

# Charles Edwin Webster

## List of Publications by Year in descending order

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104  
papers

3,858  
citations

117625

34  
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133252

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109  
all docs

109  
docs citations

109  
times ranked

4264  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Dimensions for Adsorptives. <i>Journal of the American Chemical Society</i> , 1998, 120, 5509-5516.	13.7	353
2	Rhodium Boryl Complexes in the Catalytic, Terminal Functionalization of Alkanes. <i>Journal of the American Chemical Society</i> , 2005, 127, 2538-2552.	13.7	317
3	Electrocatalytic and Photocatalytic Hydrogen Production in Aqueous Solution by a Molecular Cobalt Complex. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 5941-5944.	13.8	280
4	Experimental and Computational Evidence for a Boron-Assisted, $\sigma$ -Bond Metathesis Pathway for Alkane Borylation. <i>Journal of the American Chemical Society</i> , 2003, 125, 858-859.	13.7	177
5	Synthesis, Air Stability, Photobleaching, and DFT Modeling of Blue Light Emitting Platinum CCC-N-Heterocyclic Carbene Pincer Complexes. <i>Organometallics</i> , 2012, 31, 1664-1672.	2.3	104
6	Iridium and Ruthenium Complexes of <i>N</i> -Heterocyclic Carbene- and Pyridinol-Derived Chelates as Catalysts for Aqueous Carbon Dioxide Hydrogenation and Formic Acid Dehydrogenation: The Role of the Alkali Metal. <i>Organometallics</i> , 2017, 36, 1091-1106.	2.3	94
7	Electronic and Steric Tuning of Catalytic $H_2$ Evolution by Cobalt Complexes with Pentadentate Polypyridyl-Amine Ligands. <i>Journal of the American Chemical Society</i> , 2018, 140, 9219-9229.	13.7	88
8	The Theoretical Transition State Structure of a Model Complex Bears a Striking Resemblance to the Active Site Structure of DMSO Reductase. <i>Journal of the American Chemical Society</i> , 2001, 123, 5820-5821.	13.7	81
9	Water Oxidation by Mononuclear Ruthenium Complexes with TPA-Based Ligands. <i>Inorganic Chemistry</i> , 2011, 50, 10564-10571.	4.0	80
10	Electronic Effects on a Mononuclear Co Complex with a Pentadentate Ligand for Catalytic $H_2$ Evolution. <i>Inorganic Chemistry</i> , 2014, 53, 10094-10100.	4.0	79
11	Transmetallation from CCC-NHC pincer Zr complexes in the synthesis of air-stable CCC-NHC pincer Co( $\sigma$ -allyl) complexes and initial hydroboration trials. <i>Dalton Transactions</i> , 2016, 45, 2823-2828.	3.3	68
12	Superloading of Tin Ligands into Rhodium and Iridium Carbonyl Cluster Complexes. <i>Inorganic Chemistry</i> , 2004, 43, 7576-7578.	4.0	66
13	A Method for Characterizing Effective Pore Sizes of Catalysts. <i>Journal of Physical Chemistry B</i> , 1999, 103, 1242-1249.	2.6	65
14	Bimetallic Cluster Complexes: The Synthesis, Structures, and Bonding of Ruthenium Carbonyl Cluster Complexes Containing Palladium and Platinum with the Bulky Tri-tert-butyl-phosphine Ligand. <i>Journal of the American Chemical Society</i> , 2004, 126, 5253-5267.	13.7	64
15	Multiple Equilibrium Analysis Description of Adsorption on Na <sup>+</sup> Mordenite and H <sup>+</sup> Mordenite. <i>Journal of the American Chemical Society</i> , 1999, 121, 12127-12139.	13.7	59
16	Structures and Energetics of Models for the Active Site of Acetyl-Coenzyme A Synthase: Role of Distal and Proximal Metals in Catalysis. <i>Journal of the American Chemical Society</i> , 2004, 126, 3410-3411.	13.7	59
17	Quantum Mechanical Models of the Resting State of the Vanadium-Dependent Haloperoxidase. <i>Inorganic Chemistry</i> , 2004, 43, 4127-4136.	4.0	58
18	Exploring Surfaces and Cavities in Lipoxygenase and Other Proteins by Hyperpolarized Xenon-129 NMR. <i>Journal of the American Chemical Society</i> , 1999, 121, 9370-9377.	13.7	54

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19	Electrocatalytic reduction of CO <sub>2</sub> with CCC-NHC pincer nickel complexes. <i>Chemical Communications</i> , 2017, 53, 9442-9445.	4.1	53
20	Linkage Isomerization as a Mechanism for Photochromic Materials: Cyclopentadienylmanganese Tricarbonyl Derivatives with Chelatable Functional Groups. <i>Organometallics</i> , 2008, 27, 289-296.	2.3	52
21	Highly Active Ruthenium CNC Pincer Photocatalysts for Visible-Light-Driven Carbon Dioxide Reduction. <i>Inorganic Chemistry</i> , 2019, 58, 8012-8020.	4.0	49
22	Development of Ultrafast Photochromic Organometallics and Photoinduced Linkage Isomerization of Arene Chromium Carbonyl Derivatives. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2666-2676.	2.5	48
23	Near attack conformers dominate $\hat{\nu}^2$ -phosphoglucomutase complexes where geometry and charge distribution reflect those of substrate. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 6910-6915.	7.1	47
24	Computational Insights into Degenerate Ethylene Exchange with a Grubbs-Type Catalyst. <i>Journal of the American Chemical Society</i> , 2007, 129, 7490-7491.	13.7	44
25	Reaction of the 1,8-Bis(diphenylmethyl)naphthalenediyl Dication with Fluoride: Formation of a Cation Containing a C $\hat{\nu}$ F $\hat{\nu}$ C Bridge. <i>Journal of the American Chemical Society</i> , 2004, 126, 8189-8196.	13.7	43
26	Rhodium Silyl Boryl Hydride Complexes: Comparison of Bonding and the Rates of Elimination of Borane, Silane, and Dihydrogen. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 5474-5477.	13.8	41
27	High-Energy Intermediate or Stable Transition State Analogue: Theoretical Perspective of the Active Site and Mechanism of $\hat{\nu}^2$ -Phosphoglucomutase. <i>Journal of the American Chemical Society</i> , 2004, 126, 6840-6841.	13.7	41
28	Time-resolved IR Studies on the Mechanism for the Functionalization of Primary C $\hat{\nu}$ H Bonds by Photoactivated Cp $\hat{\nu}$ W(CO) <sub>3</sub> (Bpin). <i>Journal of the American Chemical Society</i> , 2010, 132, 1848-1859.	13.7	41
29	Synthesis, characterization, photophysical properties, and catalytic activity of an SCS bis(N-heterocyclic thione) (SCS-NHT) Pd pincer complex. <i>Dalton Transactions</i> , 2015, 44, 14475-14482.	3.3	41
30	Nickel( $\hat{\nu}$ ) pincer complexes demonstrate that the remote substituent controls catalytic carbon dioxide reduction. <i>Chemical Communications</i> , 2018, 54, 3819-3822.	4.1	39
31	A Multiple-Process Equilibrium Analysis of Silica Gel and HZSM-5. <i>Journal of the American Chemical Society</i> , 1998, 120, 538-547.	13.7	37
32	Time-Resolved Vibrational Spectroscopy of [FeFe]-Hydrogenase Model Compounds. <i>Journal of Physical Chemistry A</i> , 2012, 116, 7261-7271.	2.5	36
33	High Nuclearity Iridium $\hat{\nu}$ Platinum Clusters: Synthesis, Structures, Bonding, and Reactivity. <i>Journal of the American Chemical Society</i> , 2005, 127, 1007-1014.	13.7	34
34	Electronic and Steric Effects on Molecular Dihydrogen Activation in [Cp $\hat{\nu}$ OsH <sub>4</sub> (L)] <sup>+</sup> (L = PPh <sub>3</sub> , AsPh <sub>3</sub> ). <i>Journal of the American Chemical Society</i> , 2000, 122, 1000-1006.	13.7	33
35	Platinum CCC-NHC benzimidazolyl pincer complexes: synthesis, characterization, photostability, and theoretical investigation of a blue-green emitter. <i>Dalton Transactions</i> , 2013, 42, 8820.	3.3	33
36	Nickel $\hat{\nu}$ Manganese Sulfido Carbonyl Cluster Complexes. Synthesis, Structure, and Properties of the Unusual Paramagnetic Complexes Cp <sub>2</sub> Ni <sub>2</sub> Mn(CO) <sub>3</sub> ( $\hat{\nu}$ 3-E) <sub>2</sub> , E = S, Se. <i>Inorganic Chemistry</i> , 2004, 43, 2515-2525.	4.0	32

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37	Extreme $\pi$ -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. <i>Organometallics</i> , 2016, 35, 3452-3460.	2.3	31
38	Dinuclear Ruthenium and Iron Complexes Containing Palladium and Platinum with Tri-tert-Butylphosphine Ligands: Synthesis, Structures, and Bonding. <i>Inorganic Chemistry</i> , 2004, 43, 3921-3929.	4.0	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. <i>Organometallics</i> , 2014, 33, 952-958.	2.3	30
40	Probing the Mechanism of Carbon-Hydrogen Bond Activation by Photochemically Generated Hydridotris(pyrazolyl)borato Carbonyl Rhodium Complexes: New Experimental and Theoretical Investigations. <i>Organometallics</i> , 2008, 27, 189-201.	2.3	29
41	De Novo design in organometallic chemistry: stabilizing iridium(V). <i>Coordination Chemistry Reviews</i> , 2003, 238-239, 315-331.	18.8	28
42	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 20. Carbon-Hydrogen and Carbon-Carbon Bond Activation of Cyclopropane by Cationic Iridium(III) and Neutral Rhodium(I) and Iridium(I) Complexes. <i>Organometallics</i> , 2001, 20, 5606-5613.	2.3	27
43	$\pi$ -Boration of $\pi$ -unsaturated carbonyl compounds in ethanol and methanol catalyzed by CCC-NHC pincer Rh complexes. <i>Journal of Organometallic Chemistry</i> , 2016, 802, 32-38.	1.8	27
44	Engineering Femtosecond Organometallic Chemistry: Photochemistry and Dynamics of Ultrafast Chelation of Cyclopentadienylmanganese Tricarbonyl Derivatives with Pendant Benzenecarbonyl and Pyridinecarbonyl Groups. <i>Organometallics</i> , 2011, 30, 5611-5619.	2.3	26
45	Phosphoryl Transfers of the Phospholipase D Superfamily: A Quantum Mechanical Theoretical Study. <i>Journal of the American Chemical Society</i> , 2013, 135, 13764-13774.	13.7	26
46	Enhanced Hydrogen Evolution in Neutral Water Catalyzed by a Cobalt Complex with a Softer Polypyridyl Ligand. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 12694-12697.	13.8	25
47	<i>Organometallics</i> Roundtable 2013-2014. <i>Organometallics</i> , 2014, 33, 1505-1527.	2.3	24
48	Two Carbenes versus One in Magnesium Chemistry: Synthesis of Terminal Dihalide, Dialkyl, and Grignard Reagents. <i>Organometallics</i> , 2019, 38, 688-696.	2.3	24
49	Prediction of the reduction potential in transition-metal containing complexes: How expensive? For what accuracy?. <i>Journal of Computational Chemistry</i> , 2017, 38, 2430-2438.	3.3	23
50	Factors affecting the structure of substituted tris(pyrazolyl)borate rhodium dicarbonyl complexes. <i>Inorganica Chimica Acta</i> , 2002, 330, 268-282.	2.4	21
51	A Mononuclear Tungsten Photocatalyst for $H_2$ Production. <i>ACS Catalysis</i> , 2018, 8, 4838-4847.	11.2	21
52	Minimum Energy Structure of Hydridotris(pyrazolyl)borato Iridium(V) Tetrahydride Is Not a $C_3v$ -Capped Octahedron. <i>Journal of the American Chemical Society</i> , 2001, 123, 9822-9829.	13.7	20
53	A Theoretical Study of Phosphoryl Transfers of Tyrosyl-DNA Phosphodiesterase I (Tdp1) and the Possibility of a $\alpha$ -Dead-End-Phosphohistidine Intermediate. <i>Biochemistry</i> , 2015, 54, 4236-4247.	2.5	20
54	Singlet Oxygen Formation vs Photodissociation for Light-Responsive Protic Ruthenium Anticancer Compounds: The Oxygenated Substituent Determines Which Pathway Dominates. <i>Inorganic Chemistry</i> , 2021, 60, 2138-2148.	4.0	20

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55	The multiple equilibrium analysis quantitative prediction of single and multi-component adsorption isotherms on carbonaceous and zeolitic solids. <i>Microporous and Mesoporous Materials</i> , 1999, 33, 291-306.	4.4	19
56	Computational Investigation of the Mechanism for the Activation of CO by Oxorhenium Complexes. <i>Organometallics</i> , 2012, 31, 4055-4062.	2.3	19
57	Time-Resolved Infrared Studies of a Trimethylphosphine Model Derivative of [FeFe]-Hydrogenase. <i>Journal of Physical Chemistry B</i> , 2013, 117, 15792-15803.	2.6	19
58	Urea decomposition facilitated by a urease model complex: a theoretical investigation. <i>Dalton Transactions</i> , 2005, , 3542.	3.3	17
59	The Synthesis and Characterization of Highly Fluorescent Polycyclic Azaborine Chromophores. <i>Journal of Organic Chemistry</i> , 2016, 81, 10955-10963.	3.2	17
60	Synthesis, characterization, photophysics, and a ligand rearrangement of CCC-NHC pincer nickel complexes: Colors, polymorphs, emission, and Raman spectra. <i>Journal of Organometallic Chemistry</i> , 2017, 845, 258-265.	1.8	17
61	Carbon-Hydrogen Bond Activation in Hydridotris(pyrazolyl)borate Platinum(IV) Complexes: Comparison of Density Functionals, Basis Sets, and Bonding Patterns. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2268-2281.	5.3	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. <i>Organometallics</i> , 2014, 33, 485-497.	2.3	14
63	Catalytic H <sub>2</sub> Evolution by a Mononuclear Cobalt Complex with a Macrocyclic Pentadentate Ligand. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 2134-2139.	2.0	14
64	Forty years of Fenske-Hall molecular orbital theory. , 2005, , 1143-1165.		13
65	Ligand Displacement from TpMn(CO) <sub>2</sub> L Complexes: A Large Rate Enhancement in Comparison to the CpMn(CO) <sub>2</sub> L Analogues. <i>Organometallics</i> , 2011, 30, 3054-3063.	2.3	13
66	Metal-Ligand Synergistic Effects in the Complex Ni(II)-TEMPO: Synthesis, Structures, and Reactivity. <i>Inorganic Chemistry</i> , 2013, 52, 13882-13893.	4.0	13
67	Synthesis of <i>C</i> -Unsubstituted 1,2-Diazetidines and Their Ring-Opening Reactions via Selective N-N Bond Cleavage. <i>Journal of Organic Chemistry</i> , 2018, 83, 9497-9503.	3.2	12
68	Tris(carbene) Stabilization of Monomeric Magnesium Cations: A Neutral, Nontethered Ligand Approach. <i>Organometallics</i> , 2020, 39, 4329-4339.	2.3	12
69	Computational Analysis of the Intramolecular Oxidative Amination of an Alkene Catalyzed by the Extreme $\pi$ -Loading N-Heterocyclic Carbene Pincer Tantalum(V) Bis(imido) Complex. <i>Organometallics</i> , 2018, 37, 1671-1681.	2.3	11
70	Photocatalytic H <sub>2</sub> -Evolution by Homogeneous Molybdenum Sulfide Clusters Supported by Dithiocarbamate Ligands. <i>Inorganic Chemistry</i> , 2019, 58, 16458-16474.	4.0	11
71	Disulfido iron-manganese carbonyl cluster complexes: Synthesis, structure, bonding and properties of the radical CpFeMn <sub>2</sub> (CO) <sub>7</sub> ( $\mu$ -S) <sub>2</sub> . <i>Journal of Organometallic Chemistry</i> , 2008, 693, 2732-2738.	1.8	10
72	Degenerate Pathways for Metallacycle Ring Inversions: A Common Phenomenon Consistent with the Principle of Microscopic Reversibility. <i>Organometallics</i> , 2014, 33, 5928-5931.	2.3	10

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73	Experimental and Computational Studies of the Mechanisms of Hydroamination/Cyclisation of Unactivated $\alpha,\beta$ -Amino-alkenes with CCC-NHC Pincer Zr Complexes. <i>Australian Journal of Chemistry</i> , 2016, 69, 573.	0.9	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. <i>Inorganica Chimica Acta</i> , 2018, 469, 164-172.	2.4	10
75	Investigation of metallation/transmetallation reactions to synthesize a series of CCC-NHC Co pincer complexes and their X-ray structures. <i>Polyhedron</i> , 2018, 151, 568-574.	2.2	10
76	Structure Function Relationships in Ruthenium Carbon Dioxide Reduction Catalysts with CNC Pincers Containing Donor Groups. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 2709-2717.	2.0	10
77	The vibrational spectrum of Tp3,5-MeRh2(H2): a computational and inelastic neutron scattering study. <i>Inorganica Chimica Acta</i> , 2002, 330, 240-249.	2.4	9
78	Water Oxidation by Mononuclear Ruthenium Complex with a Pentadentate Isoquinoline-Bipyridyl Ligand. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 715-721.	2.0	9
79	Synthesis, computational, and spectroscopic analysis of tunable highly fluorescent BN-1,2-azaborine derivatives containing the N-BOH moiety. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 10172-10183.	2.8	9
80	Structure-Function Analysis of Hydrogen Production Catalyzed by Molecular Cobalt Complexes with Pentadentate Ligands in Aqueous Solutions. <i>European Journal of Inorganic Chemistry</i> , 2020, 2020, 3534-3547.	2.0	9
81	Controlling Photoisomerization Reactivity Through Single Functional Group Substitutions in Ruthenium Phosphine Sulfoxide Complexes. <i>Journal of the American Chemical Society</i> , 2018, 140, 9819-9822.	13.7	8
82	Low-Valent Cobalt(I) CNC Pincer Complexes as Catalysts for Light-Driven Carbon Dioxide Reduction. <i>ACS Catalysis</i> , 2022, 12, 8718-8728.	11.2	8
83	Phosphoramidate hydrolysis catalyzed by human histidine triad nucleotide binding protein 1 (hHint1): a cluster-model DFT computational study. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8661-8668.	2.8	7
84	Impact of the Dissolved Anion on the Electrocatalytic Reduction of CO <sub>2</sub> to CO with Ruthenium CNC Pincer Complexes. <i>ChemCatChem</i> , 2020, 12, 4879-4885.	3.7	7
85	Cheminformatic quantum mechanical enzyme model design: A catechol-O-methyltransferase case study. <i>Biophysical Journal</i> , 2021, 120, 3577-3587.	0.5	7
86	Bond Energies, Reaction Volumes, and Kinetics for $\sigma$ - and $\pi$ -Complexes of Mo(CO) <sub>5</sub> L. <i>Journal of Physical Chemistry A</i> , 2011, 115, 9004-9013.	2.5	6
87	Calibrating Reaction Enthalpies: Use of Density Functional Theory and the Correlation Consistent Composite Approach in the Design of Photochromic Materials. <i>Journal of Physical Chemistry A</i> , 2016, 120, 9982-9997.	2.5	6
88	Planar, Stair-Stepped, and Twisted: Modulating Structure and Photophysics in Pyrene- and Benzene-Fused N-Heterocyclic Boranes. <i>Chemistry - A European Journal</i> , 2020, 26, 10072-10082.	3.3	6
89	Light-responsive and Protic Ruthenium Compounds Bearing Bathophenanthroline and Dihydroxybipyridine Ligands Achieve Nanomolar Toxicity towards Breast Cancer Cells. <i>Photochemistry and Photobiology</i> , 2021, , .	2.5	6
90	A thermodynamic analysis of the Calad method with respect to gas-solid calorimetry. <i>Microporous and Mesoporous Materials</i> , 1999, 31, 205-209.	4.4	5

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91	The role of triplet states in the long wavelength absorption region of bromine nitrate. <i>Journal of Chemical Physics</i> , 2003, 119, 7864-7870.	3.0	5
92	Theoretical studies of cyclic adenosine monophosphate dependent protein kinase: native enzyme and ground-state and transition-state analogues. <i>Dalton Transactions</i> , 2014, 43, 3039-3043.	3.3	5
93	Extremely twisted and bent pyrene-fused N-heterocyclic germylenes. <i>Chemical Communications</i> , 2019, 55, 14954-14957.	4.1	5
94	Sensitized and Self-Sensitized Photocatalytic Carbon Dioxide Reduction Under Visible Light with Ruthenium Catalysts Shows Enhancements with More Conjugated Pincer Ligands. <i>European Journal of Inorganic Chemistry</i> , 2022, 2022, .	2.0	5
95	Mechanistic Studies of Oxygen-Atom Transfer (OAT) in the Homogeneous Conversion of N <sub>2</sub> O by Ru Pincer Complexes. <i>Inorganics</i> , 2022, 10, 69.	2.7	5
96	Extension of the electrostatic-covalent model to 2:1 adducts. <i>Polyhedron</i> , 1999, 18, 1097-1106.	2.2	4
97	The missing agostomer in the fluxionality of cyclohexenylmanganese tricarbonyl. <i>Journal of Organometallic Chemistry</i> , 2018, 864, 128-135.	1.8	4
98	Enhanced Hydrogen Evolution in Neutral Water Catalyzed by a Cobalt Complex with a Softer Polypyridyl Ligand. <i>Angewandte Chemie</i> , 2020, 132, 12794-12797.	2.0	3
99	Benchmarking the Fluxional Processes of Organometallic Piano-Stool Complexes. <i>Molecules</i> , 2021, 26, 2310.	3.8	3
100	Triphenylene containing blue-light emitting semi-fluorinated aryl ether polymers with excellent thermal and photostability. <i>Materials Chemistry Frontiers</i> , 2022, 6, 1391-1404.	5.9	3
101	Theoretical study of the biologically important dioxo diiron diamond core structures. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 467-478.	1.4	2
102	The trans $\leftrightarrow$ cis isomerization of Ni( $\eta^2$ -TEMPO) <sub>2</sub> : Interconnections and conformational complexity. <i>Inorganica Chimica Acta</i> , 2015, 436, 220-229.	2.4	2
103	The curious case of DMSO: A CCSD(T)/CBS(aQ56+d) benchmark and DFT study. <i>Journal of Chemical Physics</i> , 2021, 155, 114304.	3.0	2
104	Predicting Absorption and Emission Maxima of Polycyclic Aromatic Azaborines: Reliable Transition Energies and Character. <i>Journal of Physical Chemistry A</i> , 2021, 125, 3-12.	2.5	1