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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	Separation, speciation, and mechanism of astatine and bismuth extraction from nitric acid into 1-octanol and methyl anthranilate. Separation and Purification Technology, 2022, 282, 120088.	7.9	10
2	Protonating metal-metal bonds: Changing the metal-metal interaction from bonding, to nonbonding, and to antibonding. Polyhedron, 2022, 212, 115585.	2.2	3
3	Role of High-Spin Species and Pendant Amines in Electrocatalytic Alcohol Oxidation by a Nickel Phosphine Complex. ACS Catalysis, 2022, 12, 2729-2740.	11.2	6
4	Kinetic and Computational Analysis of CO Substitution in a Dinuclear Osmium Carbonyl Complex: Intersection between Dissociative and Dissociative-Interchange Mechanisms. Inorganic Chemistry, 2022, 61, 246-253.	4.0	2
5	Syntheses, Rearrangements, and Structural Analyses of Unsaturated Nitrogen Donor Ligands Derived from Diphenyldiazomethane and the Chiral Rhenium Lewis Acid [(Î·5-C5H5)Re(NO)(PPh3)]+. Dalton Transactions, 2022, , .	3.3	2
6	Sulfur Reduction Catalyst Design Inspired by Elemental Periodic Expansion Concept for Lithiumâ€“Sulfur Batteries. ACS Nano, 2022, 16, 6414-6425.	14.6	37
7	Cooperative redox and spin activity from three redox congeners of sulfur-bridged iron nitrosyl and nickel dithiolene complexes. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	4
8	Platinum(<scp>ii</scp>) alkyl complexes of chelating dibridgehead diphosphines P((CH₂)_n)₃P (n = 14, 18, 22); facile cis/trans isomerizations interconverting gyroscope and parachute like adducts. Dalton Transactions, 2021, 50, 12457-12477.	3.3	4
9	Toward Frameworks with Multiple Aligned and Interactive Fe(CO)₃ Rotators: Syntheses and Structures of Diiron Complexes Linked by Two trans-Diaxial Î±,Ï‰-Diphosphine Ligands Ar₂P(CH₂)_nPAr₂. Inorganic Chemistry, 2021, 60, 3314-3330.	4.0	1
10	Computational Investigation of Dichloromethane Ligand Substitution in the Enantiopure Cation [(Î·⁵-C₅H₅)Re(NO)(PPh₃)(ClCH₂Cl)]⁺, a Functional Equivalent of a Chiral Lewis Acid. Organometallics, 2021, 40, 742-759.	2.3	4
11	Self-Assembled Nickel-4 Supramolecular Squares and Assays for HER Electrocatalysts Derived Therefrom. Inorganic Chemistry, 2021, 60, 7051-7061.	4.0	0
12	Unsupported Lanthanideâ€“Transition Metal Bonds: Ionic vs Polar Covalent?. Inorganic Chemistry, 2021, 60, 9394-9401.	4.0	13
13	Efficient Redox-Neutral Photocatalytic Formate to Carbon Monoxide Conversion Enabled by Long-Range Hot Electron Transfer from Mn-Doped Quantum Dots. Journal of the American Chemical Society, 2021, 143, 10292-10300.	13.7	17
14	Macrocyclic Complexes Derived from Four cisâ€Ł₂Pt Corners and Four Butadiynediyl Linkers; Syntheses, Electronic Structures, and Square versus Skew Rhombus Geometries. Chemistry - A European Journal, 2021, 27, 10021-10039.	3.3	4
15	Frontispiece: Macrocyclic Complexes Derived from Four cisâ€Ł₂Pt Corners and Four Butadiynediyl Linkers; Syntheses, Electronic Structures, and Square versus Skew Rhombus Geometries. Chemistry - A European Journal, 2021, 27, .	3.3	0
16	Syntheses, Structures, Reactivities, and Basicities of Quinolinyl and Isoquinolinyl Complexes of an Electron Rich Chiral Rhenium Fragment and Their Electrophilic Addition Products. Chemistry - A European Journal, 2021, 27, 13399-13417.	3.3	2
17	Nickelâ€“Borolide Complexes and Their Complex Electronic Structure. Inorganic Chemistry, 2021, 60, 16160-16167.	4.0	3
18	Silylation of Pyridine, Picolines, and Quinoline with a Zinc Catalyst. ACS Omega, 2020, 5, 1528-1539.	3.5	8

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19	Full Conformational Analyses of the Ultrafast Isomerization in Penta-coordinated Ru(S2C2(CF3)2)(CO)(PPh3)2: One Compound, Two Crystal Structures, Three CO Frequencies, 24 Stereoisomers, and 48 Transition States. Inorganic Chemistry, 2020, 59, 11757-11769.	4.0	1
20	Controlling Pâ€“C/Câ€“H Bond Cleavage in Nickel Bis(diphosphine) Complexes: Reactivity Scope, Mechanism, and Computations. Organometallics, 2020, 39, 3306-3314.	2.3	5
21	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
22	A computational study of hydrogen bonding motifs in halide, tetrafluoroborate, hexafluorophosphate, and tetraarylborate salts of chiral cationic ruthenium and cobalt guanidinobenzimidazole hydrogen bond donor catalysts; acceptor properties of the â€œBArfâ€•anion. Polyhedron, 2020, 187, 114618.	2.2	11
23	Role of aromatic amino acids in amyloid self-assembly. International Journal of Biological Macromolecules, 2020, 156, 949-959.	7.5	42
24	Astatine partitioning between nitric acid and conventional solvents: indication of covalency in ketone complexation of AtO⁺. Chemical Communications, 2020, 56, 9004-9007.	4.1	13
25	Stacking interactions of resonance-assisted hydrogen-bridged rings and C₆-aromatic rings. Physical Chemistry Chemical Physics, 2020, 22, 13721-13728.	2.8	8
26	Electrocatalytic Hydrogen Evolution and Oxidation with Rhenium Tris(thiolate) Complexes: A Competition between Rhenium and Sulfur for Electrons and Protons. ACS Catalysis, 2020, 10, 3778-3789.	11.2	22
27	What Is Special about Aromaticâ€“Aromatic Interactions? Significant Attraction at Large Horizontal Displacement. ACS Central Science, 2020, 6, 420-425.	11.3	44
28	Computational Investigations of Enantioselection in Carbonâ€“Carbon Bond Forming Reactions of Ruthenium Guanidinobenzimidazole Second Coordination Sphere Hydrogen Bond Donor Catalysts. Organometallics, 2020, 39, 1149-1162.	2.3	19
29	Triisopropylsilyl (TIPS) Alkynes as Building Blocks for Syntheses of Platinum Triisopropylsilylpolyynyl and Diplatinum Polyynediyl Complexes. Organometallics, 2019, 38, 3294-3310.	2.3	13
30	Stacking Interactions of Resonance-Assisted Hydrogen-Bridged Rings. A Systematic Study of Crystal Structures and Quantum-Chemical Calculations. Crystal Growth and Design, 2019, 19, 5619-5628.	3.0	8
31	Photoinduced Terminal Hydride of [FeFe]-Hydrogenase Biomimetic Complexes. Inorganic Chemistry, 2019, 58, 13737-13741.	4.0	5
32	Controlling O₂ Reactivity in Synthetic Analogues of [NiFeS]- and [NiFeSe]-Hydrogenase Active Sites. Journal of the American Chemical Society, 2019, 141, 15338-15347.	13.7	15
33	Oxygen uptake in complexes related to [NiFeS]- and [NiFeSe]-hydrogenase active sites. Chemical Science, 2019, 10, 1368-1373.	7.4	21
34	Influence of chelate ring type on chelateâ€“chelate and chelateâ€“aryl stacking: the case of nickel bis(dithiolene). Physical Chemistry Chemical Physics, 2019, 21, 1198-1206.	2.8	7
35	MÃ¶ssbauer Spectroscopy and Theoretical Studies of Iron Bimetallic Complexes Showing Electrocatalytic Hydrogen Evolution. Inorganic Chemistry, 2019, 58, 7069-7077.	4.0	12
36	Stacking interaction potential energy surfaces of square-planar metal complexes containing chelate rings. Advances in Inorganic Chemistry, 2019, , 159-189.	1.0	4

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37	Theoretical Analysis of Competing Pathways for Carbonâ€“Hydrogen Activation of Cyclopentadienylâ€“Triphenylphosphineâ€“Iridium in Benzene. Inorganic Chemistry, 2019, 58, 16553-16558.	4.0	1
38	Origin of Shielding and Deshielding Effects in NMR Spectra of Organic Conjugated Polyynes. Organic Letters, 2019, 21, 753-757.	4.6	19
39	Study of stacking interactions between two neutral tetrathiafulvalene molecules in Cambridge Structural Database crystal structures and by quantum chemical calculations. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 1-7.	1.1	9
40	Recent computational studies on transitionâ€metal carbonâ€“hydrogen bond activation of alkanes. International Journal of Quantum Chemistry, 2018, 118, e25605.	2.0	4
41	Nickel Fluorocarbene Metathesis with Fluoroalkenes. Angewandte Chemie, 2018, 130, 5874-5878.	2.0	11
42	Nickel Fluorocarbene Metathesis with Fluoroalkenes. Angewandte Chemie - International Edition, 2018, 57, 5772-5776.	13.8	25
43	Influence of metal ion on chelateâ€“aryl stacking interactions. International Journal of Quantum Chemistry, 2018, 118, e25629.	2.0	8
44	Unraveling the Role of a Flexible Tetradentate Ligand in the Aerobic Oxidative Carbonâ€“Carbon Bond Formation with Palladium Complexes: A Computational Mechanistic Study. Journal of the American Chemical Society, 2018, 140, 3929-3939.	13.7	12
45	Probing the Carbonâ€“Hydrogen Activation of Alkanes Following Photolysis of Tpâ€²Rh(CNR)(carbodiimide): A Computational and Time-Resolved Infrared Spectroscopic Study. Journal of the American Chemical Society, 2018, 140, 1842-1854.	13.7	27
46	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
47	Structural and Electronic Responses to the Three Redox Levels of Fe(NO)N₂S₂â€Fe(NO)₂. Chemistry - A European Journal, 2018, 24, 16003-16008.	3.3	13
48	Cobalt Pincer Complexes in Catalytic Câ€“H Borylation: The Pincer Ligand Flips Rather Than Dearomatizes. ACS Catalysis, 2018, 8, 10606-10618.	11.2	39
49	Towards understanding of lanthanideâ€“transition metal bonding: investigations of the first Ceâ€“Fe bonded complex. Chemical Communications, 2018, 54, 10893-10896.	4.1	32
50	Cyanide Docking and Linkage Isomerism in Models for the Artificial [FeFe]-Hydrogenase Maturation Process. Journal of the American Chemical Society, 2018, 140, 9904-9911.	13.7	7
51	Structure and Magnetization Dynamics of Dyâ€'Fe and Dyâ€'Ru Bonded Complexes. Angewandte Chemie, 2018, 130, 8276-8280.	2.0	3
52	Structure and Magnetization Dynamics of Dyâ€'Fe and Dyâ€'Ru Bonded Complexes. Angewandte Chemie - International Edition, 2018, 57, 8144-8148.	13.8	38
53	Stacking of cyclopentadienyl organometallic sandwich and half-sandwich compounds. Strong interactions of sandwiches at large offsets. CrystEngComm, 2018, 20, 4506-4514.	2.6	11
54	Comparisons of MN₂S₂vs. bipyridine as redox-active ligands to manganese and rhenium in (Lâ€“L)Mâ€²(CO)₃Cl complexes. Dalton Transactions, 2017, 46, 5175-5182.	3.3	11

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55	Noncovalent bonding: Stacking interactions of chelate rings of transition metal complexes. Coordination Chemistry Reviews, 2017, 345, 318-341.	18.8	81
56	The Distinctive Electronic Structures of Rhenium Tris(thiolate) Complexes, an Unexpected Contrast to the Valence Isoelectronic Ruthenium Tris(thiolate) Complexes. Inorganic Chemistry, 2017, 56, 583-593.	4.0	12
57	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
58	A matrix of heterobimetallic complexes for interrogation of hydrogen evolution reaction electrocatalysts. Chemical Science, 2017, 8, 8291-8300.	7.4	47
59	Molybdenum Trihydride Complexes: Computational Model of Oxidatively Induced Reductive Elimination of Dihydrogen. Inorganic Chemistry, 2017, 56, 9653-9659.	4.0	2
60	Biomimetics of [NiFe]-Hydrogenase: Nickel- or Iron-Centered Proton Reduction Catalysis?. Journal of the American Chemical Society, 2017, 139, 18065-18070.	13.7	64
61	Unexpected Importance of Aromaticâ€“Aliphatic and Aliphatic Side Chainâ€“Backbone Interactions in the Stability of Amyloids. Chemistry - A European Journal, 2017, 23, 11046-11053.	3.3	12
62	Methane Activations by Titanium Neopentylidene Complexes: Electronic Resilience and Steric Control. Inorganic Chemistry, 2017, 56, 9264-9272.	4.0	7
63	Interactions of Aromatic Residues in Amyloids: A Survey of Protein Data Bank Crystallographic Data. Crystal Growth and Design, 2017, 17, 6353-6362.	3.0	15
64	Flexible Zirconium Metalâ€Organic Frameworks as Bioinspired Switchable Catalysts. Angewandte Chemie - International Edition, 2016, 55, 10776-10780.	13.8	179
65	Cyanide-bridged iron complexes as biomimetics of tri-iron arrangements in maturases of the H cluster of the di-iron hydrogenase. Chemical Science, 2016, 7, 3710-3719.	7.4	20
66	Carbon-hydrogen bond activation by a titanium neopentylidene complex. Journal of Coordination Chemistry, 2016, 69, 1759-1768.	2.2	8
67	Hemilabile Bridging Thiolates as Proton Shuttles in Bioinspired H₂ Production Electrocatalysts. Journal of the American Chemical Society, 2016, 138, 12920-12927.	13.7	78
68	The Rich Structural Chemistry Displayed by the Carbon Monoxide as a Ligand to Metal Complexes. Structure and Bonding, 2016, , 199-248.	1.0	10
69	InnenrÃ¼cktitelbild: Flexible Zirconium Metalâ€Organic Frameworks as Bioinspired Switchable Catalysts (Angew. Chem. 36/2016). Angewandte Chemie, 2016, 128, 11079-11079.	2.0	0
70	Facile Pâˆ'C/Câˆ'H Bondâ€Cleavage Reactivity of Nickel Bis(diphosphine) Complexes. Chemistry - A European Journal, 2016, 22, 9493-9497.	3.3	3
71	The stacking interactions of bipyridine complexes: the influence of the metal ion type on the strength of interactions. Journal of Molecular Modeling, 2016, 22, 30.	1.8	7
72	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

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73	A Reduced 2Fe2S Cluster Probe of Sulfurâ€“Hydrogen versus Sulfurâ€“Gold Interactions. Angewandte Chemie - International Edition, 2015, 54, 11102-11106.	13.8	9
74	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
75	Molybdenum Trihydride Complexes: Computational Determinations of Hydrogen Positions and Rearrangement Mechanisms. Inorganic Chemistry, 2015, 54, 6380-6385.	4.0	6
76	Carbonâ€“Hydrogen Bond Activation in Bis(2,6-dimethylbenzenethiolato)tris(trimethylphosphine)ruthenium(II): Ligand Dances and Solvent Transformations. Organometallics, 2015, 34, 3129-3140.	2.3	4
77	Hostâ€“Guest Behavior of a Heavy-Atom Heterocycle Re4(CO)16(Î¼-SbPh2)2(Î¼-H)2 Obtained from a Palladium-Assisted Ring Opening Dimerization of Re2(CO)8(Î¼-SbPh2)(Î¼-H). Inorganic Chemistry, 2015, 54, 3536-3544.	4.0	6
78	Addition of ethylene to a Ï€-conjugated two-dimensional nickel-based organometallic framework with implications for olefin separation. Journal of Molecular Modeling, 2015, 21, 107.	1.8	9
79	Regioselectivity in Ligand Substitution Reactions on Diiron Complexes Governed by Nucleophilic and Electrophilic Ligand Properties. Inorganic Chemistry, 2015, 54, 3523-3535.	4.0	12
80	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
81	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
82	Understanding the Radical Nature of an Oxidized Ruthenium Tris(thiolate) Complex and Its Role in the Chemistry. Journal of the American Chemical Society, 2015, 137, 15616-15619.	13.7	13
83	Influence of the Density Functional and Basis Set on the Relative Stabilities of Oxygenated Isomers of Diiron Models for the Active Site of [FeFe]-Hydrogenase. Journal of Chemical Theory and Computation, 2015, 11, 205-214.	5.3	13
84	Redox active iron nitrosyl units in proton reduction electrocatalysis. Nature Communications, 2014, 5, 3684.	12.8	58
85	Theoretical investigation on the reaction of HS+ with CH3NH2. Chemical Papers, 2014, 68, .	2.2	2
86	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
87	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
88	Carbonâ€“Hydrogen Activation of Cycloalkanes by Cyclopentadienylcarbonylrhodiumâ€”A Lifetime Enigma. Journal of the American Chemical Society, 2014, 136, 8614-8625.	13.7	32
89	Computational study of the cycloaddition reactivity of the osmium silylyne. Inorganica Chimica Acta, 2014, 422, 40-46.	2.4	3
90	Computational Exploration of Alternative Catalysts for Olefin Purification: Cobalt and Copper Analogues Inspired by Nickel Bis(dithiolene) Electrocatalysis. Inorganic Chemistry, 2014, 53, 9679-9691.	4.0	18

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91	Theoretical investigation on the mechanism of FeCl3-catalysed cross-coupling reaction of alcohols with alkenes. Molecular Physics, 2014, 112, 2107-2113.	1.7	1
92	Uptake of One and Two Molecules of 1,3-Butadiene by Platinum Bis(dithiolene): A Theoretical Study. Inorganic Chemistry, 2014, 53, 9692-9702.	4.0	16
93	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
94	Ambidentate Thiocyanate and Cyanate Ligands in Dinitrosyl Iron Complexes. Inorganic Chemistry, 2013, 52, 2119-2124.	4.0	39
95	Understanding Pdâ€“Pd Bond Length Variation in (PNP)Pdâ€“Pd(PNP) Dimers. Inorganic Chemistry, 2013, 52, 2317-2322.	4.0	15
96	The mechanism of addition of aldehydes to germene in different solvents: A DFT study. Journal of Organometallic Chemistry, 2013, 748, 8-12.	1.8	4
97	Comparative Insight into Electronic Properties and Reactivities toward Câ€“H Bond Activation by Iron(IV)â€“Nitrido, Iron(IV)â€“Oxo, and Iron(IV)â€“Sulfido Complexes: A Theoretical Investigation. Inorganic Chemistry, 2013, 52, 2684-2696.	4.0	23
98	Apparent Anti-Woodwardâ€“Hoffmann Addition to a Nickel Bis(dithiolene) Complex: The Reaction Mechanism Involves Reduced, Dimetallic Intermediates. Inorganic Chemistry, 2013, 52, 3711-3723.	4.0	28
99	A mechanism for the addition of ethylene to nickel bisâ€dithiolene. International Journal of Quantum Chemistry, 2013, 113, 1621-1625.	2.0	12
100	Stacking Interactions of Ni(acac) Chelates with Benzene: Calculated Interaction Energies. ChemPhysChem, 2013, 14, 1797-1800.	2.1	16
101	Carbon Monoxide Induced Reductive Elimination of Disulfide in an N-Heterocyclic Carbene (NHC)/ Thiolate Dinitrosyl Iron Complex (DNIC). Journal of the American Chemical Society, 2013, 135, 8423-8430.	13.7	25
102	Analysis of an alternative to the H-atom abstraction mechanism in methane Câ€“H bond activation by nonheme iron(iv)-oxo oxidants. Dalton Transactions, 2013, 42, 10260.	3.3	15
103	Investigating the Electronic Structure of the Atox1 Copper(I) Transfer Mechanism with Density Functional Theory. Inorganic Chemistry, 2013, 52, 10387-10393.	4.0	6
104	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
105	Measuring the internal energies of species emitted from hypervelocity nanoprojectile impacts on surfaces using recalibrated benzylpyridinium probe ions. Journal of Chemical Physics, 2013, 138, 214301.	3.0	17
106	The effect of the axial ligand on distinct reaction tunneling for methane hydroxylation by nonheme iron(iv)â€“oxo complexes. Physical Chemistry Chemical Physics, 2012, 14, 12863.	2.8	19
107	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
108	Î±-Cleavage of Phenyl Groups from GePh₃Ligands in Iridium Carbonyl Cluster Complexes. A Mechanism and Its Role in the Synthesis of Bridging Germylene Ligands. Organometallics, 2012, 31, 2621-2630.	2.3	14

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109	Bonding and Reactivity in the Electronically Unsaturated Hydrogen-Bridged Dimer [Ru₃(CO)₈(Î¼₃-CMe)(Î¼-H)₂(Î¼₃-H)]₂. Organometallics, 2012, 31, 50-53.	4.0	4
110	Computational Insights into Uranium Complexes Supported by Redox-Active Î±-Diimine Ligands. Inorganic Chemistry, 2012, 51, 2058-2064.	4.0	25
111	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
112	Computational Studies on Ethylene Addition to Nickel Bis(dithiolene). Journal of Physical Chemistry A, 2012, 116, 476-482.	2.5	37
113	Comparison of the FeO²⁺ and FeS²⁺ complexes in the cyanide and isocyanide ligand environment for methane hydroxylation. Journal of Computational Chemistry, 2012, 33, 1448-1457.	3.3	4
114	Diruthenium Naphthalene and Anthracene Complexes Containing a Doubly Linked Dicyclopentadienyl Ligand. Organometallics, 2012, 31, 4838-4848.	2.3	14
115	Combined experimental and theoretical investigation into Câ€“H activation of cyclic alkanes by Cpâ€²Rh(CO)2 (Cpâ€² = Î·5-C5H5 or Î·5-C5Me5). Dalton Transactions, 2011, 40, 1751.	3.3	18
116	cis-Dithiolatonickel as metalloligand to dinitrosyl iron units: the di-metallic structure of Ni(Î¼-SR)[Fe(NO)2] and an unexpected, abbreviated metalloadamantyl cluster, Ni2(Î¼-SR)4[Fe(NO)2]3. Dalton Transactions, 2011, 40, 6047.	3.3	17
117	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
118	Computational Investigation of the Concerted Dismutation of Chlorite Ion by Water-Soluble Iron Porphyrins. Inorganic Chemistry, 2011, 50, 7928-7930.	4.0	19
119	Carbonâ€“Bromine Bond Formation through a Nickel-Centered Spin-Crossing Mechanism. Organometallics, 2011, 30, 6365-6371.	2.3	19
120	Allyl Ligand Reactivity in Tantalum(V) Compounds: Experimental and Computational Evidence for Allyl Transfer to the Formamidinate Ligand in fac-Ta(NMe₂)₃(Î·¹-allyl)[ⁱPrNC(H)NⁱPr] via a Metallo-Claisen Rearrangement. Organometallics, 2011, 30, 5832-5843.	2.3	7
121	Modeling Structures and Vibrational Frequencies for Dinitrosyl Iron Complexes (DNICs) with Density Functional Theory. Inorganic Chemistry, 2011, 50, 8532-8540.	4.0	37
122	Observation of Inductive Effects That Cause a Change in the Rate-Determining Step for the Conversion of Rhenium Azides to Imido Complexes. Inorganic Chemistry, 2011, 50, 10505-10514.	4.0	16
123	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
124	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
125	Computational Investigations into Hydrogen-Atom Abstraction from Rhodium Hydride Complexes by Methyl Radicals in Aqueous Solution. European Journal of Inorganic Chemistry, 2011, 2011, 4901-4905.	2.0	1
126	Theoretical study on the reaction of PH+ with H2O. Computational and Theoretical Chemistry, 2011, 966, 328-333.	2.5	0

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127	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
128	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
129	Oxygen atom transfer catalysis: Ligand effects on the key reaction barrier in molybdenum (VI) dioxo systemsâ˜†. Journal of Molecular Catalysis A, 2010, 324, 15-23.	4.8	11
130	Unexpected Î¼-oxo five-member ring intermediates for oxygen atom transfer between osmium complexes. Journal of Coordination Chemistry, 2010, 63, 2846-2853.	2.2	0
131	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
132	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
133	Thermal Decomposition Pathways of Hydroxylamine: Theoretical Investigation on the Initial Steps. Journal of Physical Chemistry A, 2010, 114, 9262-9269.	2.5	52
134	Crystallographic Evidence of a Base-Free Uranium(IV) Terminal Oxo Species. Inorganic Chemistry, 2010, 49, 7620-7622.	4.0	72
135	Ortho-Metalation Dynamics and Ligand Fluxionality in the Conversion of Os₃(CO)₁₀(dppm) to HOs₃(CO)₈[Î¼-PhP(C₆H₄-Î¼₂,Î·¹)CH₂PPh₂]. Experimental and DFT Evidence for the Participation of Agostic Câ^'H and Ï€-Aryl Intermediates at an Intact Triosmium Cluster. Organometallics, 2010, 29, 4041-4057.	2.8	38
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