co Complex with a Pentadentate Ligand for Catalytic H₂ Evolution. Inorganic Chemistry, 2014, 53, 10094-10100.	1.9	79
11	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.	1.6	68
12	Superloading of Tin Ligands into Rhodium and Iridium Carbonyl Cluster Complexes. Inorganic Chemistry, 2004, 43, 7576-7578.	1.9	66
13	A Method for Characterizing Effective Pore Sizes of Catalysts. Journal of Physical Chemistry B, 1999, 103, 1242-1249.	1.2	65
14	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.	6.6	64
15	Multiple Equilibrium Analysis Description of Adsorption on Naâ^'Mordenite and Hâ^'Mordenite. Journal of the American Chemical Society, 1999, 121, 12127-12139.	6.6	59
16	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.	6.6	59
17	Quantum Mechanical Models of the Resting State of the Vanadium-Dependent Haloperoxidase. Inorganic Chemistry, 2004, 43, 4127-4136.	1.9	58
18	Exploring Surfaces and Cavities in Lipoxygenase and Other Proteins by Hyperpolarized Xenon-129 NMR. Journal of the American Chemical Society, 1999, 121, 9370-9377.	6.6	54

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19	Electrocatalytic reduction of CO₂ with CCC-NHC pincer nickel complexes. Chemical Communications, 2017, 53, 9442-9445.	2.2	53
20	Linkage Isomerization as a Mechanism for Photochromic Materials: Cyclopentadienylmanganese Tricarbonyl Derivatives with Chelatable Functional Groups. Organometallics, 2008, 27, 289-296.	1.1	52
21	Highly Active Ruthenium CNC Pincer Photocatalysts for Visible-Light-Driven Carbon Dioxide Reduction. Inorganic Chemistry, 2019, 58, 8012-8020.	1.9	49
22	Development of Ultrafast Photochromic Organometallics and Photoinduced Linkage Isomerization of Arene Chromium Carbonyl Derivatives. Journal of Physical Chemistry A, 2009, 113, 2666-2676.	1.1	48
23	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.	3.3	47
24	Computational Insights into Degenerate Ethylene Exchange with a Grubbs-Type Catalyst. Journal of the American Chemical Society, 2007, 129, 7490-7491.	6.6	44
25	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.	6.6	43
26	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.	7.2	41
27	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.	6.6	41
28	Time-resolved IR Studies on the Mechanism for the Functionalization of Primary Câ^'H Bonds by Photoactivated Cp*W(CO)₃(Bpin). Journal of the American Chemical Society, 2010, 132, 1848-1859.	6.6	41
29	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.	1.6	41
30	Nickel(<scp>ii</scp>) pincer complexes demonstrate that the remote substituent controls catalytic carbon dioxide reduction. Chemical Communications, 2018, 54, 3819-3822.	2.2	39
31	A Multiple-Process Equilibrium Analysis of Silica Gel and HZSM-5. Journal of the American Chemical Society, 1998, 120, 538-547.	6.6	37
32	Time-Resolved Vibrational Spectroscopy of [FeFe]-Hydrogenase Model Compounds. Journal of Physical Chemistry A, 2012, 116, 7261-7271.	1.1	36
33	High Nuclearity Iridiumâ^'Platinum Clusters:Â Synthesis, Structures, Bonding, and Reactivity. Journal of the American Chemical Society, 2005, 127, 1007-1014.	6.6	34
34	Electronic and Steric Effects on Molecular Dihydrogen Activation in [Cp*OsH4(L)]+(L = PPh3, AsPh3,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	6.6	33
35	Platinum CCC-NHC benzimidazolyl pincer complexes: synthesis, characterization, photostability, and theoretical investigation of a blue-green emitter. Dalton Transactions, 2013, 42, 8820.	1.6	33
36	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.	1.9	32

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37	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.	1.1	31
38	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.	1.9	30
39	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.	1.1	30
40	Probing the Mechanism of Carbonâ^'Hydrogen Bond Activation by Photochemically Generated Hydridotris(pyrazolyl)borato Carbonyl Rhodium Complexes: New Experimental and Theoretical Investigations. Organometallics, 2008, 27, 189-201.	1.1	29
41	De Novo design in organometallic chemistry: stabilizing iridium(V). Coordination Chemistry Reviews, 2003, 238-239, 315-331.	9.5	28
42	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.	1.1	27
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.	0.8	27
44	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.	1.1	26
45	Phosphoryl Transfers of the Phospholipase D Superfamily: A Quantum Mechanical Theoretical Study. Journal of the American Chemical Society, 2013, 135, 13764-13774.	6.6	26
46	Enhanced Hydrogen Evolution in Neutral Water Catalyzed by a Cobalt Complex with a Softer Polypyridyl Ligand. Angewandte Chemie - International Edition, 2020, 59, 12694-12697.	7.2	25
47	Organometallics Roundtable 2013â€“2014. Organometallics, 2014, 33, 1505-1527.	1.1	24
48	Two Carbenes versus One in Magnesium Chemistry: Synthesis of Terminal Dihalide, Dialkyl, and Grignard Reagents. Organometallics, 2019, 38, 688-696.	1.1	24
49	Prediction of the reduction potential in transitionâ€metal containing complexes: How expensive? For what accuracy?. Journal of Computational Chemistry, 2017, 38, 2430-2438.	1.5	23
50	Factors affecting the structure of substituted tris(pyrazolyl)borate rhodium dicarbonyl complexes. Inorganica Chimica Acta, 2002, 330, 268-282.	1.2	21
51	A Mononuclear Tungsten Photocatalyst for H₂ Production. ACS Catalysis, 2018, 8, 4838-4847.	5.5	21
52	Minimum Energy Structure of Hydridotris(pyrazolyl)borato Iridium(V) Tetrahydride Is Not aC3vCapped Octahedron. Journal of the American Chemical Society, 2001, 123, 9822-9829.	6.6	20
53	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.	1.2	20
54	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.	1.9	20

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55	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.	2.2	19
56	Computational Investigation of the Mechanism for the Activation of CO by Oxorhenium Complexes. Organometallics, 2012, 31, 4055-4062.	1.1	19
57	Time-Resolved Infrared Studies of a Trimethylphosphine Model Derivative of [FeFe]-Hydrogenase. Journal of Physical Chemistry B, 2013, 117, 15792-15803.	1.2	19
58	Urea decomposition facilitated by a urease model complex: a theoretical investigation. Dalton Transactions, 2005, , 3542.	1.6	17
59	The Synthesis and Characterization of Highly Fluorescent Polycyclic Azaborine Chromophores. Journal of Organic Chemistry, 2016, 81, 10955-10963.	1.7	17
60	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.	0.8	17
61	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.	2.3	14
62	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.	1.1	14
63	Catalytic H₂ Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand. European Journal of Inorganic Chemistry, 2019, 2019, 2134-2139.	1.0	14
64	Forty years of Fenske-Hall molecular orbital theory. , 2005, , 1143-1165.		13
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.	1.1	13
66	Metalâ€“Ligand Synergistic Effects in the Complex Ni(Î·²-TEMPO)₂: Synthesis, Structures, and Reactivity. Inorganic Chemistry, 2013, 52, 13882-13893.	1.9	13
67	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.	1.7	12
68	Tris(carbene) Stabilization of Monomeric Magnesium Cations: A Neutral, Nontethered Ligand Approach. Organometallics, 2020, 39, 4329-4339.	1.1	12
69	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.	1.1	11
70	Photocatalytic H₂-Evolution by Homogeneous Molybdenum Sulfide Clusters Supported by Dithiocarbamate Ligands. Inorganic Chemistry, 2019, 58, 16458-16474.	1.9	11
71	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.	0.8	10
72	Degenerate Pathways for Metallacycle Ring Inversions: A Common Phenomenon Consistent with the Principle of Microscopic Reversibility. Organometallics, 2014, 33, 5928-5931.	1.1	10

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73	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.	0.5	10
74	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.	1.2	10
75	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.	1.0	10
76	Structure Function Relationships in Ruthenium Carbon Dioxide Reduction Catalysts with CNC Pincers Containing Donor Groups. European Journal of Inorganic Chemistry, 2020, 2020, 2709-2717.	1.0	10
77	The vibrational spectrum of Tp3,5-MeRhH2(H2): a computational and inelastic neutron scattering study. Inorganica Chimica Acta, 2002, 330, 240-249.	1.2	9
78	Water Oxidation by Mononuclear Ruthenium Complex with a Pentadentate Isoquinoline-Bipyridyl Ligand. European Journal of Inorganic Chemistry, 2014, 2014, 715-721.	1.0	9
79	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.	1.5	9
80	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.	1.0	9
81	Controlling Photoisomerization Reactivity Through Single Functional Group Substitutions in Ruthenium Phosphine Sulfoxide Complexes. Journal of the American Chemical Society, 2018, 140, 9819-9822.	6.6	8
82	Low-Valent Cobalt(I) CNC Pincer Complexes as Catalysts for Light-Driven Carbon Dioxide Reduction. ACS Catalysis, 2022, 12, 8718-8728.	5.5	8
83	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.	1.5	7
84	Impact of the Dissolved Anion on the Electrocatalytic Reduction of CO 2 to CO with Ruthenium CNC Pincer Complexes. ChemCatChem, 2020, 12, 4879-4885.	1.8	7
85	Cheminformatic quantum mechanical enzyme model design: A catechol-O-methyltransferase case study. Biophysical Journal, 2021, 120, 3577-3587.	0.2	7
86	Bond Energies, Reaction Volumes, and Kinetics for Ïƒ- and Ï€-Complexes of Mo(CO)5L. Journal of Physical Chemistry A, 2011, 115, 9004-9013.	1.1	6
87	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.	1.1	6
88	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.	1.7	6
89	Lightâ€responsive and Protic Ruthenium Compounds Bearing Bathophenanthroline and Dihydroxybipyridine Ligands Achieve Nanomolar Toxicity towards Breast Cancer Cells. Photochemistry and Photobiology, 2021, , .	1.3	6
90	A thermodynamic analysis of the Calâ€“Ad method with respect to gasâ€“solid calorimetry. Microporous and Mesoporous Materials, 1999, 31, 205-209.	2.2	5

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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.	1.2	5
92	Theoretical studies of cyclic adenosine monophosphate dependent protein kinase: native enzyme and ground-state and transition-state analogues. Dalton Transactions, 2014, 43, 3039-3043.	1.6	5
93	Extremely twisted and bent pyrene-fused N-heterocyclic germylenes. Chemical Communications, 2019, 55, 14954-14957.	2.2	5
94	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, .	1.0	5
95	Mechanistic Studies of Oxygen-Atom Transfer (OAT) in the Homogeneous Conversion of N2O by Ru Pincer Complexes. Inorganics, 2022, 10, 69.	1.2	5
96	Extension of the electrostatic-covalent model to 2:1 adducts. Polyhedron, 1999, 18, 1097-1106.	1.0	4
97	The missing agostomer in the fluxionality of cyclohexenylmanganese tricarbonyl. Journal of Organometallic Chemistry, 2018, 864, 128-135.	0.8	4
98	Enhanced Hydrogen Evolution in Neutral Water Catalyzed by a Cobalt Complex with a Softer Polypyridyl Ligand. Angewandte Chemie, 2020, 132, 12794-12797.	1.6	3
99	Benchmarking the Fluxional Processes of Organometallic Piano-Stool Complexes. Molecules, 2021, 26, 2310.	1.7	3
100	Triphenylene containing blue-light emitting semi-fluorinated aryl ether polymers with excellent thermal and photostability. Materials Chemistry Frontiers, 2022, 6, 1391-1404.	3.2	3
101	Theoretical study of the biologically important dioxo diiron diamond core structures. Theoretical Chemistry Accounts, 2008, 120, 467-478.	0.5	2
102	The transâ€“cis isomerization of Ni(Î·2-TEMPO)2: Interconnections and conformational complexity. Inorganica Chimica Acta, 2015, 436, 220-229.	1.2	2
103	The curious case of DMSO: A CCSD(T)/CBS(aQ56+d) benchmark and DFT study. Journal of Chemical Physics, 2021, 155, 114304.	1.2	2
104	Predicting Absorption and Emission Maxima of Polycyclic Aromatic Azaborines: Reliable Transition Energies and Character. Journal of Physical Chemistry A, 2021, 125, 3-12.	1.1	1