Feliu Maseras

List of Publications by Year in Descending Order

285 papers	14,621 citations	60 h-index	108 g-index
315 ext. papers	15,655 ext. citations	7.5 avg, IF	6.71 L-index

#	Paper	IF	Citations
285	Mechanistic Studies on the Synthesis of Pyrrolidines and Piperidines via Copper-Catalyzed Intramolecular C-H Amination.. *Organometallics*, **2022**, 41, 1099-1105	3.8	1
284	An Expanded SET Model Associated with the Functional Hindrance Dominates the Amide-Directed Distal sp C-H Functionalization. *Journal of the American Chemical Society*, **2021**, 143, 19406-19416	16.4	1
283	Computational insights into metal-catalyzed asymmetric hydrogenation. *Advances in Catalysis*, **2021**, 68, 385-426	2.4	1
282	Two Copper-Carbenes from One Diazo Compound. *Journal of the American Chemical Society*, **2021**, 143, 4837-4843	16.4	6
281	Redefining the Mechanistic Scenario of Carbon-Sulfur Nucleophilic Coupling via High-Valent Cp*Co Species. *Angewandte Chemie - International Edition*, **2021**, 60, 11217-11221	16.4	5
280	Redefining the Mechanistic Scenario of Carbon–Sulfur Nucleophilic Coupling via High-Valent Cp*CoIV Species. *Angewandte Chemie*, **2021**, 133, 11317-11321	3.6	0
279	The Effect of Added Ligands on the Reactions of [Ni(COD)(dppf)] with Alkyl Halides: Halide Abstraction May Be Reversible. *Organometallics*, **2021**, 40, 1997-2007	3.8	3
278	Understanding Ball Milling Mechanochemical Processes with DFT Calculations and Microkinetic Modeling. *ChemSusChem*, **2021**, 14, 2763-2768	8.3	3
277	Photolytic Activation of Late-Transition-Metal–Carbon Bonds and Their Reactivity toward Oxygen. *Organometallics*, **2021**, 40, 4077-4091	3.8	0
276	Intermolecular Allene Functionalization by Silver-Nitrene Catalysis. *Journal of the American Chemical Society*, **2020**, 142, 13062-13071	16.4	14
275	The Challenge of Reproducing with Calculations Raw Experimental Kinetic Data for an Organic Reaction. *Organic Letters*, **2020**, 22, 2873-2877	6.2	12
274	A Quantitative Model for Alkane Nucleophilicity Based on C–H Bond Structural/Topological Descriptors. *Angewandte Chemie*, **2020**, 132, 3136-3140	3.6	2
273	A Quantitative Model for Alkane Nucleophilicity Based on C-H Bond Structural/Topological Descriptors. *Angewandte Chemie - International Edition*, **2020**, 59, 3112-3116	16.4	11
272	Water oxidation electrocatalysis using ruthenium coordination oligomers adsorbed on multiwalled carbon nanotubes. *Nature Chemistry*, **2020**, 12, 1060-1066	17.6	27
271	Photosynthesis of a Dihydroimidazopyridine Chelate Shines Light on the Reactions of a Photoactivated Iron(III) Complex with O. *Inorganic Chemistry*, **2020**, 59, 16281-16290	5.1	2
270	Computational Modeling of Selected Photoactivated Processes. *Topics in Organometallic Chemistry*, **2020**, 131-152	0.6	
269	Unexpected Nickel Complex Speciation Unlocks Alternative Pathways for the Reactions of Alkyl Halides with dppf-Nickel(0). *ACS Catalysis*, **2020**, 10, 10717-10725	13.1	9

268	Caesium fluoride-mediated hydrocarboxylation of alkenes and allenes: scope and mechanistic insights. *Chemical Science*, **2019**, 10, 10072-10078	9.4	5
267	Four Oxidation States in a Single Photoredox Nickel-Based Catalytic Cycle: A Computational Study. *Angewandte Chemie - International Edition*, **2019**, 58, 3898-3902	16.4	17
266	Four Oxidation States in a Single Photoredox Nickel-Based Catalytic Cycle: A Computational Study. *Angewandte Chemie*, **2019**, 131, 3938-3942	3.6	2
265	Scope and Challenge of Computational Methods for Studying Mechanism and Reactivity in Homogeneous Catalysis. *ACS Catalysis*, **2019**, 9, 6803-6813	13.1	91
264	Mechanistic Study on the Asymmetric Synthesis of the Wieland-Miescher Ketone and Analogs. *ChemCatChem*, **2019**, 11, 4064-4071	5.2	3
263	Diastereodivergent Enantioselective [8 + 2] Annulation of Tropones and Enals Catalyzed by N-Heterocyclic Carbenes. *Organic Letters*, **2019**, 21, 3187-3192	6.2	25
262	Copper-Catalyzed N-F Bond Activation for Uniform Intramolecular C-H Amination Yielding Pyrrolidines and Piperidines. *Angewandte Chemie - International Edition*, **2019**, 58, 8912-8916	16.4	45
261	Eine Kupfer-katalysierte N-F-Bindungsaktivierung f□die einheitliche intramolekulare C-H-Aminierung zu Pyrrolidinen und Piperidinen. *Angewandte Chemie*, **2019**, 131, 9004-9009	3.6	5
260	The Role of Electron-Donor Substituents in the Family of OPBAN-Cu Water Oxidation Catalysts: Effect on the Degradation Pathways and Efficiency. *European Journal of Inorganic Chemistry*, **2019**, 2019, 2109-2114	2.3	7
259	Computational Characterization of Single-Electron Transfer Steps in Water Oxidation. *Inorganics*, **2019**, 7, 32	2.9	8
258	DFT characterization of the mechanism for Staudinger/aza-Wittig tandem organocatalysis. *Tetrahedron*, **2019**, 75, 1852-1859	2.4	4
257	Enantioselective Synthesis of 3-Heterosubstituted-2-amino-1-ols by Sequential Metal-Free Diene Aziridination/Kinetic Resolution. *Chemistry - A European Journal*, **2019**, 25, 12628-12635	4.8	3
256	A Career in Catalysis: Odile Eisenstein. *ACS Catalysis*, **2019**, 9, 10375-10388	13.1	1
255	The diverse mechanisms for the oxidative addition of C-Br bonds to Pd(PR) and Pd(PR) complexes. *Dalton Transactions*, **2019**, 48, 16242-16248	4.3	10
254	On the Use of Thermodynamic Cycles for the Calculation of Standard Potentials for the Oxidation of Solid Metals in Solution. *ChemPhysChem*, **2019**, 20, 159-162	3.2	
253	GARLEEK: Adding an extra flavor to ONIOM. *Journal of Computational Chemistry*, **2019**, 40, 381-386	3.5	6
252	Exploring the Role of Coinage Metalates in Trifluoromethylation: A Combined Experimental and Theoretical Study. *Chemistry - A European Journal*, **2019**, 25, 9390-9394	4.8	9
251	Elucidating the Mechanism of Aryl Aminations Mediated by NHC-Supported Nickel Complexes: Evidence for a Nonradical Ni(0)/Ni(II) Pathway. *ACS Catalysis*, **2018**, 8, 3733-3742	13.1	41

250	Copper-Catalyzed Borylative Ring Closing C□C Coupling toward Spiro- and Dispiroheterocycles. *ACS Catalysis*, **2018**, 8, 2833-2838	13.1	31
249	Computational Description of a Huisgen Cycloaddition Inside a Self-Assembled Nanocapsule. *European Journal of Organic Chemistry*, **2018**, 2018, 2103-2109	3.2	11
248	A Domino Process toward Functionally Dense Quaternary Carbons through Pd-Catalyzed Decarboxylative C(sp)-C(sp) Bond Formation. *Journal of the American Chemical Society*, **2018**, 140, 3981-3987	16.4	87
247	Enantioselective Synthesis of Aminodiols by Sequential Rhodium-Catalysed Oxyamination/Kinetic Resolution: Expanding the Substrate Scope of Amidine-Based Catalysis. *Chemistry - A European Journal*, **2018**, 24, 4635-4642	4.8	13
246	Oxidative Coupling Mechanisms: Current State of Understanding. *ACS Catalysis*, **2018**, 8, 1161-1172	13.1	56
245	Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. *Journal of Physical Chemistry A*, **2018**, 122, 1392-1399	2.8	82
244	A DFT-based mechanistic proposal for the light-driven insertion of dioxygen into Pt(ii)-C bonds. *Chemical Science*, **2018**, 9, 5039-5046	9.4	15
243	Computationally Guided Design of a Readily Assembled Phosphite□Thioether Ligand for a Broad Range of Pd-Catalyzed Asymmetric Allylic Substitutions. *ACS Catalysis*, **2018**, 8, 3587-3601	13.1	18
242	Computational Characterization of the Mechanism for the Oxidative Coupling of Benzoic Acid and Alkynes by Rhodium/Copper and Rhodium/Silver Systems. *Chemistry - A European Journal*, **2018**, 24, 12383-12388	4.8	20
241	Accelerated Ru-Cu Trinuclear Cooperative C-H Bond Functionalization of Carbazoles: A Kinetic and Computational Investigation. *Chemistry - A European Journal*, **2018**, 24, 15178-15184	4.8	9
240	The Acetate Proton Shuttle between Mutually Trans Ligands. *Organometallics*, **2018**, 37, 2645-2651	3.8	8
239	Measuring the Relative Reactivity of the Carbon-Hydrogen Bonds of Alkanes as Nucleophiles. *Angewandte Chemie - International Edition*, **2018**, 57, 13848-13852	16.4	25
238	Expanding the Range of Force Fields Available for ONIOM Calculations: The SICTWO Interface. *Journal of Chemical Information and Modeling*, **2018**, 58, 1828-1835	6.1	16
237	Titelbild: Measuring the Relative Reactivity of the Carbon□Hydrogen Bonds of Alkanes as Nucleophiles (Angew. Chem. 42/2018). *Angewandte Chemie*, **2018**, 130, 13885-13885	3.6	
236	Searching for Hidden Descriptors in the Metal-Ligand Bond through Statistical Analysis of Density Functional Theory (DFT) Results. *Inorganic Chemistry*, **2018**, 57, 14660-14670	5.1	15
235	Measuring the Relative Reactivity of the Carbon□Hydrogen Bonds of Alkanes as Nucleophiles. *Angewandte Chemie*, **2018**, 130, 14044-14048	3.6	6
234	Photoinduced O-Dependent Stepwise Oxidative Deglycination of a Nonheme Iron(III) Complex. *Journal of the American Chemical Society*, **2018**, 140, 14150-14160	16.4	7
233	Copper-mediated reduction of azides under seemingly oxidising conditions: catalytic and computational studies. *Catalysis Science and Technology*, **2018**, 8, 5763-5773	5.5	11

232	Steric effects determine the mechanisms of reactions between bis(N-heterocyclic carbene)-nickel(0) complexes and aryl halides. *Chemical Communications*, **2018**, 54, 10646-10649	5.8	21
231	New Vistas in Transmetalation with Discrete "AgCF " Species: Implications in Pd-Mediated Trifluoromethylation Reactions. *Chemistry - A European Journal*, **2018**, 24, 11895-11898	4.8	16
230	Microkinetic modeling in homogeneous catalysis. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2018**, 8, e1372	7.9	60
229	Palladium-Catalyzed Aerobic Homocoupling of Alkynes: Full Mechanistic Characterization of a More Complex Oxidase-Type Behavior. *ACS Catalysis*, **2018**, 8, 7495-7506	13.1	20
228	Single Electron Transfer Steps in Water Oxidation Catalysis. Redefining the Mechanistic Scenario. *ACS Catalysis*, **2017**, 7, 1712-1719	13.1	51
227	Functional-Group-Tolerant, Silver-Catalyzed N-N Bond Formation by Nitrene Transfer to Amines. *Journal of the American Chemical Society*, **2017**, 139, 2216-2223	16.4	45
226	Light-Driven Enantioselective Organocatalytic Benzylation of Enals. *Angewandte Chemie - International Edition*, **2017**, 56, 3304-3308	16.4	43
225	Light-Driven Enantioselective Organocatalytic Benzylation of Enals. *Angewandte Chemie*, **2017**, 129, 3352-3356	3.6	14
224	Computational study on the mechanism of the reaction of carbon dioxide with siloxy silanes. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	3
223	Halide Abstraction Competes with Oxidative Addition in the Reactions of Aryl Halides with [Ni(PMe Ph)]. *Chemistry - A European Journal*, **2017**, 23, 16728-16733	4.8	36
222	Computational characterization of the mechanism for the light-driven catalytic trichloromethylation of acylpyridines. *Organic and Biomolecular Chemistry*, **2017**, 15, 8641-8647	3.9	16
221	Catalytic Nitrene Transfer To Alkynes: A Novel and Versatile Route for the Synthesis of Sulfinamides and Isothiazoles. *Angewandte Chemie*, **2017**, 129, 13022-13027	3.6	8
220	Catalytic Nitrene Transfer To Alkynes: A Novel and Versatile Route for the Synthesis of Sulfinamides and Isothiazoles. *Angewandte Chemie - International Edition*, **2017**, 56, 12842-12847	16.4	28
219	Cyclobutene vs 1,3-Diene Formation in the Gold-Catalyzed Reaction of Alkynes with Alkenes: The Complete Mechanistic Picture. *Journal of the American Chemical Society*, **2017**, 139, 10302-10311	16.4	52
218	ONIOM(QM:AMOEBA09) Study on Binding Energies and Binding Preference of OH, HCO, and CH3 Radicals on Hexagonal Water Ice (Ih). *Journal of Physical Chemistry C*, **2017**, 121, 15223-15232	3.8	13
217	Mechanistic Studies on Gold-Catalyzed Direct Arene CH Bond Functionalization by Carbene Insertion: The Coinage-Metal Effect. *Organometallics*, **2017**, 36, 172-179	3.8	41
216	Stereoselective and Versatile Preparation of Tri- and Tetrasubstituted Allylic Amine Scaffolds under Mild Conditions. *Journal of the American Chemical Society*, **2016**, 138, 11970-8	16.4	109
215	Mechanistic Investigation of Iridium-Catalyzed CH Borylation of Methyl Benzoate: Ligand Effects in Regioselectivity and Activity. *Organometallics*, **2016**, 35, 3221-3226	3.8	18

214	Cooperative Reductive Elimination: The Missing Piece in the Oxidative-Coupling Mechanistic Puzzle. *Angewandte Chemie*, **2016**, 128, 2814-2817	3.6	11
213	DFT Rationalization of the Diverse Outcomes of the Iodine(III)-Mediated Oxidative Amination of Alkenes. *Chemistry - A European Journal*, **2016**, 22, 7545-53	4.8	31
212	Cooperative Reductive Elimination: The Missing Piece in the Oxidative-Coupling Mechanistic Puzzle. *Angewandte Chemie - International Edition*, **2016**, 55, 2764-7	16.4	38
211	Computational Characterization of the Origin of Selectivity in Cycloaddition Reactions Catalyzed by Phosphoric Acid Derivatives. *Chemistry - an Asian Journal*, **2016**, 11, 411-6	4.5	18
210	Computational Study on the Mechanism of the Acceleration of 1,3-Dipolar Cycloaddition inside Cucurbit[6]uril. *ACS Catalysis*, **2015**, 5, 2445-2451	13.1	49
209	Computational study with DFT and kinetic models on the mechanism of photoinitiated aromatic perfluoroalkylations. *Organic Letters*, **2015**, 17, 2676-9	6.2	55
208	Managing the computational chemistry big data problem: the ioChem-BD platform. *Journal of Chemical Information and Modeling*, **2015**, 55, 95-103	6.1	289
207	A computational view on the reactions of hydrocarbons with coinage metal complexes. *Journal of Organometallic Chemistry*, **2015**, 784, 2-12	2.3	33
206	QM/MM Calculations on Selectivity in Homogeneous Catalysis. *Structure and Bonding*, **2015**, 59-79	0.9	5
205	Functionalization of CnH2n+2 Alkanes: Supercritical Carbon Dioxide Enhances the Reactivity towards Primary Carbon□Hydrogen Bonds. *ChemCatChem*, **2015**, 7, 3254-3260	5.2	19
204	Redox Non-innocent Ligand Controls Water Oxidation Overpotential in a New Family of Mononuclear Cu-Based Efficient Catalysts. *Journal of the American Chemical Society*, **2015**, 137, 6758-61	16.4	210
203	Rationale for the sluggish oxidative addition of aryl halides to Au(I). *Chemical Communications*, **2014**, 50, 1533-6	5.8	59
202	Toward a mechanistic understanding of oxidative homocoupling: the Glaser□Hay reaction. *Catalysis Science and Technology*, **2014**, 4, 4200-4209	5.5	46
201	On the Feasibility of Nickel-Catalyzed Trifluoromethylation of Aryl Halides. *Organometallics*, **2014**, 33, 6531-6543	3.8	35
200	Catalytic Copper-Mediated Ring Opening and Functionalization of Benzoxazoles. *ACS Catalysis*, **2014**, 4, 4215-4222	13.1	14
199	Chiral transition-metal complexes as Br□sted-acid catalysts for the asymmetric Friedel-Crafts hydroxyalkylation of indoles. *Dalton Transactions*, **2014**, 43, 11260-8	4.3	21
198	Pd-catalysed mono- and dicarbonylation of aryl iodides: insights into the mechanism and the selectivity. *Chemistry - A European Journal*, **2014**, 20, 10982-9	4.8	24
197	The Transmetalation Process in Suzuki□Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. *ChemCatChem*, **2014**, 6, 3132-3138	5.2	55

196	Computational characterization of the mechanism for coinage-metal-catalyzed carboxylation of terminal alkynes. *Journal of Organic Chemistry*, **2014**, 79, 11981-7	4.2	32
195	Silver-Catalyzed Functionalization of Esters by Carbene Transfer: The Role of Ylide Zwitterionic Intermediates. *ChemCatChem*, **2014**, 6, 2206-2210	5.2	19
194	Chemo-, regio-, and stereoselective silver-catalyzed aziridination of dienes: scope, mechanistic studies, and ring-opening reactions. *Journal of the American Chemical Society*, **2014**, 136, 5342-50	16.4	76
193	An unusual example of hypervalent silicon: a five-coordinate silyl group bridging two palladium or nickel centers through a nonsymmetrical four-center two-electron bond. *Angewandte Chemie - International Edition*, **2014**, 53, 1103-8	16.4	32
192	╫H Abstraction/1,3-CH Bond Addition as a Mechanism for the Activation of CH Bonds at Early Transition Metal Centers. *Organometallics*, **2014**, 33, 7270-7278	3.8	15
191	Reaction of alkynes and azides: not triazoles through copper-acetylides but oxazoles through copper-nitrene intermediates. *Chemistry - A European Journal*, **2014**, 20, 3463-74	4.8	37
190	Computational perspective on Pd-catalyzed C-C cross-coupling reaction mechanisms. *Accounts of Chemical Research*, **2013**, 46, 2626-34	24.3	253
189	Catalytic cross-coupling of diazo compounds with coinage metal-based catalysts: an experimental and theoretical study. *Dalton Transactions*, **2013**, 42, 4132-8	4.3	55
188	Computational characterization of a mechanism for the copper-catalyzed aerobic oxidative trifluoromethylation of terminal alkynes. *Chemical Communications*, **2013**, 49, 10486-8	5.8	33
187	A general mechanism for the copper- and silver-catalyzed olefin aziridination reactions: concomitant involvement of the singlet and triplet pathways. *Journal of the American Chemical Society*, **2013**, 135, 1338-48	16.4	136
186	Oxidative Additions of Aryl Halides to Palladium Proceed through the Monoligated Complex. *ChemCatChem*, **2013**, 5, 3604-3609	5.2	62
185	A computational study on the intriguing mechanisms of the gas-phase thermal activation of methane by bare [Ni(H)(OH)]+. *Physical Chemistry Chemical Physics*, **2012**, 14, 9306-10	3.6	9
184	Mild, reversible reaction of iridium(III) amido complexes with carbon dioxide. *Inorganic Chemistry*, **2012**, 51, 9683-93	5.1	17
183	Substitution reactions in dinuclear Ru-Hbpp complexes: an evaluation of through-space interactions. *Inorganic Chemistry*, **2012**, 51, 1889-901	5.1	21
182	Merging sustainability with organocatalysis in the formation of organic carbonates by using CO(2) as a feedstock. *ChemSusChem*, **2012**, 5, 2032-8	8.3	247
181	Homogeneous Computational Catalysis: The Mechanism for Cross-Coupling and Other C-C Bond Formation Processes. *NATO Science for Peace and Security Series B: Physics and Biophysics*, **2012**, 185-206	0.2	1
180	Transition metal catalysis by density functional theory and density functional theory/molecular mechanics. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2012**, 2, 375-385	7.9	78
179	Synthesis of PCP-supported nickel complexes and their reactivity with carbon dioxide. *Chemistry - A European Journal*, **2012**, 18, 6915-27	4.8	63

178	The role of cyclobutenes in gold(I)-catalysed skeletal rearrangement of 1,6-enynes. *Organic and Biomolecular Chemistry*, **2012**, 10, 6105-11	3.9	49
177	Mechanism of the gold-catalyzed cyclopropanation of alkenes with 1,6-enynes. *Chemical Science*, **2011**, 2, 141-149	9.4	83
176	Quantum mechanics/molecular mechanics methods can be more accurate than full quantum mechanics in systems involving dispersion correlations. *Physical Chemistry Chemical Physics*, **2011**, 13, 10520-6	3.6	18
175	Phosphine and solvent effects on oxidative addition of CH3Br to Pd(PR3) and Pd(PR3)2 complexes. *Dalton Transactions*, **2011**, 40, 11089-94	4.3	44
174	Theoretical Evaluation of Phosphine Effects in Cross-Coupling Reactions. *Catalysis By Metal Complexes*, **2011**, 57-84		10
173	Aromatic versus Benzylic CH Bond Activation of Alkylaromatics by a Transient η2-Cyclopropene Complex. *Organometallics*, **2011**, 30, 3999-4007	3.8	15
172	Mechanism of Side Reactions in Alkane C?H Bond Functionalization by Diazo Compounds Catalyzed by Ag and Cu Homoscorpionate Complexes□A DFT Study. *ChemCatChem*, **2011**, 3, 1646-1652	5.2	37
171	The importance of conformational search: a test case on the catalytic cycle of the Suzuki□Miyaura cross-coupling. *Theoretical Chemistry Accounts*, **2011**, 128, 639-646	1.9	57
170	A computational study on the role of chiral N-oxides in enantioselective Pauson-Khand reactions. *Chemistry - A European Journal*, **2011**, 17, 10050-7	4.8	14
169	Mechanistic and computational studies of the atom transfer radical addition of CCl4 to styrene catalyzed by copper homoscorpionate complexes. *Inorganic Chemistry*, **2011**, 50, 2458-67	5.1	35
168	A DFT Study of the Effect of the Ligands in the Reductive Elimination from Palladium Bis(allyl) Complexes□ *Organometallics*, **2010**, 29, 4983-4991	3.8	52
167	Copper(I)□Olefin Complexes: The Effect of the Trispyrazolylborate Ancillary Ligand in Structure and Reactivity. *Organometallics*, **2010**, 29, 3481-3489	3.8	29
166	Mechanism for Hydride-Assisted Rearrangement from Ethylidene to Ethylene in Iridium Cationic Complexes. *Organometallics*, **2010**, 29, 2040-2045	3.8	27
165	C-H bond activation of benzene by unsaturated η2-cyclopropene and η2-benzyne complexes of niobium. *Journal of the American Chemical Society*, **2010**, 132, 14239-50	16.4	35
164	Mechanistic study of amine to imine oxidation in a dinuclear Cu(II) complex containing an octaaza dinucleating ligand. *Inorganic Chemistry*, **2010**, 49, 5977-85	5.1	27
163	Highly modular P-OP ligands for asymmetric hydrogenation: synthesis, catalytic activity, and mechanism. *Chemistry - A European Journal*, **2010**, 16, 6495-508	4.8	61
162	Metal-arene interactions in dialkylbiarylphosphane complexes of copper, silver, and gold. *Chemistry - A European Journal*, **2010**, 16, 5324-32	4.8	135
161	Through-space ligand interactions in enantiomeric dinuclear Ru complexes. *Chemistry - A European Journal*, **2010**, 16, 7965-8	4.8	20

160	Competitive and selective Csp3-Br versus Csp2-Br bond activation in palladium-catalysed Suzuki cross-coupling: an experimental and theoretical study of the role of phosphine ligands. *Chemistry - A European Journal*, **2010**, 16, 13390-7	4.8	62
159	Palladium round trip in the Negishi coupling of trans-[PdMeCl(PMePh2)2] with ZnMeCl: an experimental and DFT study of the transmetalation step. *Chemistry - A European Journal*, **2010**, 16, 8596-9	4.8	70
158	Origin of enantioselectivity in asymmetric Pauson□hand reactions catalyzed by [(BINAP)Co2(CO)6]?. *Journal of Molecular Catalysis A*, **2010**, 324, 127-132		10
157	Structural analysis of zincocenes with substituted cyclopentadienyl rings. *Chemistry - A European Journal*, **2009**, 15, 924-35	4.8	15
156	Br□sted acid catalyzed Morita-Baylis-Hillman reaction: a new mechanistic view for thioureas revealed by ESI-MS(/MS) monitoring and DFT calculations. *Chemistry - A European Journal*, **2009**, 15, 12460-9	4.8	69
155	The role of amide ligands in the stabilization of Pd(II) tricoordinated complexes: is the Pd□NR2 bond order single or higher?. *Theoretical Chemistry Accounts*, **2009**, 123, 75-84	1.9	8
154	Agostic interactions in alkyl derivatives of sterically hindered tris(pyrazolyl)borate complexes of niobium. *Coordination Chemistry Reviews*, **2009**, 253, 635-646	23.2	44
153	Protonation of transition-metal hydrides: a not so simple process. *Chemical Society Reviews*, **2009**, 38, 957-66	58.5	93
152	Why is the Suzuki-Miyaura cross-coupling of sp3 carbons in alpha-bromo sulfoxide systems fast and stereoselective? A DFT study on the mechanism. *Journal of Organic Chemistry*, **2009**, 74, 4049-54	4.2	52
151	C□ Coupling Constants, JCC, Are Reliable Probes for □C□ Agostic Structures. *Organometallics*, **2009**, 28, 940-943	3.8	23
150	The Nature of M□B Versus M?B Bonds in Cationic Terminal Borylene Complexes: Structure and Energy Analysis in the Borylene Complexes [(□5-C5H5)(CO)2M{B(□5-C5Me5)}]+, [(□5-C5H5)(CO)2M(BMes)]+, and [(□5-C5H5)(CO)2M(BNMe2)]+ (M = Fe, Ru, Os). *Organometallics*, **2009**, 28, 6442-6449	3.8	19
149	Vinyl acetate synthesis on homogeneous and heterogeneous Pd-based catalysts: a theoretical analysis on the reaction mechanisms. *Journal of Physical Chemistry A*, **2009**, 113, 11758-62	2.8	10
148	The Mechanism of the Catalytic Functionalization of Haloalkanes by Carbene Insertion: An Experimental and Theoretical Study. *Organometallics*, **2009**, 28, 5968-5981	3.8	46
147	Gold(I)-catalyzed intermolecular hydroalkoxylation of allenes: a DFT study. *Organic Letters*, **2009**, 11, 2237-40	6.2	114
146	Mechanism of the [(NHC)Au(I)]-catalyzed rearrangement of allylic acetates. A DFT study. *Organic Letters*, **2009**, 11, 81-4	6.2	41
145	Oxidative dehydrogenation of an amine group of a macrocyclic ligand in the coordination sphere of a Cu(II) complex. *Dalton Transactions*, **2009**, 6013-20	4.3	17
144	A DFT/MM analysis of the effect of ligand substituents on asymmetric hydrogenation catalyzed by rhodium complexes with phosphine□phosphinite ligands. *Canadian Journal of Chemistry*, **2009**, 87, 1273-1279	0.9	29
143	C-C reductive elimination in palladium complexes, and the role of coupling additives. A DFT study supported by experiment. *Journal of the American Chemical Society*, **2009**, 131, 3650-7	16.4	167

142	QM/MM methods in inorganic chemistry. *Dalton Transactions*, **2008**, 2911-9	4.3	69
141	Direct arylation of arene C-H bonds by cooperative action of NHcarbene-ruthenium(II) catalyst and carbonate via proton abstraction mechanism. *Journal of the American Chemical Society*, **2008**, 130, 1156-7	16.4	347
140	On the Origin of □and #Agostic Distortions in Early-Transition-Metal Alkyl Complexes. *Organometallics*, **2008**, 27, 1128-1134	3.8	51
139	Towards configurationally stable [4]helicenes: enantioselective synthesis of 12-substituted 7,8-dihydro[4]helicene quinones. *Chemistry - A European Journal*, **2008**, 14, 603-20	4.8	65
138	Selective homogeneous and heterogeneous gold catalysis with alkynes and alkenes: similar behavior, different origin. *ChemPhysChem*, **2008**, 9, 1624-9	3.2	111
137	DFT modeling of reactivity in an ionic liquid: How many ion pairs?. *Journal of Computational Chemistry*, **2008**, 29, 892-9	3.5	24
136	DFT/MM Study on Copper-Catalyzed Cyclopropanation □Enantioselectivity with No Enthalpy Barrier. *European Journal of Organic Chemistry*, **2008**, 2008, 5614-5621	3.2	18
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