Michael B Hall

List of Publications by Year
in descending order

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		18482	30087
351	14,928	62	103
papers	citations	h-index	g-index

367	367	367	8628
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical Studies on Reactions of Transition-Metal Complexes. Chemical Reviews, 2000, 100, 353-406.	47.7	811
2	Electronic structure and bonding in methyl- and perfluoromethyl(pentacarbonyl)manganese. Inorganic Chemistry, 1972, 11, 768-775.	4.0	531
3	Basis sets for transition metals: Optimized outerp functions. Journal of Computational Chemistry, 1996, 17, 1359-1370.	3.3	412
4	Computational Studies of [NiFe] and [FeFe] Hydrogenases. Chemical Reviews, 2007, 107, 4414-4435.	47.7	383
5	A Capable Bridging Ligand for Fe-Only Hydrogenase:Â Density Functional Calculations of a Low-Energy Route for Heterolytic Cleavage and Formation of Dihydrogen. Journal of the American Chemical Society, 2001, 123, 3828-3829.	13.7	334
6	Rhodium Boryl Complexes in the Catalytic, Terminal Functionalization of Alkanes. Journal of the American Chemical Society, 2005, 127, 2538-2552.	13.7	317
7	Theoretical Characterization of the Reaction Intermediates in a Model of the Nickelâ^'Iron Hydrogenase ofDesulfovibrio gigas. Journal of the American Chemical Society, 1999, 121, 4000-4007.	13.7	191
8	Fundamental properties of small molecule models of Fe-only hydrogenase: computations relative to the definition of an entatic state in the active site. Coordination Chemistry Reviews, 2003, 238-239, 255-266.	18.8	186
9	Monomeric and Oligomeric Amineâ^'Borane Ïƒ-Complexes of Rhodium. Intermediates in the Catalytic Dehydrogenation of Amineâ^'Boranes. Journal of the American Chemical Society, 2009, 131, 15440-15456.	13.7	183
10	Flexible Zirconium Metalâ€Organic Frameworks as Bioinspired Switchable Catalysts. Angewandte Chemie - International Edition, 2016, 55, 10776-10780.	13.8	179
11	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
12	Thermally Stable Homogeneous Catalysts for Alkane Dehydrogenation S.O. thanks the German Academic Exchange Service (DAAD) for financing a research stay with W.C.K. in the USA. This work was supported by the National Science Foundation (CHE 9800184 to M.B.H.), by the University of California Energy Institute and University of California Santa Barbara (to W.C.K.), and by the German Research Association (DFG, to M.W.H). We thank Dr. R. Mynott and Mrs. C. Wirtz, MPI fÃ¼r Kohlenforschung, for	13.8	175
13	Modeling the Active Sites of Metalloenzymes. 3. Density Functional Calculations on Models for [Fe]-Hydrogenase:Â Structures and Vibrational Frequencies of the Observed Redox Forms and the Reaction Mechanism at the Diiron Active Center. Journal of the American Chemical Society, 2001, 123, 3734-3742.	13.7	169
14	Monoiron Hydrogenase Catalysis: Hydrogen Activation with the Formation of a Dihydrogen, Feâ^'H^{Î´â^'}Â·Â·Â·H^{Î´+}â^'O, Bond and Methenyl-H₄MPT⁺ Triggered Hydride Transfer. Journal of the American Chemical Society, 2009, 131, 10901-10908.	13.7	158
15	Electronic Effects Steer the Mechanism of Asymmetric Hydrogenations of Unfunctionalized Aryl-Substituted Alkenes. Journal of the American Chemical Society, 2004, 126, 16688-16689.	13.7	150
16	De Novo Design of Synthetic Di-Iron(I) Complexes as Structural Models of the Reduced Form of Ironâ^'Iron Hydrogenase. Inorganic Chemistry, 2006, 45, 1552-1559.	4.0	145
17	Tetrarhena-heterocycle from the Palladium-Catalyzed Dimerization of Re₂(CO)₈(Î¼-SbPh₂)(Î¼-H) Exhibits an Unusual Hostâ€“Guest Behavior. Journal of the American Chemical Society, 2011, 133, 12994-12997.	13.7	144
18	Dual Electron Uptake by Simultaneous Iron and Ligand Reduction in an N-Heterocyclic Carbene Substituted [FeFe] Hydrogenase Model Compound. Inorganic Chemistry, 2005, 44, 5550-5552.	4.0	136

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19	Two-State Reactivity in Low-Valent Iron-Mediated Câ€“H Activation and the Implications for Other First-Row Transition Metals. Journal of the American Chemical Society, 2016, 138, 3715-3730.	13.7	136
20	The Catalytic Dehydrogenation of Ammonia-Borane Involving an Unexpected Hydrogen Transfer to Ligated Carbene and Subsequent Carbonâ^'Hydrogen Activation. Journal of the American Chemical Society, 2008, 130, 1798-1799.	13.7	135
21	Mechanism of Water Splitting and Oxygenâ^'Oxygen Bond Formation by a Mononuclear Ruthenium Complex. Journal of the American Chemical Society, 2010, 132, 120-130.	13.7	133
22	Hydrogen-Substituted Osmium Silylene Complexes:Â Effect of Charge Localization on Catalytic Hydrosilation. Journal of the American Chemical Society, 2006, 128, 428-429.	13.7	128
23	Methane Metathesis at a Cationic Iridium Center. Journal of the American Chemical Society, 1996, 118, 6068-6069.	13.7	118
24	Synthesis of Carboxylic Acid-Modified [FeFe]-Hydrogenase Model Complexes Amenable to Surface Immobilization. Organometallics, 2007, 26, 3976-3984.	2.3	115
25	Theoretical Calculations of Metal-Dioxygen Complexes. Chemical Reviews, 1994, 94, 639-658.	47.7	113
26	Theoretical Studies on Models for the Oxo-Transfer Reaction of Dioxomolybdenum Enzymes. Inorganic Chemistry, 1996, 35, 1273-1278.	4.0	111
27	Series of Mixed Valent Fe(II)Fe(I) Complexes That Model the H_{ox} State of [FeFe]Hydrogenase: Redox Properties, Density-Functional Theory Investigation, and Reactivities with Extrinsic CO. Inorganic Chemistry, 2008, 47, 7009-7024.	4.0	111
28	Origins of the Selectivity for Borylation of Primary over Secondary Câ^'H Bonds Catalyzed by Cp*-Rhodium Complexes. Journal of the American Chemical Society, 2010, 132, 3078-3091.	13.7	110
29	Theoretical studies of inorganic and organometallic reaction mechanisms. 2. The trans effect in square-planar platinum(II) and rhodium(I) substitution reactions. Inorganic Chemistry, 1991, 30, 646-651.	4.0	100
30	Carbonâ^'Hydrogen Bond Activation:â€‰ Two, Three, or More Mechanisms?. Journal of the American Chemical Society, 2007, 129, 12068-12069.	13.7	100
31	Mechanistic Insights into Iridium-Catalyzed Asymmetric Hydrogenation of Dienes. Chemistry - A European Journal, 2005, 11, 6859-6868.	3.3	95
32	Transition metal polyhydride complexes: a theoretical view. Coordination Chemistry Reviews, 1994, 135-136, 845-879.	18.8	91
33	Inter- and Intramolecular Câ^'H Activation by a Cationic Iridium(III) Center via Oxidative-Addition Reductive-Elimination and Ïƒ-Bond Metathesis Pathways. Journal of the American Chemical Society, 1998, 120, 6169-6170.	13.7	90
34	Synthesis, Reactivity, and DFT Studies of Tantalum Complexes Incorporating Diamido-N-heterocyclic Carbene Ligands. Facile Endocyclic Câ^'H Bond Activation. Journal of the American Chemical Society, 2006, 128, 12531-12543.	13.7	87
35	Mechanism of the Formation of Carboxylate from Alcohols and Water Catalyzed by a Bipyridine-Based Ruthenium Complex: A Computational Study. Journal of the American Chemical Society, 2014, 136, 383-395.	13.7	85
36	Density functional study of the catalytic cycle of nickelâ€“iron [NiFe] hydrogenases and the involvement of high-spin nickel(II). Journal of Biological Inorganic Chemistry, 2006, 11, 286-306.	2.6	83

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37	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
38	Structural and Spectroscopic Features of Mixed Valent Fe^{II}Fe^I Complexes and Factors Related to the Rotated Configuration of Diiron Hydrogenase. Journal of the American Chemical Society, 2012, 134, 13089-13102.	13.7	81
39	Noncovalent bonding: Stacking interactions of chelate rings of transition metal complexes. Coordination Chemistry Reviews, 2017, 345, 318-341.	18.8	81
40	Prediction of the Geometries of Simple Transition Metal Polyhydride Complexes by Symmetry Analysis. Journal of the American Chemical Society, 1999, 121, 1348-1358.	13.7	79
41	IR spectroelectrochemical study of the binding of carbon monoxide to the active site of Desulfovibrio fructosovorans Ni-Fe hydrogenase. Journal of Biological Inorganic Chemistry, 2002, 7, 318-326.	2.6	78
42	Hemilabile Bridging Thiolates as Proton Shuttles in Bioinspired H₂ Production Electrocatalysts. Journal of the American Chemical Society, 2016, 138, 12920-12927.	13.7	78
43	A Theoretical Investigation of Ruthenium-Catalyzed Alkene Hydrosilation:Â Evidence To Support an Exciting New Mechanistic Proposal. Journal of the American Chemical Society, 2004, 126, 13564-13565.	13.7	77
44	Theoretical studies of inorganic and organometallic reaction mechanisms. 6. Methane activation on transient cyclopentadienylcarbonylrhodium. Organometallics, 1993, 12, 3118-3126.	2.3	76
45	The molecular and electronic structure of carbonâ€“hydrogen bond activation and transition metal assisted hydrogen transfer. Coordination Chemistry Reviews, 2009, 253, 1202-1218.	18.8	76
46	Computational Mechanistic Studies on Reactions of Transition Metal Complexes with Noninnocent Pincer Ligands: Aromatizationâ€“Dearomatization or Not. ACS Catalysis, 2015, 5, 1895-1913.	11.2	75
47	Assignment of Molecular Structures to the Electrochemical Reduction Products of Diiron Compounds Related to [Feâ˜Fe] Hydrogenase:Â A Combined Experimental and Density Functional Theory Study. Inorganic Chemistry, 2007, 46, 384-394.	4.0	73
48	Mechanism of electrocatalytic hydrogen production by a di-iron model of ironâ€“iron hydrogenase: A density functional theory study of proton dissociation constants and electrode reduction potentials. Dalton Transactions, 2010, 39, 3093.	3.3	73
49	Force constants and the electronic structure of carbonyl groups. d6 Carbonyl halides and dihalides. Inorganic Chemistry, 1972, 11, 1619-1624.	4.0	72
50	A group theoretical analysis on transition-metal complexes with metal-ligand multiple bonds. Coordination Chemistry Reviews, 1993, 123, 149-167.	18.8	72
51	Crystallographic Evidence of a Base-Free Uranium(IV) Terminal Oxo Species. Inorganic Chemistry, 2010, 49, 7620-7622.	4.0	72
52	Electrochemical oxidation of organometallic complexes. Carbene and Lewis base complexes of chromium, molybdenum, and tungsten carbonyls. Journal of the Chemical Society Dalton Transactions, 1973, , 1743.	1.1	69
53	Sulfur Oxygenates of Biomimetics of the Diiron Subsite of the [FeFe]-Hydrogenase Active Site: Properties and Oxygen Damage Repair Possibilities. Journal of the American Chemical Society, 2009, 131, 8296-8307.	13.7	69
54	Analysis of a Pentacoordinate Iron Dicarbonyl as Synthetic Analogue of the Hmd or Monoâ€Iron Hydrogenase Active Site. Chemistry - A European Journal, 2010, 16, 3083-3089.	3.3	69

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55	Nature of metal-metal interactions in systems with bridging ligands. 1. Electronic structure and bonding in octacarbonyldicobalt. Inorganic Chemistry, 1991, 30, 1079-1086.	4.0	68
56	Better than platinum? Fuel cells energized by enzymes. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 16911-16912.	7.1	67
57	A reexamination of the propensities of amino acids towards a particular secondary structure: classification of amino acids based on their chemical structure. Journal of Molecular Modeling, 2008, 14, 769-775.	1.8	67
58	Role of the Chemically Non-Innocent Ligand in the Catalytic Formation of Hydrogen and Carbon Dioxide from Methanol and Water with the Metal as the Spectator. Journal of the American Chemical Society, 2015, 137, 12330-12342.	13.7	67
59	Superloading of Tin Ligands into Rhodium and Iridium Carbonyl Cluster Complexes. Inorganic Chemistry, 2004, 43, 7576-7578.	4.0	66
60	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
61	Biomimetics of [NiFe]-Hydrogenase: Nickel- or Iron-Centered Proton Reduction Catalysis?. Journal of the American Chemical Society, 2017, 139, 18065-18070.	13.7	64
62	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 15. Catalytic Alkane Dehydrogenation by Iridium(III) Complexes. Journal of the American Chemical Society, 1999, 121, 3992-3999.	13.7	63
63	A Theoretical Study of the Primary Oxo Transfer Reaction of a Dioxo Molybdenum(VI) Compound with Imine Thiolate Chelating Ligands:Â A Molybdenum Oxotransferase Analogue. Journal of the American Chemical Society, 2001, 123, 3995-4002.	13.7	63
64	Nonparameterized MO calculations of ligand-bridged M2(CO)8-(U2-X)2-type dimers containing metalî—¸metal interactions: Evidence for dictation of stereochemistry by one-electron and two-electron metalî—¸metal Ïƒ-type bonds. Journal of Organometallic Chemistry, 1974, 70, 413-420.	1.8	62
65	Theoretical studies of inorganic and organometallic reaction mechanisms. 3. The origin of the difference in the barrier for the kinetic and thermodynamic products for the oxidative addition of dihydrogen to a square-planar iridium complex. Journal of the American Chemical Society, 1992, 114, 517-522.	13.7	62
66	Theoretical studies of inorganic and organometallic reaction mechanisms. 4. Oxidative addition of dihydrogen to d8 square-planar iridium complexes with trans phosphines. Inorganic Chemistry, 1992, 31, 317-321.	4.0	62
67	The Osmiumâ€“Silicon Triple Bond: Synthesis, Characterization, and Reactivity of an Osmium Silylyne Complex. Journal of the American Chemical Society, 2013, 135, 11780-11783.	13.7	62
68	Modeling the Active Sites of Metalloenzymes. 4. Predictions of the Unready States of [NiFe]Desulfovibrio gigasHydrogenase from Density Functional Theory. Inorganic Chemistry, 2001, 40, 18-24.	4.0	61
69	Modeling the Active Sites in Metalloenzymes 5. The Heterolytic Bond Cleavage of H2in the [NiFe] Hydrogenase ofDesulfovibrio gigasby a Nucleophilic Addition Mechanism. Inorganic Chemistry, 2001, 40, 6201-6203.	4.0	61
70	Use of spin-orbit coupling in the interpretation of photoelectron spectra. I. Application to substituted rhenium pentacarbonyls. Journal of the American Chemical Society, 1975, 97, 2057-2065.	13.7	60
71	Generalized molecular orbital calculations on transition-metal dioxygen complexes. Models for iron and cobalt porphyrins. Inorganic Chemistry, 1984, 23, 4627-4632.	4.0	60
72	Density functional study of the complete pathway for the Heck reaction with palladium diphosphines. Journal of Organometallic Chemistry, 2008, 693, 1552-1563.	1.8	60

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73	Theoretical Study of Alternative Pathways for the Heck Reaction through Dipalladium and â€œLigand-Freeâ€•Palladium Intermediates. Organometallics, 2008, 27, 6222-6232.	2.3	60
74	Preparation and Thermal Decomposition of N,N'-Diacyl-N,N'-Dialkoxyhydrazines: Synthetic Applications and Mechanistic Insights. Journal of the American Chemical Society, 1995, 117, 4870-4874.	13.7	59
75	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
76	Quantum Mechanical Models of the Resting State of the Vanadium-Dependent Haloperoxidase. Inorganic Chemistry, 2004, 43, 4127-4136.	4.0	58
77	Redox active iron nitrosyl units in proton reduction electrocatalysis. Nature Communications, 2014, 5, 3684.	12.8	58
78	Understanding the Effects of Bidentate Directing Groups: A Unified Rationale for sp2 and sp3 Câ€“H Bond Activations. Journal of Organic Chemistry, 2015, 80, 4672-4682.	3.2	58
79	Ab Initio Calculations of the Geometries and Bonding Energies of Alkane and Fluoroalkane Complexes with Tungsten Pentacarbonyl. Journal of Physical Chemistry A, 1997, 101, 4646-4652.	2.5	56
80	Mechanistic Investigation of the Oxygen-Atom-Transfer Reactivity of Dioxo-molybdenum(VI) Complexes. Chemistry - A European Journal, 2006, 12, 7501-7509.	3.3	56
81	Problems in the theoretical description of metal-metal multiple bonds or how I learned to hate the electron correlation problem. Polyhedron, 1987, 6, 679-684.	2.2	54
82	Interruption of conjugation in polyenes bound to transition-metal fragments. Journal of the American Chemical Society, 1983, 105, 4930-4941.	13.7	53
83	Trigger Mechanism for the Catalytic Hydrogen Activation by Monoiron (Ironâ^'Sulfur Cluster-Free) Hydrogenase. Journal of the American Chemical Society, 2008, 130, 14036-14037.	13.7	52
84	Thermal Decomposition Pathways of Hydroxylamine: Theoretical Investigation on the Initial Steps. Journal of Physical Chemistry A, 2010, 114, 9262-9269.	2.5	52
85	Origins of Selective C(sp²)â€“H Activation Using Transition Metal Complexes with N,N-Bidentate Directing Groups: A Combined Theoreticalâ€“Experimental Study. ACS Catalysis, 2014, 4, 649-656.	11.2	51
86	How Electron Flow Controls the Thermochemistry of the Addition of Olefins to Nickel Dithiolenes:Â Predictions by Density Functional Theory. Journal of the American Chemical Society, 2002, 124, 12076-12077.	13.7	48
87	Computational definition of a mixed valent Fe(II)Fe(I) model of the [FeFe]hydrogenase active site resting state. Journal of Inorganic Biochemistry, 2007, 101, 1752-1757.	3.5	48
88	Prediction of the Reactive Intermediates in Alkane Activation by Tris(pyrazolyl borate)rhodium Carbonyl. Journal of Physical Chemistry A, 1998, 102, 1963-1964.	2.5	47
89	A matrix of heterobimetallic complexes for interrogation of hydrogen evolution reaction electrocatalysts. Chemical Science, 2017, 8, 8291-8300.	7.4	47
90	Tuning Reactivity of Bioinspired [NiFe]-Hydrogenase Models by Ligand Design and Modeling the CO Inhibition Process. ACS Catalysis, 2018, 8, 10658-10667.	11.2	47

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91	Comparison of Hartreeâ^'Fock, Density Functional, MÃ¸llerâ^'Plesset Perturbation, Coupled Cluster, and Configuration Interaction Methods for the Migratory Insertion of Nitric Oxide into a Cobaltâ^'Carbon Bond. Journal of Physical Chemistry A, 1997, 101, 1360-1365.	2.5	46
92	What Is Special about Aromaticâ€"Aromatic Interactions? Significant Attraction at Large Horizontal Displacement. ACS Central Science, 2020, 6, 420-425.	11.3	44
93	Photoelectron spectra and molecular orbital calculations on bis(cyclopentadienyldicarbonylchromium, -molybdenum, and -tungsten): nature of the bonding of linear semibridging carbonyls. Journal of the American Chemical Society, 1984, 106, 5079-5083.	13.7	43
94	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 9. Intermolecular versus Intramolecular Carbonâ^'Hydrogen Bond Activation in Zirconium, Rhodium, and Iridium Complexes. Organometallics, 1996, 15, 1889-1897.	2.3	43
95	High-Spin Ni(II), a Surprisingly Good Structural Model for [NiFe] Hydrogenase. Journal of the American Chemical Society, 2002, 124, 394-395.	13.7	43
96	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
97	Understanding the factors affecting the activation of alkane by Cp ^{â€²} Rh(CO) ₂ (Cp ^{â€²} Â=ÂCp or Cp*). Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20178-20183.	7.1	43
98	Determination of copper binding sites in peptides containing basic residues: a combined experimental and theoretical study. International Journal of Mass Spectrometry, 2001, 204, 31-46.	1.5	42
99	Role of aromatic amino acids in amyloid self-assembly. International Journal of Biological Macromolecules, 2020, 156, 949-959.	7.5	42
100	Transition metal polyhydride complexes. 2. Theoretical methods for the determination of stabilities of classical and nonclassical isomers. Journal of the American Chemical Society, 1992, 114, 2928-2932.	13.7	41
101	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
102	The Mechanism of Alkene Addition to a Nickel Bis(dithiolene) Complex: The Role of the Reduced Metal Complex. Journal of the American Chemical Society, 2012, 134, 4481-4484.	13.7	41
103	Transition-metal polyhydride complexes. 3. Relative stabilities of classical and nonclassical isomers. Journal of the American Chemical Society, 1992, 114, 6102-6108.	13.7	40
104	Photoreversible Multiple Additions of Hydrogen to a Highly Unsaturated Platinumâ^'Rhenium Cluster Complex. Journal of the American Chemical Society, 2007, 129, 986-1000.	13.7	40
105	Refining the Active Site Structure of Ironâ^'Iron Hydrogenase Using Computational Infrared Spectroscopy. Inorganic Chemistry, 2008, 47, 2380-2388.	4.0	40
106	Self-Assembly of Dinitrosyl Iron Units into Imidazolate-Edge-Bridged Molecular Squares: Characterization Including MÃ¶ssbauer Spectroscopy. Journal of the American Chemical Society, 2011, 133, 20426-20434.	13.7	40
107	Interplay of hemilability and redox activity in models of hydrogenase active sites. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E9775-E9782.	7.1	40
108	Density functional theory on the larger active site models for [NiFe] hydrogenases: Two-state reactivity?. Comptes Rendus Chimie, 2008, 11, 790-804.	0.5	39

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109	Ambidentate Thiocyanate and Cyanate Ligands in Dinitrosyl Iron Complexes. Inorganic Chemistry, 2013, 52, 2119-2124.	4.0	39
110	Cobalt Pincer Complexes in Catalytic Câ€“H Borylation: The Pincer Ligand Flips Rather Than Dearomatizes. ACS Catalysis, 2018, 8, 10606-10618.	11.2	39
111	Transition Metal Polyhydride Complexes. 10. Intramolecular Hydrogen Exchange in the Octahedral Iridium(III) Dihydrogen Dihydride Complexes IrXH2(Î·2-H2)(PR3)2(X = Cl, Br, I). Journal of the American Chemical Society, 2000, 122, 2903-2910.	13.7	38
112	Theoretical Studies of Inorganic and Organometallic Reaction Mechanisms. 18. Catalytic Transfer Dehydrogenation of Alkanes by an Iridium(III) Pincer Complex. Organometallics, 2001, 20, 2153-2160.	2.3	38
113	Intramolecular Iron-Mediated Câ€“H Bond Heterolysis with an Assist of Pendant Base in a [FeFe]-Hydrogenase Model. Journal of the American Chemical Society, 2014, 136, 16817-16823.	13.7	38
114	Structure and Magnetization Dynamics of Dyâ^'Fe and Dyâ^'Ru Bonded Complexes. Angewandte Chemie - International Edition, 2018, 57, 8144-8148.	13.8	38
115	High energy photoelectron spectroscopy of transition metal complexes. Part 3.â€"Direct measurement and interpretation of the core level shifts between free and complexed CO, and the bonding in some substituted manganese pentacarbonyls. Journal of the Chemical Society, Faraday Transactions 2, 1973, 69, 1677-1684.	1.1	37
116	Problems in the theoretical structure of organometallic molecules: generalized molecular orbital, configuration interaction calculations on ferrocene. Chemical Physics Letters, 1985, 114, 338-342.	2.6	37
117	Small Yttriumâ^'Carbon and Lanthanumâ^'Carbon Clusters:Â Rings Are Most Stable. The Journal of Physical Chemistry, 1996, 100, 18007-18009.	2.9	37
118	Synthesis, Characterization, and Electronic Structures of a Series of Two-Dimensional Trimetallic Cluster Complexes, Ru₃(CO)₉(Î¼-SnPh₂)₃[Pt(PBu^t₃)]_x = 0â^'3. Journal of the American Chemical Society, 2007, 129, 12328-12340.	13.7	37
119	Modeling Structures and Vibrational Frequencies for Dinitrosyl Iron Complexes (DNICs) with Density Functional Theory. Inorganic Chemistry, 2011, 50, 8532-8540.	4.0	37
120	Density Functional Calculations on Protonation of the [FeFe]â€Hydrogenase Model Complex Fe₂(Î¼â€pdt)(CO)₄(PMe₃)₂ and Subsequent Isomerization Pathways. European Journal of Inorganic Chemistry, 2011, 2011, 1080-1093.	2.0	37
121	Computational Studies on Ethylene Addition to Nickel Bis(dithiolene). Journal of Physical Chemistry A, 2012, 116, 476-482.	2.5	37
122	Sulfur Reduction Catalyst Design Inspired by Elemental Periodic Expansion Concept for Lithiumâ€"Sulfur Batteries. ACS Nano, 2022, 16, 6414-6425.	14.6	37
123	Electronic structure of metal clusters. 1. Photoelectron spectra and molecular orbital calculations on alkylidynetricobalt nonacarbonyl clusters. Inorganic Chemistry, 1981, 20, 4419-4425.	4.0	36
124	Cluster synthesisâ€"XXIII. The synthesis, structure and bonding of Fe4(CO)10(Î¼-CO)(Î¼4-S)2. Polyhedron, 1989, 8, 1885-1890.	2.2	36
125	Geometric distortions in four-legged piano-stool cyclopentadienyl transition-metal complexes. Organometallics, 1993, 12, 19-23.	2.3	36
126	Correlation between computed gas-phase and experimentally determined solution-phase infrared spectra: Models of the ironâ€"iron hydrogenase enzyme active site. Journal of Computational Chemistry, 2006, 27, 1454-1462.	3.3	36

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127	[4 + 2] Dimerization and Cycloaddition Reactions of Î±,Î²-Unsaturated Selenoaldehydes and Selenoketones. Journal of Organic Chemistry, 1999, 64, 1565-1575.	3.2	35
128	Density functional theory study of the mechanism for Ni(NHC)2 catalyzed dehydrogenation of ammoniaâ€“borane for chemical hydrogen storage. Journal of Organometallic Chemistry, 2009, 694, 2831-2838.	1.8	35
129	Ortho-Metalation Dynamics and Ligand Fluxionality in the Conversion of Os₃(CO)₁₀(dppm) to HOs₃(CO)₈[Î¼-PhP(C₆H₄-Î¼₂,Î·¹)C₆H₄PPh₂]. Experimental and DFT Evidence for the Participation of Agostic Câ€”H and Î€-Aryl Intermediates at an Intact Triosmium Cluster. Organometallics, 2010, 29, 4041-4057.	2.3	35
130	Linear semibridging carbonyls. 2. Heterobimetallic complexes containing a coordinatively unsaturated late transition metal center. Journal of the American Chemical Society, 1989, 111, 1563-1569.	13.7	34
131	High Nuclearity Iridiumâ€“Platinum Clusters:Â Synthesis, Structures, Bonding, and Reactivity. Journal of the American Chemical Society, 2005, 127, 1007-1014.	13.7	34
132	Density Functional Theory Investigation into the Mechanism for Î·2-Alkyne to Vinylidene Isomerization by the Addition of Phenylacetylene to [(Î·3-C3H5)Rh(PiPr3)2]. Organometallics, 2008, 27, 4325-4333.	2.3	34
133	Invoking Side-Chain Functionality for the Mediation of Regioselectivity during Ring-Opening Polymerization of Glucose Carbonates. Journal of the American Chemical Society, 2020, 142, 16974-16981.	13.7	34
134	Hydride locations and bonding studies in some silyl polyhydride rhenium complexes. Inorganic Chemistry, 1991, 30, 2569-2572.	4.0	33
135	On the Behavior of Î±,Î²-Unsaturated Thioaldehydes and Thioketones in the Dielsâ€“Alder Reaction. Journal of Organic Chemistry, 2000, 65, 6601-6612.	3.2	33
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