Eric Clot

List of Publications by Year
in descending order

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155 papers	10,316 citations	26630 56 h-index	37204 96 g-index
170 all docs	170 docs citations	170 times ranked	6912 citing authors

#	Article	IF	Citations
1	Supramolecular Chirogenesis in Bis-Porphyrin: Crystallographic Structure and CD Spectra for a Complex with a Chiral Guanidine Derivative. Symmetry, 2021, 13, 275.	2.2	7
2	Chirogenesis in Zinc Porphyrins: Theoretical Evaluation of Electronic Transitions, Controlling Structural Factors and Axial Ligation. ChemPhysChem, 2021, 22, 1817-1833.	2.1	3
3	Impact of the Alkali Metal on the Structural and Dynamic Properties of the Anionic Pentahydride Ruthenium Complexes [M(THF)x][RuH5(PCy3)2] (M = Li, Na, K). Organometallics, 2021, 40, 3024-3032.	2.3	0
4	Supramolecular chirogenesis in zinc porphyrins: Complexation with enantiopure thiourea derivatives, binding studies and chirality transfer mechanism. Journal of Porphyrins and Phthalocyanines, 2020, 24, 840-849.	0.8	5
5	Stepwise Functionalization of N₂ at Mo: Nitrido to Imido to Amido â€“ Factors Favoring Amine Elimination from the Amido Complex. European Journal of Inorganic Chemistry, 2020, 2020, 1499-1505.	2.0	12
6	Regiospecificity in Ligand-Free Pd-Catalyzed Câ€“H Arylation of Indoles: LiHMDS as Base and Transient Directing Group. ACS Catalysis, 2020, 10, 2713-2719.	11.2	32
7	Benchmarking computational methods and influence of guest conformation on chirogenesis in zinc porphyrin complexes. Physical Chemistry Chemical Physics, 2020, 22, 11025-11037.	2.8	5
8	Efficient alkene hydrosilation with bis(8-quinolyl)phosphine (NPN) nickel catalysts. The dominant role of silyl-over hydrido-nickel catalytic intermediates. Chemical Science, 2020, 11, 5043-5051.	7.4	7
9	A Career in Catalysis: Odile Eisenstein. ACS Catalysis, 2019, 9, 10375-10388.	11.2	2
10	Aerobic and Ligand-Free Manganese-Catalyzed Homocoupling of Arenes or Aryl Halides via in Situ Formation of Aryllithiums. Journal of Organic Chemistry, 2019, 84, 4413-4420.	3.2	19
11	Isolation and structural characterization of a titanacyclopropane as key intermediate in the double aryl Grignard addition to 2-(arylethynyl)pyridine derivatives. Chemical Communications, 2018, 54, 2228-2231.	4.1	4
12	Ta-Catalyzed Hydroaminoalkylation of Alkenes: Insights into Ligand-Modified Reactivity Using DFT. Organometallics, 2018, 37, 4387-4394.	2.3	24
13	Selective mono N-methylation of anilines with methanol catalyzed by rhenium complexes: An experimental and theoretical study. Journal of Catalysis, 2018, 366, 300-309.	6.2	58
14	Dehydrogenative coupling of 4-substituted pyridines mediated by a zirconium(ii) synthon: reaction pathways and dead ends. Chemical Science, 2018, 9, 5223-5232.	7.4	13
15	Roomâ€Temperature Functionalization of N₂ to Borylamine at a Molybdenum Complex. Angewandte Chemie, 2018, 130, 13047-13050.	2.0	15
16	Roomâ€Temperature Functionalization of N₂ to Borylamine at a Molybdenum Complex. Angewandte Chemie - International Edition, 2018, 57, 12865-12868.	13.8	39
17	Domino Pd⁰â€Catalyzed C(sp³)â€“H Arylation/Electrocyclic Reactions via Benzazetidine Intermediates. Angewandte Chemie, 2018, 130, 12307-12311.	2.0	10
18	Domino Pd⁰â€Catalyzed C(sp³)â€“H Arylation/Electrocyclic Reactions via Benzazetidine Intermediates. Angewandte Chemie - International Edition, 2018, 57, 12131-12135.	13.8	22

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19	New Titanium Borylimido Compounds: Synthesis, Structure, and Bonding. Inorganic Chemistry, 2017, 56, 10794-10814.	4.0	12
20	Reactions of Titanium Imides and Hydrazides with Boranes. Organometallics, 2017, 36, 3329-3342.	2.3	7
21	Mild Decarboxylative Câ^'H Alkylation: Computational Insights for Solventâ€Robust Ruthenium(II) Domino Manifold. Chemistry - A European Journal, 2017, 23, 17449-17453.	3.3	53
22	Nâ€Heterocyclic Carbene Iron Silyl Hydride Complexes. Israel Journal of Chemistry, 2017, 57, 1216-1221.	2.3	11
23	New Scandium Borylimido Chemistry: Synthesis, Bonding, and Reactivity. Journal of the American Chemical Society, 2017, 139, 11165-11183.	13.7	23
24	Hydrogenation of Carbonyl Derivatives with a Wellâ€Defined Rhenium Precatalyst. ChemCatChem, 2017, 9, 80-83.	3.7	39
25	A mechanochemical approach to access the prolineâ€“proline diketopiperazine framework. Beilstein Journal of Organic Chemistry, 2017, 13, 2169-2178.	2.2	14
26	Î·⁶â€Areneâ€Zirconiumâ€PNPâ€Pincer Complexes: Mechanism of Their Hydrogenolytic Formation and Their Reactivity as Zirconium(II) Synthons. Chemistry - A European Journal, 2016, 22, 9283-9292.	3.3	27
27	Deciphering Selectivity in Organic Reactions: A Multifaceted Problem. Accounts of Chemical Research, 2016, 49, 1070-1078.	15.6	31
28	Small molecule activation. Dalton Transactions, 2016, 45, 14419-14420.	3.3	17
29	Azaphilic versus Carbophilic Coupling at Cï£¾N Bonds: Key Steps in Titaniumâ€Assisted Multicomponent Reactions. Chemistry - A European Journal, 2015, 21, 18730-18738.	3.3	9
30	A Highly Effective Ruthenium System for the Catalyzed Dehydrogenative Cyclization of Amineâ€“Boranes to Cyclic Boranes under Mild Conditions. Chemistry - A European Journal, 2015, 21, 13080-13090.	3.3	19
31	Controlling the Selectivity of Câ€“H Activation in Pyridinium Triazolylidene Iridium Complexes: Mechanistic Details and Influence of Remote Substituents. Organometallics, 2015, 34, 858-869.	2.3	28
32	Reactions of Titanium Hydrazides with Silanes and Boranes: Nâ€“N Bond Cleavage and N Atom Functionalization. Journal of the American Chemical Society, 2015, 137, 10140-10143.	13.7	21
33	Efficient Pd⁰-Catalyzed Asymmetric Activation of Primary and Secondary Câ€“H Bonds Enabled by Modular Binepine Ligands and Carbonate Bases. ACS Catalysis, 2015, 5, 4300-4308.	11.2	84
34	Bâ€“C Bond Cleavage and Ruâ€“C Bond Formation from a Phosphinoborane: Synthesis of a Bis-Ïƒ Borane Aryl-Ruthenium Complex. Organometallics, 2014, 33, 7157-7163.	2.3	12
35	Bï£¿H, Cï£¿H, and Bï£¿C Bond Activation: The Role of Two Adjacent Agostic Interactions. Angewandte Chemie - International Edition, 2014, 53, 7569-7573.	13.8	46
36	Mechanistic Study of the Selectivity of Olefin versus Cyclobutene Formation by Palladium(0)-Catalyzed Intramolecular C(sp³)â€“H Activation. Journal of Organic Chemistry, 2014, 79, 11903-11910.	3.2	48

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37	Linear-Selective Hydroarylation of Unactivated Terminal and Internal Olefins with Trifluoromethyl-Substituted Arenes. Journal of the American Chemical Society, 2014, 136, 13098-13101.	13.7	263
38	Synergy between experiment and theory. Dalton Transactions, 2014, 43, 11092.	3.3	3
39	Monosubstituted Borane Ruthenium Complexes RuH₂(Î·²:Î·²-H₂BR)(PRâ€²₃)₂: A General Approach to the Geminal Bis(Ïƒ-Bâ€“H) Coordination Mode. Organometallics, 2013, 32, 4868-4877.	2.3	32
40	Synthesis of a ruthenium bis(diisopropylamino(isocyano)borane) complex from the activation of an amino(cyano)borane. Dalton Transactions, 2013, 42, 776-781.	3.3	4
41	Ligand-controlled Î²-selective C(sp3)â€“H arylation of N-Boc-piperidines. Chemical Science, 2013, 4, 2241.	7.4	122
42	Synthesis, Bonding and Reactivity of a Terminal Titanium Alkylidene Hydrazido Compound. Chemistry - A European Journal, 2013, 19, 4198-4216.	3.3	30
43	Synthesis and Reactions of a Cyclopentadienyl-Amidinate Titanium tert-Butoxyimido Compound. Organometallics, 2013, 32, 7520-7539.	2.3	21
44	Site selectivity and reversibility in the reactions of titanium hydrazides with Siâ€“H, Siâ€“X, Câ€“X and H+ reagents: Tiî€Nα 1,2-silane addition, Nβ alkylation, Nα protonation and Ïƒ-bond metathesis. Dalton Transactions, 2012, 41, 2277.	3.3	32
45	Hydride Ligands Make the Difference: Density Functional Study of the Mechanism of the Murai Reaction Catalyzed by [Ru(H)₂(H₂)₂(PR₃)₂] (R=cyclohexyl). Chemistry - A European Journal, 2012, 18, 11449-11458.	3.3	22
46	On the Mechanism of the Palladiumâ€Catalyzed Î²â€Arylation of Ester Enolates. Chemistry - A European Journal, 2012, 18, 1932-1944.	3.3	72
47	New Sandwich and Half-Sandwich Titanium Hydrazido Compounds. Organometallics, 2011, 30, 2295-2307.	2.3	24
48	Siâ€“H and Siâ€“Cl bond activation reactions of titanium hydrazides with silanes and subsequent Tiâ€“H/Eâ€“H (E = Si or H) Ïƒ-bond metathesis. Chemical Communications, 2011, 47, 3147.	4.1	32
49	Câˆ’F and Câˆ’H Bond Activation of Fluorobenzenes and Fluoropyridines at Transition Metal Centers: How Fluorine Tips the Scales. Accounts of Chemical Research, 2011, 44, 333-348.	15.6	430
50	Reactions of Cyclopentadienylâˆ’Amidinate Titanium Hydrazides with CO₂, CS₂, and Isocyanates: Tiâ•N_{Î±} Cycloaddition, Cycloadditionâˆ’Insertion, and Cycloadditionâˆ’NNR₂ Group Transfer Reactions. Organometallics, 2011, 30, 1182-1201.	2.3	41
51	Ruthenium Agostic (Phosphinoaryl)borane Complexes: Multinuclear Solid-State and Solution NMR, X-ray, and DFT Studies. Journal of the American Chemical Society, 2011, 133, 17232-17238.	13.7	39
52	Titanium alkoxyimido (Tiî€Nâ€“OR) complexes: reductive Nâ€“O bond cleavage at the boundary between hydrazide and peroxide ligands. Chemical Communications, 2011, 47, 4926.	4.1	19
53	Titanium tert-Butoxyimido Compounds. Inorganic Chemistry, 2011, 50, 12155-12171.	4.0	15
54	Reaction Site Diversity in the Reactions of Titanium Hydrazides with Organic Nitriles, Isonitriles and Isocyanates: Tï£¾N_{Î±} Cycloaddition, Tï£¾N_{Î±} Insertion and N_{Î±}ï£¿N_{Î²} Bond Cleavage. Chemistry - A European Journal, 2011, 17, 265-285.	3.3	52

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55	Dimethylaminoborane (H₂BNMe₂) Coordination to Late Transition Metal Centers: Snapshots of the Bâ€“H Oxidative Addition Process.. Inorganic Chemistry, 2011, 50, 11039-11045.	4.0	49
56	Ruthenium Bis(Ïƒâ€Bï£¿H) Aminoborane Complexes from Dehydrogenation of Amineâ€“Boranes: Trapping of H₂Bï£¿NH₂. Angewandte Chemie - International Edition, 2010, 49, 918-920.	13.8	145
57	Palladiumâ€Catalyzed Î²â€…Arylation of Carboxylic Esters. Angewandte Chemie - International Edition, 2010, 49, 7261-7265.	13.8	190
58	Mechanistic investigation of vinylic carbonâ€“fluorine bond activation of perfluorinated cycloalkenes using Cp*2ZrH2 and Cp*2ZrHF. Journal of Fluorine Chemistry, 2010, 131, 1122-1132.	1.7	42
59	Dielsâ€“Alder reaction of vinylene carbonate and 2,5-dimethylfuran: kinetic vs. thermodynamic control. New Journal of Chemistry, 2010, 34, 517.	2.8	20
60	Intramolecular Palladium-Catalyzed Alkane Câ^'H Arylation from Aryl Chlorides. Journal of the American Chemical Society, 2010, 132, 10706-10716.	13.7	218
61	Mâ•NÎ±Cycloaddition and NÎ±â^'NÎ²Insertion in the Reactions of Titanium Hydrazido Compounds with Alkynes: A Combined Experimental and Computational Study. Journal of the American Chemical Society, 2010, 132, 10484-10497.	13.7	53
62	Single and double substrate insertion into the Tiî€N_{Î±}bonds of terminal titanium hydrazides. Chemical Communications, 2010, 46, 85-87.	4.1	37
63	Câ€”H Bond Activation in Transition Metal Species from a Computational Perspective. Chemical Reviews, 2010, 110, 749-823.	47.7	959
64	Importance of palladiumâ€“carbon bond energies in direct arylation of polyfluorinated benzenes. Dalton Transactions, 2010, 39, 10510.	3.3	54
65	DFT study of the mechanism of benzocyclobutene formation by palladium-catalysed C(sp3)â€“H activation: role of the nature of the base and the phosphine. Dalton Transactions, 2010, 39, 10528.	3.3	59
66	Synthesis, structure, and reductive elimination in the series Tpâ€²Rh(PR3)(ArF)H; Determination of rhodiumâ€“carbon bond energies of fluoroaryl substituents. Dalton Transactions, 2010, 39, 10495.	3.3	35
67	Ruthenium, Rhodium, and Iridium Bis(Ïƒ-Bâ^'H) Diisopropylaminoborane Complexes. Organometallics, 2010, 29, 5591-5595.	2.3	71
68	Ionâ€Pairing in Organometallic Chemistry: Structure and Influence on Proton Transfer from a Computational Perspective. European Journal of Inorganic Chemistry, 2009, 2009, 2319-2328.	2.0	49
69	Phosphinoborane and Sulfidoborohydride as Chelating Ligands in Polyhydride Ruthenium Complexes: Agostic Ïƒâ€Borane versus Dihydroborate Coordination. Angewandte Chemie - International Edition, 2009, 48, 2964-2968.	13.8	64
70	Energetics of Câ^'H Bond Activation of Fluorinated Aromatic Hydrocarbons Using a [Tpâ€²Rh(CNneopentyl)] Complex. Journal of the American Chemical Society, 2009, 131, 13464-13473.	13.7	117
71	Self-Aggregation Tendency of All Species Involved in the Catalytic Cycle of Bifunctional Transfer Hydrogenation. Organometallics, 2009, 28, 960-967.	2.3	17
72	Exceptional Sensitivity of Metalâ^'Aryl Bond Energies to ortho-Fluorine Substituents: Influence of the Metal, the Coordination Sphere, and the Spectator Ligands on Mâ^'C/Hâ^'C Bond Energy Correlations. Journal of the American Chemical Society, 2009, 131, 7817-7827.	13.7	172

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73	Synthesis and structure of â€œ16-electronâ€•rhodium(iii) catalysts for transfer hydrogenation of a cyclic imine: mechanistic implications. Chemical Communications, 2009, , 6801.	4.1	35
74	Reactions of cyclopentadienyl-amidinate titanium imido compounds with CO2: cycloaddition-extrusion vs. cycloaddition-insertion. Dalton Transactions, 2009, , 5960.	3.3	58
75	Syntheses, Reactivity and DFT Studies of Groupâ€…2 and Group 12 Metal Complexes of Tris(pyrazolyl)methanides Featuring â€œFreeâ€•Pyramidal Carbanions. Chemistry - A European Journal, 2008, 14, 5918-5934.	3.3	57
76	A NMR, X-ray, and DFT combined study on the regio-chemistry of nucleophilic addition to platinum(II) coordinated terminal olefins. Journal of Organometallic Chemistry, 2008, 693, 2819-2827.	1.8	17
77	Synthesis of Benzocyclobutenes by Palladium-Catalyzed Câ^'H Activation of Methyl Groups: Method and Mechanistic Study. Journal of the American Chemical Society, 2008, 130, 15157-15166.	13.7	290
78	A Weak Donor, Planar Chelating Bitriazole N-Heterocyclic Carbene Ligand for Ruthenium(II), Palladium(II), and Rhodium. Organometallics, 2008, 27, 2128-2136.	2.3	98
79	Mechanism of Homogeneous Iridium-Catalyzed Alkylation of Amines with Alcohols from a DFT Study. Organometallics, 2008, 27, 2529-2535.	2.3	149
80	Cycloaddition reactions of transition metal hydrazides with alkynes and heteroalkynes: coupling of Tiî€NNPh2 with PhCCMe, PhCCH, MeCN and tBuCP. Chemical Communications, 2008, , 5101.	4.1	38
81	Stereochemical Nonrigidity of a Chiral Rhodium Boryl Hydride Complex:Â A Ïƒ-Borane Complex as Transition State for Isomerization. Journal of the American Chemical Society, 2008, 130, 4375-4385.	13.7	20
82	Î²-H Transfer from the Metallacyclobutane: A Key Step in the Deactivation and Byproduct Formation for the Well-Defined Silica-Supported Rhenium Alkylidene Alkene Metathesis Catalyst. Journal of the American Chemical Society, 2008, 130, 6288-6297.	13.7	88
83	A Terminal Borylene Ruthenium Complex: From Bâ^'H Activation to Reversible Hydrogen Release. Journal of the American Chemical Society, 2008, 130, 12878-12879.	13.7	108
84	Synthesis, DFT Studies, and Reactions of Scandium and Yttrium Dialkyl Cations Containing Neutral fac-N₃ and fac-S₃ Donor Ligands. Organometallics, 2008, 27, 3458-3473.	2.3	29
85	Tiâ•NR vs Tiâ^'Râ€² Functional Group Selectivity in Titanium Imido Alkyl Cations from an Experimental Perspective. Organometallics, 2008, 27, 6096-6110.	2.3	28
86	Tiâ•NR vs Tiâ^'Râ€² Functional Group Selectivity in Titanium Imido Alkyl Cations from a DFT Perspective. Organometallics, 2008, 27, 6111-6122.	2.3	7
87	Dynamics of Silica-Supported Catalysts Determined by Combining Solid-State NMR Spectroscopy and DFT Calculations. Journal of the American Chemical Society, 2008, 130, 5886-5900.	13.7	98
88	Titanium Hydrazides Supported by Diamide-Amine and Related Ligands: A Combined Experimental and DFT Study. Organometallics, 2008, 27, 6479-6494.	2.3	41
89	Structural and dynamic properties of propane coordinated to TpRh(CNR) from a confrontation between theory and experiment. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 6939-6944.	7.1	33
90	Agostic interaction and intramolecular proton transfer from the protonation of dihydrogen ortho metalated ruthenium complexes. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 6945-6950.	7.1	52

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91	Understanding d0-Olefin Metathesis Catalysts:Â Which Metal, Which Ligands?. Journal of the American Chemical Society, 2007, 129, 8207-8216.	13.7	210
92	Computational structureâ€“activity relationships in H2storage: how placement of N atoms affects release temperatures in organic liquid storage materials. Chemical Communications, 2007, , 2231-2233.	4.1	163
93	New ligand platforms for developing the chemistry of the Tiî€Nâ€“NR2 functional group and the insertion of alkynes into the Nâ€“N bond of a Tiî€Nâ€“NPh2 ligand. Chemical Communications, 2007, , 4937.	4.1	65
94	Mesitylborane as a Bis(Ïƒ-Bâˆ’H) Ligand:Â An Unprecedented Bonding Mode to a Metal Center. Journal of the American Chemical Society, 2007, 129, 8704-8705.	13.7	91
95	Interionic Structure of Ion Pairs and Ion Quadruples of Half-Sandwich Ruthenium(II) Salts Bearing Î±-Diimine Ligands. Organometallics, 2007, 26, 3930-3946.	2.3	69
96	Aliphatic versus Aromatic Câˆ’H Activation in the Formation of Abnormal Carbenes with Iridium:â€‰ A Combined Experimental and Theoretical Study. Organometallics, 2007, 26, 5304-5314.	2.3	94
97	Imidazolium Carboxylates as Versatile and Selective N-Heterocyclic Carbene Transfer Agents:â€‰ Synthesis, Mechanism, and Applications. Journal of the American Chemical Society, 2007, 129, 12834-12846.	13.7	213
98	AlMe3and ZnMe2Adducts of a Titanium Imido Methyl Cation:Â A Combined Crystallographic, Spectroscopic, and DFT Study. Journal of the American Chemical Society, 2006, 128, 15005-15018.	13.7	62
99	Validation of the Mâˆ’C/Hâˆ’C Bond Enthalpy Relationship through Application of Density Functional Theory. Journal of the American Chemical Society, 2006, 128, 8350-8357.	13.7	73
100	Carbonylâ‹¯carbonyl interactions in first-row transition metal complexes. CrystEngComm, 2006, 8, 563-570.	2.6	35
101	DFT calculations of d0M(NR)(CHtBu)(X)(Y) (M = Mo, W; R = CPh3, 2,6-iPrâ€“C6H3; X and Y = CH2tBu, OtBu,) Tj ETQq1 1 0.784314 rgB Transactions, 2006, , 3077-3087.	3.3	58
102	Experimental and DFT Studies of Cationic Imido Titanium Alkyls:Â Agostic Interactions and Câˆ’H Bond and Solvent Activation Reactions of Isolobal Analogues of Group 4 Metallocenium Cations. Organometallics, 2006, 25, 2806-2825.	2.3	55
103	Synthesis and Ethylene Polymerization Capability of Metallocene-like Imido Titanium Dialkyl Compounds and Their Reactions with AliBu3. Organometallics, 2006, 25, 5549-5565.	2.3	31
104	Agostic Interactions from a Computational Perspective: One Name, Many Interpretations. ChemInform, 2005, 36, no.	0.0	1
105	Selectivity in Câ€“Cl bond activation of dichloroarenes by photogenerated Cp*Re(CO)2: combined experimental and DFT studies. New Journal of Chemistry, 2005, 29, 226-231.	2.8	10
106	Well-defined imidotitanium alkyl cations: agostic interactions, migratory insertion vs.[2+2] cycloaddition, and the first structurally authenticated AlMe3 adduct of any transition metal alkyl cation. Chemical Communications, 2005, , 3313.	4.1	58
107	Aggregation in solution of neutral half-sandwich Ru(ii) precatalysts for transfer hydrogenation. New Journal of Chemistry, 2005, 29, 430.	2.8	40
108	An Anion-Dependent Switch in Selectivity Results from a Change of Câˆ’H Activation Mechanism in the Reaction of an Imidazolium Salt with IrH5(PPh3)2. Journal of the American Chemical Society, 2005, 127, 16299-16311.	13.7	172

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109	Structure and Reactivity oftrans-Bis[2-(2-chloroethyl)pyridine]palladium Chloride (1). A Study on the Elimination Reaction of1and 2-(2-Chloroethyl)pyridine Induced by Quinuclidine in Acetonitrile. Journal of Organic Chemistry, 2005, 70, 10688-10692.	3.2	4
110	Understanding Structural and Dynamic Properties of Well-Defined Rhenium-Based Olefin Metathesis Catalysts, Re(â‹®CR)(CHR)(X)(Y), from DFT and QM/MM Calculations. Organometallics, 2005, 24, 1586-1597.	2.3	59
111	Reactions of Neutral and Cationic Diamide-Supported Imido Complexes with CO2 and Other Heterocumulenes:â€‰ Issues of Site Selectivity. Organometallics, 2005, 24, 2368-2385.	2.3	35
112	Pendant Arm Functionalized Benzamidinate Titanium Imido Compounds:â€‰ Experimental and Computational Studies of Their Reactions with CO2. Organometallics, 2005, 24, 2347-2367.	2.3	65
113	d0Re-Based Olefin Metathesis Catalysts, Re(â‹®CR)(CHR)(X)(Y):Â The Key Role of X and Y Ligands for Efficient Active Sites. Journal of the American Chemical Society, 2005, 127, 14015-14025.	13.7	158
114	Agostic Interactions from a Computational Perspective: One Name, Many Interpretations. Structure and Bonding, 2004, , 1-36.	1.0	132
115	Biscarbeneâ€”Ruthenium Complexes in Catalysis: Novel Stereoselective Synthesis of (1E,3E)-1,4-Disubstituted-1,3-dienes via Head-to-Head Coupling of Terminal Alkynes and Addition of Carboxylic Acids.. ChemInform, 2004, 35, no.	0.0	0
116	Defluorination of Perfluoropropene Using Cp*2ZrH2and Cp*2ZrHF:Â A Mechanism Investigation from a Joint Experimentalâ^Theoretical Perspective. Journal of the American Chemical Society, 2004, 126, 5647-5653.	13.7	85
117	Is the Allylpalladium Structure Altered between Solid and Solutions?. Journal of the American Chemical Society, 2004, 126, 9079-9084.	13.7	7
118	Ortho-Metalated Ruthenium Hydrido Dihydrogen Complexes:Â Dynamics, Exchange Couplings, and Reactivity. Organometallics, 2004, 23, 1424-1433.	2.3	48
119	Double Geminal Câ^H Activation and Reversible Î±-Elimination in 2-Aminopyridine Iridium(III) Complexes:Â The Role of Hydrides and Solvent in Flattening the Free Energy Surface. Journal of the American Chemical Society, 2004, 126, 8795-8804.	13.7	77
120	Synthesis, Reactivity, and Computational Studies of the Cationic Tungsten Methyl Complex [W(NPh)(N2Npy)Me]+and Related Compounds (N2Npy= MeC(2-C5H4N)(CH2NSiMe3)2). Organometallics, 2004, 23, 4444-4461.	2.3	33
121	PGSE and NOE NMR Evidence for Higher Order Aggregation in Some Cationic Ruthenium Complexes in Both Protic and Aprotic Solvents. Inorganic Chemistry, 2003, 42, 5465-5467.	4.0	52
122	Biscarbeneâ^Ruthenium Complexes in Catalysis: Novel Stereoselective Synthesis of (1E,3E)-1,4-Disubstituted-1,3-dienes via Head-to-Head Coupling of Terminal Alkynes and Addition of Carboxylic Acids. Journal of the American Chemical Society, 2003, 125, 11964-11975.	13.7	99
123	Outer sphere anion participation can modify the mechanism for conformer interconversion in Pd pincer complexes. Dalton Transactions, 2003, , 831-838.	3.3	84
124	cisâ€“trans Isomerisation of CpRe(CO)2(H)(ArF) (ArF= C6FnH5â^n; n = 0â€“5) is the rate determining step in Câ€“H activation of fluoroarenes: a DFT study. Dalton Transactions, 2003, , 4065-4074.	3.3	53
125	Bond energy Mâ€“C/Hâ€“C correlations: dual theoretical and experimental approach to the sensitivity of Mâ€“C bond strength to substituentsElectronic supplementary information (ESI) available: methods of calculation; Fig. S1: Comparison of calculated and experimental Câ€“H bond dissociation energies for organic molecules; Table S1, comparison of calculated and experimental CO-stretching frequencies; Table S2, total energies, BDE for Reâ€“C and Hâ€“C; Table S3, NPA charges q(C) and q(aryl) for the organic fragments C6H6â€“. Chemical Communications, 2003, , 490-491.	4.1	89
126	Ion pairing effects in intramolecular heterolytic H2 activation in an Ir(iii) complex: a combined theoretical/experimental study. New Journal of Chemistry, 2003, 27, 80-87.	2.8	69

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127	Isomerization of Double and Triple C-C Bonds at a Metal Center. Catalysis By Metal Complexes, 2002, , 137-160.	0.6	4
128	Interplay of Weak Interactions:Â An Iridium(III) System with an Agostictert-Butyl but a Nonagostic Isopropyl Group. Organometallics, 2002, 21, 575-580.	2.3	39
129	Counter-ion effects switch ligand binding from C-2 to C-5 in kinetic carbenes formed from an imidazolium salt and IrH5(PPh3)2. Chemical Communications, 2002, , 2580-2581.	4.1	82
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