Thomas R Cundari

List of Publications by Year
in descending order

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250	10,078	53939	53065
papers	citations	47 h-index	89 g-index

291	291	291	10101
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Olefin oligomerization by zirconium boratabenzene catalysts. Journal of Organometallic Chemistry, 2022, 962, 122268.	0.8	0
2	Electrocatalytic Reduction of Nitrogen to Ammonia: the Roles of Lattice O and N in Reduction at Vanadium Oxynitride Surfaces. ACS Applied Materials & Interfaces, 2022, 14, 531-542.	4.0	14
3	Copper(III) Metallacyclopentadienes via Zirconocene Transfer and Reductive Elimination to an Isolable Phenanthrocyclobutadiene. Journal of the American Chemical Society, 2022, 144, 9853-9858.	6.6	8
4	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.	6.6	52
5	Thermochemistry of Tungstenâ€”3p Elements for Density Functional Theory, Caveat Lector!. Journal of Physical Chemistry A, 2021, 125, 681-690.	1.1	0
6	Communicationâ€”Electrochemical Reduction of N₂ to Ammonia by Vanadium Oxide Thin Films at Neutral pH: Oxophilicity and the NRR Reaction. Journal of the Electrochemical Society, 2021, 168, 026504.	1.3	10
7	A Dicopper Nitrenoid by Oxidation of a CuICuI Core: Synthesis, Electronic Structure, and Reactivity. Journal of the American Chemical Society, 2021, 143, 7135-7143.	6.6	5
8	Bifunctional activation of methane by bioinspired transition metal complexes. A simple methane protease model. Computational and Theoretical Chemistry, 2021, 1198, 113180.	1.1	0
9	Is the Electrophilicity of the Metal Nitrene the Sole Predictor of Metal-Mediated Nitrene Transfer to Olefins? Secondary Contributing Factors as Revealed by a Library of High-Spin Co(II) Reagents. Organometallics, 2021, 40, 1974-1996.	1.1	8
10	DFT and TDDFT Study of the Reaction Pathway for Double Intramolecular Câ€“H Activation and Functionalization by Iron, Cobalt, and Nickelâ€“Nitridyl Complexes. Inorganic Chemistry, 2021, 60, 12299-12308.	1.9	5
11	Investigating the non-classical M-H2 bonding in OsClH3(PPh3)3. Journal of Alloys and Compounds, 2021, 894, 162445.	2.8	1
12	Reversible Câ€“C Bond Formation, Halide Abstraction, and Electromers in Complexes of Iron Containing Redox-Noninnocent Pyridine-imine Ligands. Inorganic Chemistry, 2021, 60, 18662-18673.	1.9	6
13	Synthesis, characterization, DFT calculations, and reactivity study of a nitrido-bridged dimeric vanadium(<scp>iv</scp>) complex. Dalton Transactions, 2020, 49, 1200-1206.	1.6	6
14	A Pd^{III} Sulfate Dimer Initiates Rapid Methane Monofunctionalization by H Atom Abstraction. ACS Catalysis, 2020, 10, 14782-14792.	5.5	15
15	Computational Determination of pK_a(Câ€“H) in 3d Transition Metal-Methyl Complexes. Organometallics, 2020, 39, 2803-2812.	1.1	3
16	Computational investigations of NHC-backbone configurations for applications in organocatalytic umpolung reactions. Organic and Biomolecular Chemistry, 2020, 18, 7437-7447.	1.5	3
17	Au₃-to-Ag₃coordinate-covalent bonding and other supramolecular interactions with covalent bonding strength. Chemical Science, 2020, 11, 11179-11188.	3.7	12
18	Metal and Ligand Effects on Coordinated Methane pK_a: Direct Correlation with the Methane Activation Barrier. Journal of Physical Chemistry A, 2020, 124, 7283-7289.	1.1	4

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19	Density Functional Study of Methane Activation by Frustrated Lewis Pairs with Group 13 Trihalides and Group 15 Pentahalides and a Machine Learning Analysis of Their Barrier Heights. Journal of Chemical Information and Modeling, 2020, 60, 4958-4966.	2.5	10
20	A family of structural and functional models for the active site of a unique dioxygenase: Acireductone dioxygenase (ARD). Journal of Inorganic Biochemistry, 2020, 212, 111253.	1.5	1
21	DFT Calculations Investigate Competing Pathways to Form Dimeric Neopentylpalladium(II) Amido Complexes: The Critical Importance of Dispersion. Journal of Physical Chemistry A, 2020, 124, 8798-8805.	1.1	0
22	Computational Assessment of Counterion Effect of Borate Anions on Ethylene Polymerization by Zirconocene and Hafnocene Catalysts. Organometallics, 2020, 39, 2068-2079.	1.1	18
23	Computational Study of Methane Câ€“H Activation by Main Group and Mixed Main Groupâ€“Transition Metal Complexes. Molecules, 2020, 25, 2794.	1.7	2
24	Unrealized concepts of masked alkylidenes in (PNP)FeXY systems and alternative approaches to LnXmFe(IV)=CHR. Polyhedron, 2020, 181, 114460.	1.0	6
25	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.	3.7	19
26	Revealing a Decisive Role for Secondary Coordination Sphere Nucleophiles on Methane Activation. Journal of the American Chemical Society, 2020, 142, 3125-3131.	6.6	7
27	Chemical and electronic structures of cobalt oxynitride films deposited by NH₃vs. N₂ plasma: theory vs. experiment. Physical Chemistry Chemical Physics, 2020, 22, 24640-24648.	1.3	6
28	Nitrene Insertion into Aromatic and Benzylic Câˆ’H Bonds Catalyzed by Copper Complexes of Fluorinated Bisâ€•and Tris(pyrazolyl)borates. ChemCatChem, 2019, 11, 4966-4973.	1.8	7
29	Asymmetric Ring-Opening of Donorâ€“Acceptor Cyclopropanes with Primary Arylamines Catalyzed by a Chiral Heterobimetallic Catalyst. ACS Catalysis, 2019, 9, 8285-8293.	5.5	40
30	Experimental and Computational Investigation of the Aerobic Oxidation of a Late Transition Metal-Hydride. Journal of the American Chemical Society, 2019, 141, 10830-10843.	6.6	14
31	Importance of Nitrogenâ€“Hydrogen Bond pK_a in the Catalytic Coupling of Alkenes and Amines by Amidate Tantalum Complexes: A Computational Study. Journal of Physical Chemistry A, 2019, 123, 8595-8606.	1.1	4
32	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.	1.1	20
33	Effect of Appended S-Block Metal Ion Crown Ethers on Redox Properties and Catalytic Activity of Mnâ€“Nitride Schiff Base Complexes: Methane Activation. Inorganic Chemistry, 2019, 58, 12254-12263.	1.9	9
34	DFT and QSAR Studies of Ethylene Polymerization by Zirconocene Catalysts. ACS Catalysis, 2019, 9, 9339-9349.	5.5	25
35	Computational Analysis of Proton-Coupled Electron Transfer in Hydrotris(triazolyl)borate Midâ€“Late 3d and 4d Transition Metal Complexes. Organometallics, 2019, 38, 3521-3531.	1.1	3
36	Copperâ€Catalyzed C(sp³)âˆ’H Amidation: Sterically Driven Primary and Secondary Câˆ’H Siteâ€Selectivity. Angewandte Chemie - International Edition, 2019, 58, 3421-3425.	7.2	61

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37	Copperâ€Catalyzed C(sp³)â^'H Amidation: Sterically Driven Primary and Secondary Câ^'H Siteâ€Selectivity. Angewandte Chemie, 2019, 131, 3459-3463.	1.6	15
38	Direct Anti-Markovnikov Addition of Water to Olefin To Synthesize Primary Alcohols: A Theoretical Study. Journal of Physical Chemistry A, 2019, 123, 958-965.	1.1	11
39	Tungstenâ€"Ligand Bond Strengths for 2p Elements Including Ïƒ- and Ï€-Bond Strength Components, A Density Functional Theory and ab Initio Study. Journal of Physical Chemistry A, 2019, 123, 7940-7949.	1.1	2
40	Intramolecular Câ€"H Functionalization Followed by a [2_{Ïƒ} + 2_{Ï€}] Addition via an Intermediate Nickelâ€"Nitridyl Complex. Inorganic Chemistry, 2019, 58, 7131-7135.	1.9	23
41	Oxidative Additions to Ti(IV) in [(dadi)^{4â€"}]Ti^{IV}(THF) Involve Carbonâ€"Carbon Bond Formation and Redox-Noninnocent Behavior. Organometallics, 2019, 38, 1502-1515.	1.1	7
42	Computational Study of 3d Metals and Their Influence on the Acidity of Methane Câ€"H Bonds. ACS Omega, 2019, 4, 20159-20163.	1.6	11
43	Genetic Mutations in the S-loop of Human Glutathione Synthetase: Links Between Substrate Binding, Active Site Structure and Allostery. Computational and Structural Biotechnology Journal, 2019, 17, 31-38.	1.9	7
44	Carbon(sp3)-nitrogen bond-forming reductive elimination from phosphine-ligated alkylpalladium(II) amide complexes: A DFT study. Tetrahedron, 2019, 75, 137-143.	1.0	5
45	Cooperative Metal + Ligand Oxidative Addition and Ïƒ-Bond Metathesis: A DFT Study. Organometallics, 2018, 37, 309-313.	1.1	5
46	DFT study of substituent effects in the hydroxylation of methane and toluene mediated by an ethylbenzene dehydrogenase active site model. Journal of Organometallic Chemistry, 2018, 864, 44-49.	0.8	9
47	Dispersion forces play a role in (Me₂IPr)Fe(î€NAd)R₂ (Ad = adamantyl; R =) Tj ETQq1 1 0.784314 rgBT /Ove Transactions, 2018, 47, 6025-6030.	1.6	15
48	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.	6.6	21
49	H₂ addition to (^{Me4}PCP)Ir(CO): studies of the isomerization mechanism. Dalton Transactions, 2018, 47, 16119-16125.	1.6	9
50	Reductive Elimination to Form C(sp³)â€"N Bonds from Palladium(II) Primary Alkyl Complexes. Organometallics, 2018, 37, 3243-3247.	1.1	12
51	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.	1.1	22
52	Câ€"H Activation of Methane by Nickelâ€"Methoxide Complexes: A Density Functional Theory Study. Organometallics, 2018, 37, 3111-3121.	1.1	12
53	Computational study of acetylene hydration by bio-inspired group six catalyst models. Polyhedron, 2018, 154, 114-122.	1.0	9
54	Complexes of [(dadi)Ti(L/X)]^m That Reveal Redox Non-Innocence and a Stepwise Carbene Insertion into a Carbonâ€"Carbon Bond. Organometallics, 2018, 37, 3488-3501.	1.1	13

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55	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.	5.5	36
56	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.	1.9	19
57	Mechanistic Studies of Single-Step Styrene Production Using a Rhodium(I) Catalyst. Journal of the American Chemical Society, 2017, 139, 1485-1498.	6.6	36
58	5d Metal(IV) Imide Complexes. The Impact (or Lack Thereof) of d-Orbital Occupation on Methane Activation and Functionalization. Inorganic Chemistry, 2017, 56, 1823-1829.	1.9	7
59	Redox non-innocence permits catalytic nitrene carbonylation by (dadi)Tiî€NAd (Ad = adamantyl). Chemical Science, 2017, 8, 3410-3418.	3.7	39
60	Elusive Terminal Copper Arylnitrene Intermediates. Angewandte Chemie - International Edition, 2017, 56, 6426-6430.	7.2	45
61	An Uncanny Dehydrogenation Mechanism: Polar Bond Control over Stepwise or Concerted Transition States. Inorganic Chemistry, 2017, 56, 5519-5524.	1.9	23
62	Three-Coordinate Copper(II) Aryls: Key Intermediates in Câ€“O Bond Formation. Journal of the American Chemical Society, 2017, 139, 9112-9115.	6.6	34
63	Elusive Terminal Copper Arylnitrene Intermediates. Angewandte Chemie, 2017, 129, 6526-6530.	1.6	11
64	Computational Study of Methane Câ€“H Activation by Earth-Abundant Metal Amide/Aminyl Complexes. Organometallics, 2017, 36, 3987-3994.	1.1	5
65	A DFT Survey of the Effects of dâ€Electron Count and Metal Identity on the Activation and Functionalization of Câ^'H Bonds for Mid to Late Transition Metals. Israel Journal of Chemistry, 2017, 57, 1023-1031.	1.0	7
66	Control of Câ€“H Bond Activation by Mo-Oxo Complexes: pK_a or Bond Dissociation Free Energy (BDFE)?. Inorganic Chemistry, 2017, 56, 12319-12327.	1.9	18
67	Heterobimetallic Silverâ€“Iron Complexes Involving Fe(CO)5 Ligands. Journal of the American Chemical Society, 2017, 139, 14292-14301.	6.6	22
68	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.	1.9	17
69	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.	6.6	42
70	Heterolytic Hâ€“H and Hâ€“B Bond Cleavage Reactions of {(IPr)Ni(Î¼-S)}₂. Inorganic Chemistry, 2017, 56, 9922-9930.	1.9	12
71	Computational Analysis of Transition Metal-Terminal Boride Complexes. Journal of Physical Chemistry A, 2017, 121, 9358-9368.	1.1	6
72	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.	1.0	15

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73	Toward a More Rational Design of the Direct Synthesis of Aniline: A Density Functional Theory Study. ACS Omega, 2017, 2, 3214-3227.	1.6	1
74	Comparison of PdII vs RhI-catalyzed catalytic cycle for single step styrene production. Computational and Theoretical Chemistry, 2017, 1115, 313-322.	1.1	3
75	Effect of Ancillary Ligands (A) on Oxidative Addition of CH₄ to Rhenium(III) Complexes: A = B, Al, CH, SiH, N, and P Using MP2, CCSD(T), and MCSCF Methods. Journal of Physical Chemistry A, 2017, 121, 5341-5351.	1.1	3
76	Effect of Ancillary Ligands on Oxidative Addition of CH₄ to Ta(III) Complexes Ta(OC₂H₄)₃A (A = B, Al, CH, SiH, N, P): A Density Functional Theory Study. Organometallics, 2017, 36, 64-73.	1.1	5
77	Methane Manifesto: A Theoristâ€™s Perspective on Catalytic Light Alkane Functionalization. Comments on Inorganic Chemistry, 2017, 37, 219-237.	3.0	6
78	Reactivity of Hydrogen on and in Nanostructured Molybdenum Nitride: Crotonaldehyde Hydrogenation. ACS Catalysis, 2016, 6, 5797-5806.	5.5	44
79	Aqueous Hydricity from Calculations of Reduction Potential and Acidity in Water. Journal of Physical Chemistry B, 2016, 120, 12911-12919.	1.2	16
80	The Mechanism of Nâ€“N Double Bond Cleavage by an Iron(II) Hydride Complex. Journal of the American Chemical Society, 2016, 138, 12112-12123.	6.6	34
81	N-Heterocyclic Carbene Based Nickel and Palladium Complexes: A DFT Comparison of the Mizorokiâ€“Heck Catalytic Cycles. Organometallics, 2016, 35, 3170-3181.	1.1	48
82	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.	1.0	22
83	A Dinitrogen Dicopper(I) Complex via a Mixedâ€Valence Dicopper Hydride. Angewandte Chemie - International Edition, 2016, 55, 9927-9931.	7.2	38
84	A Dinitrogen Dicopper(I) Complex via a Mixedâ€Valence Dicopper Hydride. Angewandte Chemie, 2016, 128, 10081-10085.	1.6	10
85	Solvent-Dependent Thermochemistry of an Iridium/Ruthenium H₂ Evolution Catalyst. Inorganic Chemistry, 2016, 55, 12042-12051.	1.9	18
86	Goldâ€Mediated Isomerization of ÂCyclooctyne to Ring Fused Olefinic Bicycles. European Journal of Inorganic Chemistry, 2016, 2016, 995-1001.	1.0	6
87	Theoretical Study of Two Possible Side Reactions for Reductive Functionalization of 3d Metalâ€“Methyl Complexes by Hydroxide Ion: Deprotonation and Metalâ€“Methyl Bond Dissociation. Organometallics, 2016, 35, 950-958.	1.1	13
88	Iron-Catalyzed Homogeneous Hydrogenation of Alkenes under Mild Conditions by a Stepwise, Bifunctional Mechanism. ACS Catalysis, 2016, 6, 2127-2135.	5.5	108
89	Reductive functionalization of 3d metalâ€“methyl complexes: The greater importance of ligand than metal. Computational and Theoretical Chemistry, 2015, 1069, 86-95.	1.1	8
90	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.	7.2	37

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91	Methane Is the Best Substrate for C(sp³)â€“H Activation with Cp*(PMe₃)Co(Me)(OTf): A Density Functional Theory Study. Organometallics, 2015, 34, 4032-4038.	1.1	9
92	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.	1.1	18
93	A rhodium catalyst for single-step styrene production from benzene and ethylene. Science, 2015, 348, 421-424.	6.0	94
94	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.	6.6	44
95	Effect of Ligand Connectivity and Charge State on the Amination of Câ€“H Bonds by Copper Amide Complexes. Organometallics, 2015, 34, 5045-5050.	1.1	2
96	Zinc(II)-Mediated Carbene Insertion into Câ€“H Bonds in Alkanes. Inorganic Chemistry, 2015, 54, 11043-11045.	1.9	24
97	DFT Modeling of the Aldehydeâ€“Water Shift Reaction with a Cationic Cp*Ir Catalyst. ACS Catalysis, 2015, 5, 225-232.	5.5	19
98	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.	1.1	33
99	Impact of divalent metal cations on the catalysis of peptide bonds: a DFT study. Journal of Coordination Chemistry, 2014, 67, 3920-3931.	0.8	2
100	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.	1.1	15
101	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.	1.9	20
102	Disparate reactivity from isomeric {Me 2 C(CH 2 N CHpy) 2 } and {Me 2 C(CH NCH 2 py) 2 } chelates in iron complexation. Polyhedron, 2014, 84, 182-191.	1.0	8
103	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.	1.1	58
104	The Curious Case of Mesityl Azide and Its Reactivity with bpyNiEt₂. Inorganic Chemistry, 2014, 53, 11633-11639.	1.9	3
105	Reductive functionalization of a rhodium(iii)â€“methyl bond by electronic modification of the supporting ligand. Dalton Transactions, 2014, 43, 8273.	1.6	26
106	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.	3.7	37
107	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.	6.6	115
108	Copper(II) Anilides in sp³ C-H Amination. Journal of the American Chemical Society, 2014, 136, 10930-10940.	6.6	99

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109	Oxygen Atom Insertion into Iron(II) Phenyl and Methyl Bonds: A Key Step for Catalytic Hydrocarbon Functionalization. Organometallics, 2014, 33, 5597-5605.	1.1	13
110	Iridium, Rhodium, and Ruthenium Catalysts for the â€œAldehydeâ€“Water Shiftâ€•Reaction. ACS Catalysis, 2014, 4, 3034-3038.	5.5	50
111	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.	1.9	39
112	Molecular and Electronic Structure of Cyclic Trinuclear Gold(I) Carbeniate Complexes: Insights for Structure/Luminescence/Conductivity Relationships. Inorganic Chemistry, 2014, 53, 7485-7499.	1.9	32
113	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.	5.5	36
114	Impact of d-Orbital Occupation on Metalâ€“Carbon Bond Functionalization. Inorganic Chemistry, 2014, 53, 7789-7798.	1.9	12
115	Chemical bonding involving d-orbitals. Chemical Communications, 2013, 49, 9521.	2.2	7
116	Activation of carbonâ€“hydrogen bonds and dihydrogen by 1,2-CH-addition across metalâ€“heteroatom bonds. Dalton Transactions, 2013, 42, 16646.	1.6	76
117	Methane Câ€“H Bond Activation by â€œNakedâ€•Alkali Metal Imidyl and Alkaline Earth Metal Imide Complexes. The Role of Ligand Spin and Nucleophilicity. Journal of Physical Chemistry A, 2013, 117, 9245-9251.	1.1	8
118	Spin Crossover during Î²-Hydride Elimination in High-Spin Iron(II)â€“ and Cobalt(II)â€“Alkyl Complexes. Organometallics, 2013, 32, 4741-4751.	1.1	63
119	Computational study of carbonâ€“hydrogen bond deprotonation by alkali metal superbases. Computational and Theoretical Chemistry, 2013, 1019, 85-93.	1.1	19
120	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.	1.0	20
121	Selective Extraction of N₂ from Air by Diarylimine Iron Complexes. Journal of the American Chemical Society, 2013, 135, 3511-3527.	6.6	17
122	Mechanism of Hydrogenolysis of an Iridiumâ€“Methyl Bond: Evidence for a Methane Complex Intermediate. Journal of the American Chemical Society, 2013, 135, 1217-1220.	6.6	33
123	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.	1.9	51
124	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.	1.1	36
125	Periodic Trends in 3d Metal Mediated CO2 Activation. ACS Symposium Series, 2013, , 67-88.	0.5	3
126	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.	2.1	15

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127	Câ€“H Activation by Multiply Bonded Complexes with Potentially Noninnocent Ligands: A Computational Study. Inorganic Chemistry, 2013, 52, 8106-8113.	1.9	23
128	Pt^{II}-Catalyzed Ethylene Hydrophenylation: Influence of Dipyridyl Chelate Ring Size on Catalyst Activity and Longevity. ACS Catalysis, 2013, 3, 1165-1171.	5.5	45
129	Cooperative Carbon Capture Capabilities in Multivariate MOFs Decorated with Amino Acid Side Chains: A Computational Study. Journal of Physical Chemistry C, 2013, 117, 14717-14722.	1.5	13
130	Lewis Bases Trigger Intramolecular CH-Bond Activation: (tBu3SiO)2W=NtBu [rlhar2] (tBu3SiO)(Î¹O,Î¹C-tBu2SiOCMe2CH2)HW=NtBu. European Journal of Inorganic Chemistry, 2013, 2013, 4056-4067.	1.0	6
131	Pt^{II} and Rh^{III} Hydrocarbyl Complexes Bearing Coordinated Oxygen Atom Delivery Reagents. European Journal of Inorganic Chemistry, 2013, 2013, 4515-4525.	1.0	9
132	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.	6.6	44
133	Reductive Elimination of Alkylamines from Low-Valent, Alkylpalladium(II) Amido Complexes. Journal of the American Chemical Society, 2012, 134, 15281-15284.	6.6	28
134	Carbon Dioxide Migration Pathways in Proteins. Journal of Physical Chemistry Letters, 2012, 3, 830-833.	2.1	9
135	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.	1.9	36
136	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.	1.1	22
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