Thomas R Cundari

List of Publications by Year
in descending order

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250 papers	10,078 citations	47 h-index	89 g-index
		47006	46799
291 all docs	291 docs citations	291 times ranked	9006 citing authors

#	Article	IF	Citations
1	Effective core potential methods for the lanthanides. Journal of Chemical Physics, 1993, 98, 5555-5565.	3.0	1,155
2	Copperâ€“Nitrene Complexes in Catalytic Cï£¿H Amination. Angewandte Chemie - International Edition, 2008, 47, 9961-9964.	13.8	325
3	Metal Effect on the Supramolecular Structure, Photophysics, and Acidâ^'Base Character of Trinuclear Pyrazolato Coinage Metal Complexesâ€. Inorganic Chemistry, 2005, 44, 8200-8210.	4.0	274
4	Variational Transition State Theory with Multidimensional Tunneling. Reviews in Computational Chemistry, 2007, , 125-232.	1.5	273
5	Applications of Support Vector Machines in Chemistry. Reviews in Computational Chemistry, 2007, , 291-400.	1.5	261
6	Stepwise Reduction of Dinitrogen Bond Order by a Low-Coordinate Iron Complex. Journal of the American Chemical Society, 2001, 123, 9222-9223.	13.7	227
7	The Reactivity Patterns of Low-Coordinate Ironâ^'Hydride Complexes. Journal of the American Chemical Society, 2008, 130, 6624-6638.	13.7	179
8	Computational Studies of Transition Metalâ^'Main Group Multiple Bonding. Chemical Reviews, 2000, 100, 807-818.	47.7	156
9	Catalytic Cï£¿H Amination with Unactivated Amines through Copper(II) Amides. Angewandte Chemie - International Edition, 2010, 49, 8850-8855.	13.8	155
10	Coordination-Number Dependence of Reactivity in an Imidoiron(III) Complex. Angewandte Chemie - International Edition, 2006, 45, 6868-6871.	13.8	143
11	Selectivity and Mechanism of Hydrogen Atom Transfer by an Isolable Imidoiron(III) Complex. Journal of the American Chemical Society, 2011, 133, 9796-9811.	13.7	128
12	Reversible Beta-Hydrogen Elimination of Three-Coordinate Iron(II) Alkyl Complexes:Â Mechanistic and Thermodynamic Studies. Organometallics, 2004, 23, 5226-5239.	2.3	125
13	Câ€“H Functionalization Reactivity of a Nickelâ€“Imide. Journal of the American Chemical Society, 2012, 134, 10114-10121.	13.7	122
14	Ab Initio Quantum Simulation in Solid State Chemistry. Reviews in Computational Chemistry, 2005, , 1-125.	1.5	120
15	A Versatile Tripodal Cu(I) Reagent for Câ€“N Bond Construction via Nitrene-Transfer Chemistry: Catalytic Perspectives and Mechanistic Insights on Câ€“H Aminations/Amidinations and Olefin Aziridinations. Journal of the American Chemical Society, 2014, 136, 11362-11381.	13.7	115
16	Born-Oppenheimer Direct Dynamics Classical Trajectory Simulations. Reviews in Computational Chemistry, 2003, , 79-146.	1.5	108
17	Iron-Catalyzed Homogeneous Hydrogenation of Alkenes under Mild Conditions by a Stepwise, Bifunctional Mechanism. ACS Catalysis, 2016, 6, 2127-2135.	11.2	108
18	Rational Design of Macrometallocyclic Trinuclear Complexes with Superior Ï€-Acidity and Ï€-Basicity. Journal of the American Chemical Society, 2008, 130, 1669-1675.	13.7	107

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19	Carbonâ^'Hydrogen Bond Activation by Titanium Imido Complexes. Computational Evidence for the Role of Alkane Adducts in Selective Câ^'H Activation. Journal of the American Chemical Society, 2002, 124, 1481-1487.	13.7	105
20	Molecular Quantum Similarity: Theory and Applications. Reviews in Computational Chemistry, 2005, , 127-207.	1.5	105
21	Calculation of the Electronic Spectra of Large Molecules. Reviews in Computational Chemistry, 2004, , 153-218.	1.5	102
22	Copper(II) Anilides in sp³ C-H Amination. Journal of the American Chemical Society, 2014, 136, 10930-10940.	13.7	99
23	Inter- and Intramolecular Experimental and Calculated Equilibrium Isotope Effects for (silox)2(tBu3SiND)TiR + RH (silox =tBu3SiO):Â Inferred Kinetic Isotope Effects for RH/D Addition to Transient (silox)2TiNSitBu3. Journal of the American Chemical Society, 2000, 122, 7953-7975.	13.7	98
24	Towards the intrinsic error of the correlation consistent Composite Approach (ccCA). Molecular Physics, 2009, 107, 1107-1121.	1.7	96
25	Accurate thermochemistry for transition metal complexes from first-principles calculations. Journal of Chemical Physics, 2009, 131, 024106.	3.0	95
26	Three-Coordinate Terminal Imidoiron(III) Complexes: Structure, Spectroscopy, and Mechanism of Formation. Inorganic Chemistry, 2010, 49, 6172-6187.	4.0	95
27	Linear-Scaling Methods in Quantum Chemistry. Reviews in Computational Chemistry, 2007, , 1-82.	1.5	94
28	A rhodium catalyst for single-step styrene production from benzene and ethylene. Science, 2015, 348, 421-424.	12.6	94
29	Synthesis and Characterization of the Gold(I) Tris(ethylene) Complex [Au(C₂H₄)₃][SbF₆]. Angewandte Chemie - International Edition, 2008, 47, 556-559.	13.8	92
30	Intertrimer and Intratrimer Metallophilic and Excimeric Bonding in the Ground and Phosphorescent States of Trinuclear Coinage Metal Pyrazolates:Â A Computational Study. Journal of Physical Chemistry A, 2006, 110, 5823-5830.	2.5	87
31	Activation of Carbonâ^'Hydrogen Bonds via 1,2-Addition across Mâ^'X (X = OH or NH2) Bonds of d6Transition Metals as a Potential Key Step in Hydrocarbon Functionalization:Â A Computational Study. Journal of the American Chemical Society, 2007, 129, 13172-13182.	13.7	77
32	Activation of carbonâ€“hydrogen bonds and dihydrogen by 1,2-CH-addition across metalâ€“heteroatom bonds. Dalton Transactions, 2013, 42, 16646.	3.3	76
33	Computational Study of Methane Activation by TpRe(CO)2 and CpRe(CO)2 with a Stereoelectronic Comparison of Cyclopentadienyl and Scorpionate Ligands. Organometallics, 2003, 22, 2331-2337.	2.3	71
34	Effective core potential studies of lanthanide complexes. Journal of Chemical Physics, 1995, 103, 7058-7063.	3.0	70
35	The Poisson-Boltzmann Equation. Reviews in Computational Chemistry, 2003, , 147-365.	1.5	69
36	Unusual Electronic Features and Reactivity of the Dipyridylazaallyl Ligand: Characterizations of (smif)2M [M = Fe, Co, Co+, Ni; smif = {(2-py)CH}2N] and [(TMS)2NFe]2(smif)2. Journal of the American Chemical Society, 2009, 131, 3428-3429.	13.7	68

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37	Spin Crossover during Î²-Hydride Elimination in High-Spin Iron(II)â€“ and Cobalt(II)â€“Alkyl Complexes. Organometallics, 2013, 32, 4741-4751.	2.3	63
38	Copperâ€Catalyzed C(sp³)âˆ’H Amidation: Sterically Driven Primary and Secondary Câˆ’H Siteâ€Selectivity. Angewandte Chemie - International Edition, 2019, 58, 3421-3425.	13.8	61
39	Valence Bond Theory, Its History, Fundamentals, and Applications: A Primer. Reviews in Computational Chemistry, 2004, , 1-100.	1.5	58
40	Experimental and Computational Studies of the Ruthenium-Catalyzed Hydrosilylation of Alkynes: Mechanistic Insights into the Regio- and Stereoselective Formation of Vinylsilanes. Organometallics, 2014, 33, 6937-6944.	2.3	58
41	Bonding and Structure of Copper Nitrenes. Inorganic Chemistry, 2008, 47, 10067-10072.	4.0	56
42	Computational Study of Methane Câˆ’H Activation by First-Row Late Transition Metal L_nMâ•E (M: Fe, Co, Ni) Complexes. Inorganic Chemistry, 2010, 49, 2038-2046.	4.0	56
43	Ligand Lone-Pair Influence on Hydrocarbon Câˆ’H Activation: A Computational Perspective. Organometallics, 2010, 29, 6801-6815.	2.3	53
44	Enantioselective Câ€“H Amination Catalyzed by Nickel Iminyl Complexes Supported by Anionic Bisoxazoline (BOX) Ligands. Journal of the American Chemical Society, 2021, 143, 817-829.	13.7	52
45	Câ€“C Bond Formation and Related Reactions at the CNC Backbone in (smif)FeX (smif =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Hydrogenations and Alkyne Trimerization (X = N(TMS)2, dpma = (Di-(2-pyridyl-methyl)-amide)). Inorganic Chemistry, 2013, 52, 3295-3312.	4.0	51
46	Iridium, Rhodium, and Ruthenium Catalysts for the â€œAldehydeâ€“Water Shiftâ€•Reaction. ACS Catalysis, 2014, 4, 3034-3038.	11.2	50
47	Robust Fuzzy Principal Component Analysis (FPCA). A Comparative Study Concerning Interaction of Carbonâˆ’Hydrogen Bonds with Molybdenumâˆ’Oxo Bonds. Journal of Chemical Information and Computer Sciences, 2002, 42, 1363-1369.	2.8	49
48	Olefin Substitution in (silox)₃M(olefin) (silox = ^tBu₃SiO;) Tj ETQq0 0 0 rgBT /Overlock 10 of the American Chemical Society, 2008, 130, 1183-1196.	13.7	48
49	N-Heterocyclic Carbene Based Nickel and Palladium Complexes: A DFT Comparison of the Mizorokiâ€“Heck Catalytic Cycles. Organometallics, 2016, 35, 3170-3181.	2.3	48
50	Conical Intersections in Molecular Systems. Reviews in Computational Chemistry, 2007, , 83-124.	1.5	47
51	Effective Core Potential Approaches to the Chemistry of the Heavier Elements. Reviews in Computational Chemistry, 2007, , 145-202.	1.5	46
52	Application of the Correlation Consistent Composite Approach (ccCA) to Third-Row (Gaâˆ’Kr) Molecules. Journal of Chemical Theory and Computation, 2008, 4, 328-334.	5.3	46
53	Density functional theory study of palladium-catalyzed aryl-nitrogen and aryl-oxygen bond formation. Journal of Physical Organic Chemistry, 2005, 18, 417-425.	1.9	45
54	Pt^{II}-Catalyzed Ethylene Hydrophenylation: Influence of Dipyridyl Chelate Ring Size on Catalyst Activity and Longevity. ACS Catalysis, 2013, 3, 1165-1171.	11.2	45

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55	Elusive Terminal Copper Arylnitrene Intermediates. Angewandte Chemie - International Edition, 2017, 56, 6426-6430.	13.8	45
56	Methane Activation by Group VB Bis(imido) Complexes. Organometallics, 1994, 13, 2987-2994.	2.3	44
57	CO₂-Formatics: How Do Proteins Bind Carbon Dioxide?. Journal of Chemical Information and Modeling, 2009, 49, 2111-2115.	5.4	44
58	Carbonâ€“Oxygen Bond Formation via Organometallic Baeyerâ€“Villiger Transformations: A Computational Study on the Impact of Metal Identity. Journal of the American Chemical Society, 2012, 134, 2332-2339.	13.7	44
59	Oxyfunctionalization with Cp*Ir^{III}(NHC)(Me)(Cl) with O₂: Identification of a Rare Bimetallic Ir^{IV} Î¼-Oxo Intermediate. Journal of the American Chemical Society, 2015, 137, 3574-3584.	13.7	44
60	Reactivity of Hydrogen on and in Nanostructured Molybdenum Nitride: Crotonaldehyde Hydrogenation. ACS Catalysis, 2016, 6, 5797-5806.	11.2	44
61	PM3(tm) parameterization using genetic algorithms. International Journal of Quantum Chemistry, 2000, 77, 421-432.	2.0	43
62	Methane activation by d0 and d2 imidos: effects of d orbital occupation and comparison of [2 + 2] and oxidative addition. Organometallics, 1993, 12, 4971-4978.	2.3	42
63	Single-Electron Oxidation of Monomeric Copper(I) Alkyl Complexes:â€‰ Evidence for Reductive Elimination through Bimolecular Formation of Alkanes. Organometallics, 2006, 25, 4097-4104.	2.3	42
64	Rare Examples of Fe(IV) Alkyl-Imide Migratory Insertions: Impact of Feâ€”C Covalency in (Me₂IPr)Fe(â•NAd)R₂ (R = ^{neo}Pe, 1-nor). Journal of the American Chemical Society, 2017, 139, 12145-12148.	13.7	42
65	Methane activation by tris(imido) complexes: the effect of metal, ligand and d orbital occupation. Journal of Organometallic Chemistry, 1995, 504, 1-13.	1.8	40
66	Asymmetric Ring-Opening of Donorâ€“Acceptor Cyclopropanes with Primary Arylamines Catalyzed by a Chiral Heterobimetallic Catalyst. ACS Catalysis, 2019, 9, 8285-8293.	11.2	40
67	Iron and Chromium Complexes Containing Tridentate Chelates Based on Nacnac and Imino- and Methyl-Pyridine Components: Triggering Câ€”X Bond Formation. Inorganic Chemistry, 2014, 53, 7467-7484.	4.0	39
68	Redox non-innocence permits catalytic nitrene carbonylation by (dadi)Tiî€•NAd (Ad = adamantyl). Chemical Science, 2017, 8, 3410-3418.	7.4	39
69	Development of Computational Models for Enzymes, Transporters, Channels, and Receptors Relevant to ADME/Tox. Reviews in Computational Chemistry, 2004, , 333-415.	1.5	38
70	A Dinitrogen Dicopper(I) Complex via a Mixedâ€Valence Dicopper Hydride. Angewandte Chemie - International Edition, 2016, 55, 9927-9931.	13.8	38
71	Hydrophenylation of ethylene using a cationic Ru(<scp>ii</scp>) catalyst: comparison to a neutral Ru(<scp>ii</scp>) catalyst. Chemical Science, 2014, 5, 4355-4366.	7.4	37
72	Nitrene Insertion into Cï£¿C and Cï£¿H Bonds of Diamide Diimine Ligands Ligated to Chromium and Iron. Angewandte Chemie - International Edition, 2015, 54, 14407-14411.	13.8	37

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73	Biomolecular Applications of Poisson-Boltzmann Methods. Reviews in Computational Chemistry, 2005, , 349-379.	1.5	36
74	Synthetic Approaches to (smif)₂Ti (smif = 1,3-di-(2-pyridyl)-2-azaallyl) Reveal Redox Non-Innocence and Câ€“C Bond-Formation. Inorganic Chemistry, 2012, 51, 8177-8186.	4.0	36
75	Use of [SbF₆]^{â^'} to Isolate Cationic Copper and Silver Adducts with More than One Ethylene on the Metal Center. Organometallics, 2013, 32, 3034-3041.	2.3	36
76	Pt^{II}-Catalyzed Hydrophenylation of Î±-Olefins: Variation of Linear/Branched Products as a Function of Ligand Donor Ability. ACS Catalysis, 2014, 4, 1607-1615.	11.2	36
77	Mechanistic Studies of Single-Step Styrene Production Using a Rhodium(I) Catalyst. Journal of the American Chemical Society, 2017, 139, 1485-1498.	13.7	36
78	Comparative Nitrene-Transfer Chemistry to Olefinic Substrates Mediated by a Library of Anionic Mn(II) Triphenylamido-Amine Reagents and M(II) Congeners (M = Fe, Co, Ni) Favoring Aromatic over Aliphatic Alkenes. ACS Catalysis, 2018, 8, 9183-9206.	11.2	36
79	Methane adducts of d0 transition metal imido complexes. Organometallics, 1993, 12, 1998-2000.	2.3	34
80	Decomposition Pathways for a Model TiN Chemical Vapor Deposition Precursor. Chemistry of Materials, 1996, 8, 189-196.	6.7	34
81	Enumerating Molecules. Reviews in Computational Chemistry, 2005, , 209-286.	1.5	34
82	The Mechanism of Nâ€“N Double Bond Cleavage by an Iron(II) Hydride Complex. Journal of the American Chemical Society, 2016, 138, 12112-12123.	13.7	34
83	Three-Coordinate Copper(II) Aryls: Key Intermediates in Câ€“O Bond Formation. Journal of the American Chemical Society, 2017, 139, 9112-9115.	13.7	34
84	Catalytic Tuning of a Phosphinoethane Ligand for Enhanced Câ^'H Activation. Journal of the American Chemical Society, 2008, 130, 13051-13058.	13.7	33
85	Mechanism of Hydrogenolysis of an Iridiumâ€“Methyl Bond: Evidence for a Methane Complex Intermediate. Journal of the American Chemical Society, 2013, 135, 1217-1220.	13.7	33
86	Understanding the Effect of Ancillary Ligands on Concerted Metalationâ€“Deprotonation by (^{dm}Phebox)Ir(OAc)₂(H₂O) Complexes: A DFT Study. Organometallics, 2014, 33, 6413-6419.	2.3	33
87	Kinetics of Substitution of Weakly Coordinating Nitrate by Chloride in (Î·5-Cp)Ru(CO)(ER3)ONO2(ER3=) Tj ETQq1 1 0.784314 rgBT /O 2270-2279.	2.3	32
88	Molecular and Electronic Structure of Cyclic Trinuclear Gold(I) Carbeniate Complexes: Insights for Structure/Luminescence/Conductivity Relationships. Inorganic Chemistry, 2014, 53, 7485-7499.	4.0	32
89	Activation of Carbonâ^'Hydrogen and Hydrogenâ^'Hydrogen Bonds by Copperâ^'Nitrenes: A Comparison of Density Functional Theory with Single- and Multireference Correlation Consistent Composite Approaches. Journal of Chemical Theory and Computation, 2009, 5, 2959-2966.	5.3	31
90	Modified embedded atom method study of the mechanical properties of carbon nanotube reinforced nickel composites. Physical Review B, 2010, 81, .	3.2	31

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91	Synthesis and Characterization of (smif)₂Mⁿ(n= 0, M = V, Cr, Mn,) Tj ETQq1 1 0.784314 rgBT /(2011, 50, 12414-12436.	4.0	29
92	Reductive Elimination of Alkylamines from Low-Valent, Alkylpalladium(II) Amido Complexes. Journal of the American Chemical Society, 2012, 134, 15281-15284.	13.7	28
93	Mechanistic Study of Oxy Insertion into Nickelâ€“Carbon Bonds with Nitrous Oxide. Organometallics, 2012, 31, 4998-5004.	2.3	28
94	Structural Analysis of Transition Metal Î²-X Substituent Interactions. Toward the Use of Soft Computing Methods for Catalyst Modeling. Journal of Chemical Information and Computer Sciences, 2000, 40, 1052-1061.	2.8	27
95	A quantum mechanics/molecular mechanics study of the steric influence of the PR3 spectator ligands on the energetics of ethylene insertion into the Rhâ€“H bond of HRh(PR3)2(CO)(Î·2-CH2î€†CH2). New Journal of Chemistry, 2002, 26, 129-135.	2.8	27
96	Ruthenium(II)-Mediated Carbonâ^'Carbon Bond Formation between Acetonitrile and Pyrrole:Â Combined Experimental and Computational Study. Organometallics, 2005, 24, 5015-5024.	2.3	27
97	Computational study of methane activation by mercury(II) complexes. Journal of Computational Chemistry, 1998, 19, 902-911.	3.3	26
98	Modeling Nonlinear Optical Properties of Transition Metal Complexes. Basis Set, Effective Core Potential, and Geometry Effects. Journal of Physical Chemistry A, 1998, 102, 2962-2966.	2.5	26
99	Molecular Modeling of Vanadiumâ^'Oxo Complexes. A Comparison of Quantum and Classical Methods. Journal of Physical Chemistry A, 1998, 102, 997-1004.	2.5	26
100	Reductive functionalization of a rhodium(iii)â€“methyl bond by electronic modification of the supporting ligand. Dalton Transactions, 2014, 43, 8273.	3.3	26
101	DFT and QSAR Studies of Ethylene Polymerization by Zirconocene Catalysts. ACS Catalysis, 2019, 9, 9339-9349.	11.2	25
102	Well-Defined Copper(I) Amido Complex and Aryl Iodides Reacting to Form Aryl Amines. Organometallics, 2011, 30, 55-57.	2.3	24
103	Zinc(II)-Mediated Carbene Insertion into Câ€“H Bonds in Alkanes. Inorganic Chemistry, 2015, 54, 11043-11045.	4.0	24
104	Conversions of Ruthenium(III) Alkyl Complexes to Ruthenium(II) through Ruâ^'Calkyl Bond Homolysis. Organometallics, 2005, 24, 1301-1305.	2.3	23
105	Câ€“H Activation by Multiply Bonded Complexes with Potentially Noninnocent Ligands: A Computational Study. Inorganic Chemistry, 2013, 52, 8106-8113.	4.0	23
106	An Uncanny Dehydrogenation Mechanism: Polar Bond Control over Stepwise or Concerted Transition States. Inorganic Chemistry, 2017, 56, 5519-5524.	4.0	23
107	Intramolecular Câ€“H Functionalization Followed by a [2_{Ïƒ} + 2_{Ï€}] Addition via an Intermediate Nickelâ€“Nitridyl Complex. Inorganic Chemistry, 2019, 58, 7131-7135.	4.0	23
108	Olefin Insertion and Subsequent Î²-X Elimination from a Pentacoordinate Tantalum Complex. A Density Functional Theory Study. Organometallics, 2003, 22, 4047-4059.	2.3	22

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109	Câ€“H Bond Activation of Methane by Pt^{II}â€“N-Heterocyclic Carbene Complexes. The Importance of Having the Ligands in the Right Place at the Right Time. Organometallics, 2012, 31, 1042-1048.	2.3	22
110	Transition Metal Mediated Câ€“H Activation and Functionalization: The Role of Poly(pyrazolyl)borate and Poly(pyrazolyl)alkane Ligands. European Journal of Inorganic Chemistry, 2016, 2016, 2296-2311.	2.0	22
111	Heterobimetallic Silverâ€“Iron Complexes Involving Fe(CO)5 Ligands. Journal of the American Chemical Society, 2017, 139, 14292-14301.	13.7	22
112	Synthesis, Photophysical Properties, and Computational Analysis of Di- and Tetranuclear Alkyne Complexes of Copper(I) Supported by a Highly Fluorinated Pyrazolate. Organometallics, 2018, 37, 4105-4118.	2.3	22
113	Reductive Elimination from Phosphine-Ligated Alkylpalladium(II) Amido Complexes To Form sp³ Carbonâ€“Nitrogen Bonds. Journal of the American Chemical Society, 2018, 140, 4893-4904.	13.7	21
114	Elimination and Activation of Methane and Larger Hydrocarbons. The Journal of Physical Chemistry, 1996, 100, 6475-6483.	2.9	20
115	Variable Selection-Spoilt for Choice?. Reviews in Computational Chemistry, 2005, , 287-348.	1.5	20
116	The Simulation of Ionic Charge Transport in Biological Ion Channels: An Introduction to Numerical Methods. Reviews in Computational Chemistry, 2006, , 229-293.	1.5	20
117	Coinage Metalâ^'Ethylene Complexes Supported by Tris(pyrazolyl)borates: A Computational Study. Organometallics, 2009, 28, 1826-1831.	2.3	20
118	Complete methane-to-methanol catalytic cycle: A DFT study of oxygen atom transfer from N2O to late-row (MNi, Cu, Zn) Î²-diketiminate CH activation catalysts. Polyhedron, 2013, 52, 945-956.	2.2	20
119	Iron Complexes Derived from {nacnac-(CH2py)2}â^' and {nacnac-(CH2py)(CHpy)}n Ligands: Stabilization of Iron(II) via Redox Noninnocence. Inorganic Chemistry, 2014, 53, 4459-4474.	4.0	20
120	Computational Mechanistic Study of Electro-Oxidation of Ammonia to N₂ by Homogenous Ruthenium and Iron Complexes. Journal of Physical Chemistry A, 2019, 123, 7973-7982.	2.5	20
121	Fuzzy Soft-Computing Methods and Their Applications in Chemistry. Reviews in Computational Chemistry, 2004, , 249-331.	1.5	19
122	Comparative Protein Modeling. Reviews in Computational Chemistry, 2006, , 57-167.	1.5	19
123	Computational study of carbonâ€“hydrogen bond deprotonation by alkali metal superbases. Computational and Theoretical Chemistry, 2013, 1019, 85-93.	2.5	19
124	DFT Modeling of the Aldehydeâ€“Water Shift Reaction with a Cationic Cp*Ir Catalyst. ACS Catalysis, 2015, 5, 225-232.	11.2	19
125	Computational Study of Methane Câ€“H Activation by Diiminopyridine Nitride/Nitridyl Complexes of 3d Transition Metals and Main-Group Elements. Inorganic Chemistry, 2018, 57, 6807-6815.	4.0	19
126	Formal oxo- and aza-[3 + 2] reactions of Î±-enaminones and quinones: a double divergent process and the roles of chiral phosphoric acid and molecular sieves. Chemical Science, 2020, 11, 9386-9394.	7.4	19

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127	Theoretical Estimation of Vibrational Frequencies Involving Transition Metal Compounds. Journal of Physical Chemistry A, 1997, 101, 5783-5788.	2.5	18
128	Novel transition metal multiple bondingâ€"myth or reality?. Inorganica Chimica Acta, 2003, 345, 70-80.	2.4	18
129	Computational study of methane functionalization by a multiply bonded, Ni-bis(phosphine) complex. Journal of Organometallic Chemistry, 2007, 692, 4551-4559.	1.8	18
130	A Computational Study of Metal-Mediated Decomposition of Nitrene Transfer Reagents. Journal of Organic Chemistry, 2009, 74, 5711-5714.	3.2	18
131	First-Row Transition Metal and Lithium Pyridine-ene-amide Complexes Exhibiting N- and C-Isomers and Ligand-Based Activation of Benzylic Câ€"H Bonds. Organometallics, 2015, 34, 4656-4668.	2.3	18
132	Solvent-Dependent Thermochemistry of an Iridium/Ruthenium H₂ Evolution Catalyst. Inorganic Chemistry, 2016, 55, 12042-12051.	4.0	18
133	Control of Câ€"H Bond Activation by Mo-Oxo Complexes: pK_a or Bond Dissociation Free Energy (BDFE)?. Inorganic Chemistry, 2017, 56, 12319-12327.	4.0	18
134	Computational Assessment of Counterion Effect of Borate Anions on Ethylene Polymerization by Zirconocene and Hafnocene Catalysts. Organometallics, 2020, 39, 2068-2079.	2.3	18
135	Selective Extraction of N₂ from Air by Diarylimine Iron Complexes. Journal of the American Chemical Society, 2013, 135, 3511-3527.	13.7	17
136	Methane Câ€"H Activation via 3d Metal Methoxide Complexes with Potentially Redox-Noninnocent Pincer Ligands: A Density Functional Theory Study. Inorganic Chemistry, 2017, 56, 12282-12290.	4.0	17
137	Aqueous Hydricity from Calculations of Reduction Potential and Acidity in Water. Journal of Physical Chemistry B, 2016, 120, 12911-12919.	2.6	16
138	Molecular Modeling of Vanadium Peroxides. Inorganic Chemistry, 1997, 36, 4029-4034.	4.0	15
139	Electronic and Charge-Transport Properties of the Au₃(CH₃Nâ•COCH₃)₃ Crystal: A Density Functional Theory Study. Journal of Physical Chemistry Letters, 2013, 4, 2186-2189.	4.6	15
140	Theoretical Study of Reductive Functionalization of Methyl Ligands of Group 9 Complexes Supported by Two Bipyridyl Ligands: A Key Step in Catalytic Hydrocarbon Functionalization. Organometallics, 2014, 33, 1936-1944.	2.3	15
141	Oxidative Hydrophenylation of Ethylene Using a Cationic Ru(II) Catalyst: Styrene Production with Ethylene as the Oxidant. Israel Journal of Chemistry, 2017, 57, 1037-1046.	2.3	15
142	Dispersion forces play a role in (Me₂IPr)Fe(î€NAd)R₂ (Ad = adamantyl; R =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Transactions, 2018, 47, 6025-6030.	3.3	15
143	Copperâ€Catalyzed C(sp³)âˆ'H Amidation: Sterically Driven Primary and Secondary Câˆ'H Siteâ€Selectivity. Angewandte Chemie, 2019, 131, 3459-3463.	2.0	15
144	A Pd^{III} Sulfate Dimer Initiates Rapid Methane Monofunctionalization by H Atom Abstraction. ACS Catalysis, 2020, 10, 14782-14792.	11.2	15

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145	Protein Structure Classification. Reviews in Computational Chemistry, 2006, , 1-55.	1.5	14
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