

Odile Eisenstein

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

338
papers

19,437
citations

76
h-index

121
g-index

385
ext. papers

20,531
ext. citations

8.5
avg, IF

6.63
L-index

#	Paper	IF	Citations
338	Computational Catalysis: A Land of Opportunities. <i>Topics in Catalysis</i> , 2022 , 65, 1-5	2.3	
337	P Chemical Shifts in Ru(II) Phosphine Complexes. A Computational Study of the Influence of the Coordination Sphere. <i>Inorganic Chemistry</i> , 2020 , 59, 17038-17048	5.1	8
336	The Grignard Reaction - Unraveling a Chemical Puzzle. <i>Journal of the American Chemical Society</i> , 2020 , 142, 2984-2994	16.4	33
335	Efficient alkene hydrosilylation with bis(8-quinolyl)phosphine (NPN) nickel catalysts. The dominant role of silyl-over hydrido-nickel catalytic intermediates. <i>Chemical Science</i> , 2020 , 11, 5043-5051	9.4	2
334	What Makes a Good (Computed) Energy Profile?. <i>Topics in Organometallic Chemistry</i> , 2020 , 1-38	0.6	9
333	Carbon-13 NMR Chemical Shift: A Descriptor for Electronic Structure and Reactivity of Organometallic Compounds. <i>Accounts of Chemical Research</i> , 2019 , 52, 2278-2289	24.3	54
332	Physical methods for mechanistic understanding: general discussion. <i>Faraday Discussions</i> , 2019 , 220, 144-178	3.6	
331	Mechanistic insight into organic and industrial transformations: general discussion. <i>Faraday Discussions</i> , 2019 , 220, 282-316	3.6	7
330	Computational and theoretical approaches for mechanistic understanding: general discussion. <i>Faraday Discussions</i> , 2019 , 220, 464-488	3.6	2
329	Concluding remarks for "Mechanistic Processes in Organometallic Chemistry": the importance of a multidisciplinary approach. <i>Faraday Discussions</i> , 2019 , 220, 489-495	3.6	4
328	σ-Bond Character in Metal-Alkyl Compounds for C-H Activation: How, When, and Why?. <i>Journal of the American Chemical Society</i> , 2019 , 141, 648-656	16.4	32
327	Modelling the surface of amorphous dehydroxylated silica: the influence of the potential on the nature and density of defects. <i>New Journal of Chemistry</i> , 2018 , 42, 1356-1367	3.6	9
326	Metal alkyls programmed to generate metal alkylidenes by β-H abstraction: prognosis from NMR chemical shift. <i>Chemical Science</i> , 2018 , 9, 1912-1918	9.4	43
325	Zirconocene-Mediated Selective C-C Bond Cleavage of Strained Carbocycles: Scope and Mechanism. <i>Journal of Organic Chemistry</i> , 2018 , 83, 3497-3515	4.2	20
324	The Key Role of the Hemiaminal Intermediate in the Iron-Catalyzed Deaminative Hydrogenation of Amides. <i>ACS Catalysis</i> , 2018 , 8, 8751-8762	13.1	38
323	NMR chemical shift analysis decodes olefin oligo- and polymerization activity of d group 4 metal complexes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, E5867-E5876	11.5	35
322	Catalytic Olefin Hydrosilylations Mediated by Ruthenium η ² -H ₂ Si η ² -Complexes of Primary and Secondary Silanes. <i>ACS Catalysis</i> , 2018 , 8, 11513-11523	13.1	6

3 ²¹	Orbital Analysis of Carbon-13 Chemical Shift Tensors Reveals Patterns to Distinguish Fischer and Schrock Carbenes. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 10127-10131	16.4	47
3 ²⁰	Orbital Analysis of Carbon-13 Chemical Shift Tensors Reveals Patterns to Distinguish Fischer and Schrock Carbenes. <i>Angewandte Chemie</i> , 2017 , 129, 10261-10265	3.6	10
3 ¹⁹	Metathesis Activity Encoded in the Metallacyclobutane Carbon-13 NMR Chemical Shift Tensors. <i>ACS Central Science</i> , 2017 , 3, 759-768	16.8	67
3 ¹⁸	How Solvent Dynamics Controls the Schlenk Equilibrium of Grignard Reagents: A Computational Study of CHMgCl in Tetrahydrofuran. <i>Journal of Physical Chemistry B</i> , 2017 , 121, 4226-4237	3.4	35
3 ¹⁷	Structure, Bonding, and Reactivity of Organoaluminum Molecular Species: A Computational Perspective 2017 , 1-32		
3 ¹⁶	Aromatic C-H Bond Activation by Ni ⁰ , Pd ⁰ , and Pt ⁰ Alkene Complexes: Concerted Oxidative Addition to Metal vs Ligand-to-Ligand H Transfer Mechanism. <i>Organometallics</i> , 2017 , 36, 2761-2771	3.8	55
3 ¹⁵	Molecular and Silica-Supported Molybdenum Alkyne Metathesis Catalysts: Influence of Electronics and Dynamics on Activity Revealed by Kinetics, Solid-State NMR, and Chemical Shift Analysis. <i>Journal of the American Chemical Society</i> , 2017 , 139, 17597-17607	16.4	60
3 ¹⁴	Selectivity of C-H Activation and Competition between C-H and C-F Bond Activation at Fluorocarbons. <i>Chemical Reviews</i> , 2017 , 117, 8710-8753	68.1	190
3 ¹³	Experimental and DFT Computational Study of β -Me and β -H Elimination Coupled with Proton Transfer: From Amides to Enamides in Cp* ₂ MX (M = La, Ce). <i>Organometallics</i> , 2017 , 36, 97-108	3.8	11
3 ¹²	Elucidating the Link between NMR Chemical Shifts and Electronic Structure in d(0) Olefin Metathesis Catalysts. <i>Journal of the American Chemical Society</i> , 2016 , 138, 2261-72	16.4	79
3 ¹¹	Coordination and insertion of alkenes and alkynes in Au(III) complexes: nature of the intermediates from a computational perspective. <i>Dalton Transactions</i> , 2016 , 45, 5504-13	4.3	18
3 ¹⁰	Deciphering Selectivity in Organic Reactions: A Multifaceted Problem. <i>Accounts of Chemical Research</i> , 2016 , 49, 1070-8	24.3	25
3 ⁰⁹	Remote functionalization of hydrocarbons with reversibility enhanced stereocontrol. <i>Chemical Science</i> , 2015 , 6, 2770-2776	9.4	57
3 ⁰⁸	Metallacyclobutanes from Schrock-Type d ⁰ Metal Alkylidene Catalysts: Structural Preferences and Consequences in Alkene Metathesis. <i>Organometallics</i> , 2015 , 34, 1668-1680	3.8	49
3 ⁰⁷	Donor-Promoted 1,2-Hydrogen Migration from Silicon to a Saturated Ruthenium Center and Access to Silaoxiranyl and Silaiminyl Complexes. <i>Journal of the American Chemical Society</i> , 2015 , 137, 9186-94	16.4	11
3 ⁰⁶	Insights from Computational Studies on d ⁰ Metal-Catalyzed Alkene and Alkyne Metathesis and Related Reactions 2015 , 159-197		2
3 ⁰⁵	Modelling and Rationalizing Organometallic Chemistry with Computation: Where Are We?. <i>Structure and Bonding</i> , 2015 , 1-37	0.9	12
3 ⁰⁴	Hydrazine N-N Bond Cleavage over Silica-Supported Tantalum-Hydrides. <i>Inorganic Chemistry</i> , 2015 , 54, 11648-59	5.1	6

303	Conformational complexity of morphine and morphinum in the gas phase and in water. A DFT and MP2 study. <i>RSC Advances</i> , 2014 , 4, 24729-24735	3.7	0
302	Linear-selective hydroarylation of unactivated terminal and internal olefins with trifluoromethyl-substituted arenes. <i>Journal of the American Chemical Society</i> , 2014 , 136, 13098-101	16.4	217
301	Cyclometalated N-heterocyclic carbene complexes of ruthenium for access to electron-rich silylene complexes that bind the Lewis acids CuOTf and AgOTf. <i>Journal of the American Chemical Society</i> , 2014 , 136, 11473-82	16.4	26
300	Nonclassical CH- π supramolecular interactions in artemisinic acid favor a single conformation, yielding high diastereoselectivity in the reduction with diazene. <i>Journal of Organic Chemistry</i> , 2014 , 79, 5939-47	4.2	13
299	1,2-hydrogen migration to a saturated ruthenium complex via reversal of electronic properties for tin in a stannylene-to-metallostannylene conversion. <i>Journal of the American Chemical Society</i> , 2014 , 136, 13991-4	16.4	25
298	Computational Studies Explain the Importance of Two Different Substituents on the Chelating Bis(amido) Ligand for Transfer Hydrogenation by Bifunctional Cp*Rh(III) Catalysts. <i>Organometallics</i> , 2014 , 33, 3433-3442	3.8	37
297	Two [1,2,4-(Me ₃ C) ₃ C ₅ H ₂] ₂ CeH molecules are involved in hydrogenation of pyridine to piperidine as shown by experiments and computations. <i>Inorganic Chemistry</i> , 2014 , 53, 6361-73	5.1	18
296	Mechanistic insights on the stereoselective nucleophilic 1,2-addition to sulfinyl imines. <i>Journal of Organic Chemistry</i> , 2014 , 79, 2514-21	4.2	16
295	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. <i>Angewandte Chemie</i> , 2014 , 126, 1121-1126	3.6	3
294	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. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 1103-8	16.4	32
293	Stereoselectivity through a network of non-classical CH weak interactions: a prospective study of a bicyclic organocatalytic scaffold. <i>New Journal of Chemistry</i> , 2014 , 38, 5975-5982	3.6	4
292	Generation and Structural Characterization of a Gold(III) Alkene Complex. <i>Angewandte Chemie</i> , 2013 , 125, 1704-1707	3.6	24
291	Theoretical Studies on the Reaction Mechanism of Metal-Assisted CH Activation 2013 , 695-726		6
290	Decamethylscandocinium-hydrido-(perfluorophenyl)borate: fixation and tandem tris(perfluorophenyl)borane catalysed deoxygenative hydrosilation of carbon dioxide. <i>Chemical Science</i> , 2013 , 4, 2152	9.4	118
289	Outer sphere hydrogenation catalysis. <i>New Journal of Chemistry</i> , 2013 , 37, 21-27	3.6	144
288	Cleaving bonds in CH ₃ OSO ₂ CF ₃ with [1,2,4-(Me ₃ C) ₃ C ₅ H ₂] ₂ CeH; an experimental and computational study. <i>New Journal of Chemistry</i> , 2013 , 37, 132-142	3.6	12
287	Generation and structural characterization of a gold(III) alkene complex. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 1660-3	16.4	56
286	Successive heterolytic cleavages of H ₂ achieve N ₂ splitting on silica-supported tantalum hydrides: a DFT proposed mechanism. <i>Inorganic Chemistry</i> , 2012 , 51, 7237-49	5.1	33

285	Selectivity in the C-H Activation Reaction of CH ₃ OSO ₂ CH ₃ with [1,2,4-(Me ₃ C) ₃ C ₅ H ₂] ₂ CeH or [1,2,4-(Me ₃ C) ₃ C ₅ H ₂][1,2-(Me ₃ C) ₂ -4-(Me ₂ CCH ₂)C ₅ H ₂]Ce: To Choose or Not To Choose. <i>Organometallics</i> , 2012 , 31, 870-881	3.8	13
284	Symmetrical hydrogen bonds in iridium(III) alkoxides with relevance to outer sphere hydrogen transfer. <i>Inorganic Chemistry</i> , 2012 , 51, 12313-23	5.1	17
283	Cp* Iridium Precatalysts for Selective C-H Oxidation via Direct Oxygen Insertion: A Joint Experimental/Computational Study. <i>ACS Catalysis</i> , 2012 , 2, 208-218	13.1	78
282	Hydrofluoroarylation of Alkynes with Ni Catalysts. C-H Activation via Ligand-to-Ligand Hydrogen Transfer, an Alternative to Oxidative Addition. <i>Organometallics</i> , 2012 , 31, 1300-1314	3.8	123
281	Structures of d ⁴ MH ₃ X: a computational study of the influence of the metal and the ligands. <i>Inorganic Chemistry</i> , 2012 , 51, 5705-15	5.1	
280	Oxo vs Imido Alkylidene d ⁰ -Metal Species: How and Why Do They Differ in Structure, Activity, and Efficiency in Alkene Metathesis?. <i>Organometallics</i> , 2012 , 31, 6812-6822	3.8	77
279	Carbon monoxide activation via O-bound CO using decamethylscandocinium-hydridoborate ion pairs. <i>Journal of the American Chemical Society</i> , 2012 , 134, 10843-51	16.4	83
278	C-F and C-H bond activation of fluorobenzenes and fluoropyridines at transition metal centers: how fluorine tips the scales. <i>Accounts of Chemical Research</i> , 2011 , 44, 333-48	24.3	391
277	Iridium-catalyzed hydrogenation of N-heterocyclic compounds under mild conditions by an outer-sphere pathway. <i>Journal of the American Chemical Society</i> , 2011 , 133, 7547-62	16.4	257
276	DFT calculations of ²⁹ Si-NMR chemical shifts in Ru(II) silyl complexes: searching for trends and accurate values. <i>Dalton Transactions</i> , 2011 , 40, 11321-6	4.3	8
275	Heterolytic cleavage of ammonia N-H bond by bifunctional activation in silica-grafted single site Ta(V) imido amido surface complex. Importance of the outer sphere NH ₃ assistance. <i>New Journal of Chemistry</i> , 2011 , 35, 1011	3.6	11
274	Half-sandwich iridium complexes for homogeneous water-oxidation catalysis. <i>Journal of the American Chemical Society</i> , 2010 , 132, 16017-29	16.4	468
273	An Experimental/theoretical Study of the Factors That Affect the Switch between Ruthenium-Catalyzed Dehydrogenative Amide Formation versus Amine Alkylation. <i>Organometallics</i> , 2010 , 29, 6548-6558	3.8	98
272	Shutting down secondary reaction pathways: the essential role of the pyrrolyl ligand in improving silica supported d ⁰ -ML ₄ alkene metathesis catalysts from DFT calculations. <i>Journal of the American Chemical Society</i> , 2010 , 132, 7750-7	16.4	113
271	Bridging Silyl Groups in σ-Bond Metathesis and [1,2]-Shifts. Experimental and Computational Study of the Reaction between Cerium Metallocenes and MeOSiMe ₃ . <i>Organometallics</i> , 2010 , 29, 5103-5110	3.8	20
270	Intermediate-valence tautomerism in decamethylterbocene complexes of methyl-substituted bipyridines. <i>Journal of the American Chemical Society</i> , 2010 , 132, 17537-49	16.4	82
269	C-H bond activation in transition metal species from a computational perspective. <i>Chemical Reviews</i> , 2010 , 110, 749-823	68.1	877
268	Manganese catalysts for C-H activation: an experimental/theoretical study identifies the stereoelectronic factor that controls the switch between hydroxylation and desaturation pathways. <i>Journal of the American Chemical Society</i> , 2010 , 132, 7605-16	16.4	94

267	Importance of palladium-carbon bond energies in direct arylation of polyfluorinated benzenes. <i>Dalton Transactions</i> , 2010 , 39, 10510-9	4.3	50
266	Catalytic hydrosilylation of olefins with organolanthanides: A DFT study. Part I: Hydrosilylation of propene by SiH ₄ . <i>Dalton Transactions</i> , 2010 , 39, 10749-56	4.3	15
265	The reaction of bis(1,2,4-tri- <i>t</i> -butylcyclopentadienyl)ceriumbenzyl, Cp' ₂ CeCH ₂ Ph, with methylhalides: a metathesis reaction that does not proceed by a metathesis transition state. <i>Dalton Transactions</i> , 2010 , 39, 6648-60	4.3	28
264	Splitting a C–D bond in dialkylethers with bis(1,2,4-tri- <i>tert</i> -butylcyclopentadienyl)cerium hydride does not occur by a σ bond metathesis pathway: a combined experimental and DFT computational study. <i>New Journal of Chemistry</i> , 2010 , 34, 2189	3.6	10
263	Catalytic hydrosilylation of olefins with organolanthanide complexes: a DFT study. Part II: Influence of the substitution on olefin and silane. <i>Dalton Transactions</i> , 2010 , 39, 10757-67	4.3	11
262	Synthesis, structure, and reductive elimination in the series Tp' [*] Rh(PR ₃)(Ar(F))H; determination of rhodium-carbon bond energies of fluoroaryl substituents. <i>Dalton Transactions</i> , 2010 , 39, 10495-509	4.3	32
261	Facile Interconversion of [Cp ₂ (Cl)Hf(SnH ₃)] and [Cp ₂ (Cl)Hf(η -H)SnH ₂]: DFT Investigations of Hafnocene Stannyl Complexes as Masked Stannylenes. <i>Angewandte Chemie</i> , 2010 , 122, 1860-1863	3.6	3
260	Facile interconversion of [Cp ₂ (Cl)Hf(SnH ₃)] and [Cp ₂ (Cl)Hf(μ -H)SnH ₂]: DFT investigations of hafnocene stannyl complexes as masked stannylenes. <i>Angewandte Chemie - International Edition</i> , 2010 , 49, 1816-9	16.4	14
259	Mechanistic investigation of vinylic carbon-fluorine bond activation of perfluorinated cycloalkenes using Cp* ₂ ZrH ₂ and Cp* ₂ ZrHF. <i>Journal of Fluorine Chemistry</i> , 2010 , 131, 1122-1132	2.1	40
258	H/D Exchange on Silica-Grafted Tantalum(V) Imido Amido [(η -SiO) ₂ Ta(V)(NH)(NH ₂)] Synthesized from Either Ammonia or Dinitrogen: IR and DFT Evidence for Heterolytic Splitting of D ₂ . <i>Topics in Catalysis</i> , 2009 , 52, 1482-1491	2.3	14
257	Bond Activations of PhSiH ₃ by Cp ₂ SmH: A Mechanistic Investigation by the DFT Method. <i>Organometallics</i> , 2009 , 28, 3767-3775	3.8	31
256	The Bond between CO and Cp* ₃ U in Cp* ₃ U(CO) Involves Back-bonding from the Cp* ₃ U Ligand-Based Orbitals of π Symmetry, where Cp* Represents a Substituted Cyclopentadienyl Ligand. <i>Organometallics</i> , 2009 , 28, 3629-3635	3.8	51
255	Hydrogen for X-Group Exchange in CH ₃ X (X = Cl, Br, I, OMe, and NMe ₂) by Monomeric [1,2,4-(Me ₃ C) ₃ C ₅ H ₂] ₂ CeH: Experimental and Computational Support for a Carbenoid Mechanism. <i>Organometallics</i> , 2009 , 28, 3173-3185	3.8	39
254	Energetics of C-H bond activation of fluorinated aromatic hydrocarbons using a [Tp' [*] Rh(CNneopentyl)] complex. <i>Journal of the American Chemical Society</i> , 2009 , 131, 13464-73	16.4	109
253	Highly active and robust Cp* iridium complexes for catalytic water oxidation. <i>Journal of the American Chemical Society</i> , 2009 , 131, 8730-1	16.4	516
252	Exceptional sensitivity of metal-aryl bond energies to ortho-fluorine substituents: influence of the metal, the coordination sphere, and the spectator ligands on M-C/H-C bond energy correlations. <i>Journal of the American Chemical Society</i> , 2009 , 131, 7817-27	16.4	149
251	Synthesis and structure of "16-electron" rhodium(III) catalysts for transfer hydrogenation of a cyclic imine: mechanistic implications. <i>Chemical Communications</i> , 2009 , 6801-3	5.8	33
250	Decamethylterbocene complexes of bipyridines and diazabutadienes: multiconfigurational ground states and open-shell singlet formation. <i>Journal of the American Chemical Society</i> , 2009 , 131, 6480-91	16.4	97

249	Molecular recognition in Mn-catalyzed C-H oxidation. Reaction mechanism and origin of selectivity from a DFT perspective. <i>Dalton Transactions</i> , 2009 , 5989-6000	4.3	25
248	Metal fragment isomerisation upon grafting a d(2) ML4 perhydrocarbyl Os complex on a silica surface: origin and consequence. <i>Dalton Transactions</i> , 2009 , 5879-86	4.3	15
247	The mechanism of N-vinylindole formation via tandem imine formation and cycloisomerisation of o-ethynylanilines. <i>Dalton Transactions</i> , 2009 , 10296-304	4.3	9
246	C-H oxidation by hydroxo manganese(v) porphyrins: a DFT study. <i>Chemical Communications</i> , 2009 , 1772-4.8	4.8	41
245	Mechanism of Homogeneous Iridium-Catalyzed Alkylation of Amines with Alcohols from a DFT Study. <i>Organometallics</i> , 2008 , 27, 2529-2535	3.8	142
244	The rebound mechanism in catalytic C-H oxidation by MnO(tpp)Cl from DFT studies: electronic nature of the active species. <i>Chemical Communications</i> , 2008 , 744-6	5.8	64
243	Stereochemical nonrigidity of a chiral rhodium boryl hydride complex: a sigma-borane complex as transition state for isomerization. <i>Journal of the American Chemical Society</i> , 2008 , 130, 4375-85	16.4	19
242	Beta-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. <i>Journal of the American Chemical Society</i> , 2008 , 130, 6288-97	16.4	85
241	Cationic methyl complexes of the rare-earth metals: an experimental and computational study on synthesis, structure, and reactivity. <i>Inorganic Chemistry</i> , 2008 , 47, 9265-78	5.1	43
240	A rational basis for the axial ligand effect in C-H oxidation by [MnO(porphyrin)(X)] ⁺ (X = H ₂ O, OH ⁻ , O ₂ ⁻) from a DFT study. <i>Inorganic Chemistry</i> , 2008 , 47, 10090-9	5.1	84
239	DFT Investigation of the Catalytic Hydromethylation of Olefins by Scandocenes. 2. Influence of the Ansa Ligand on Propene and Isobutene Hydromethylation. <i>Organometallics</i> , 2008 , 27, 2252-2257	3.8	16
238	Dynamics of silica-supported catalysts determined by combining solid-state NMR spectroscopy and DFT calculations. <i>Journal of the American Chemical Society</i> , 2008 , 130, 5886-900	16.4	88
237	A NMR, X-ray, and DFT combined study on the regio-chemistry of nucleophilic addition to platinum(II) coordinated terminal olefins. <i>Journal of Organometallic Chemistry</i> , 2008 , 693, 2819-2827	2.3	17
236	Chemoselectivity in σ -bond activation by lanthanocene complexes from a DFT perspective: reactions of Cp ₂ LnR (R = CH ₃ , H, SiH ₃) with SiH ₄ and CH ₃ SiH ₃ . <i>New Journal of Chemistry</i> , 2007 , 31, 549-555	3.6	37
235	Atom economic synthesis of amides via transition metal catalyzed rearrangement of oxaziridines. <i>Green Chemistry</i> , 2007 , 9, 976	10	31
234	Computational structure-activity relationships in H ₂ storage: how placement of N atoms affects release temperatures in organic liquid storage materials. <i>Chemical Communications</i> , 2007 , 2231-3	5.8	127
233	Single but Stronger UO, Double but Weaker UNMe Bonds: The Tale Told by Cp ₂ UO and Cp ₂ UNR. <i>Organometallics</i> , 2007 , 26, 5059-5065	3.8	90
232	Reactions of monomeric [1,2,4-(Me ₃ C) ₃ C ₅ H ₂] ₂ CeH and CO with or without H ₂ : an experimental and computational study. <i>Journal of the American Chemical Society</i> , 2007 , 129, 2529-41	16.4	64

231	Imidazolium carboxylates as versatile and selective N-heterocyclic carbene transfer agents: synthesis, mechanism, and applications. <i>Journal of the American Chemical Society</i> , 2007 , 129, 12834-46	16.4	197
230	Structural and dynamic properties of propane coordinated to TpRh(CNR) from a confrontation between theory and experiment. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 6939-44	11.5	33
229	Understanding d(0)-olefin metathesis catalysts: which metal, which ligands?. <i>Journal of the American Chemical Society</i> , 2007 , 129, 8207-16	16.4	195
228	Dinitrogen dissociation on an isolated surface tantalum atom. <i>Science</i> , 2007 , 317, 1056-60	33.3	145
227	Structure, spectroscopic and electronic properties of a well defined silica supported olefin metathesis catalyst, [(SiO)Re(CR)(CHR)(CH ₂ R)], through DFT periodic calculations: silica is just a large siloxy ligand. <i>New Journal of Chemistry</i> , 2006 , 30, 842-850	3.6	69
226	DFT studies of the methyl exchange reaction between Cp ₂ M-CH ₃ or Cp* ₂ M-CH ₃ (Cp = C ₅ H ₅ , Cp* = C ₅ Me ₅ , M = Y, Sc, Ln) and CH ₄ . Does M ionic radius control the reaction?. <i>Dalton Transactions</i> , 2006 , 3052-7	4.3	45
225	Validation of the M-C/H-C bond enthalpy relationship through application of density functional theory. <i>Journal of the American Chemical Society</i> , 2006 , 128, 8350-7	16.4	63
224	DFT calculations of d ⁰ M(NR)(CHtBu)(X)(Y) (M = Mo, W; R = CPh ₃ , 2,6-iPr-C ₆ H ₃ ; X and Y = CH ₂ tBu, OtBu, OSi(OtBu) ₃) olefin metathesis catalysts: structural, spectroscopic and electronic properties. <i>Dalton Transactions</i> , 2006 , 3077-87	4.3	52
223	A Well-Defined, Silica-Supported Tungsten Imido Alkylidene Olefin Metathesis Catalyst. <i>Organometallics</i> , 2006 , 25, 3554-3557	3.8	138
222	Silyl, Hydrido Silylene or Alternative Bonding Modes: The Many Possible Structures of [(C ₅ H ₅)(PH ₃)IrX] ⁺ (X = SiHR ₂ and SiR ₃ ; R = H, CH ₃ , SiH ₃ , and Cl). <i>Organometallics</i> , 2006 , 25, 4748-4755	3.8	9
221	DFT Investigation of the Catalytic Hydromethylation of Olefins by Metallocenes. 1. Differences between Scandium and Lutetium in Propene Hydromethylation. <i>Organometallics</i> , 2006 , 25, 5699-5708	3.8	31
220	DFT calculations of NMR J _{CâH} coupling constants: An additional tool to characterize the π -agostic interaction in high oxidation state M-alkylidene complexes (M=Re, Mo and Ta). <i>Polyhedron</i> , 2006 , 25, 339-348	2.7	32
219	Selectivity in CâCl bond activation of dichloroarenes by photogenerated Cp*Re(CO) ₂ : combined experimental and DFT studies. <i>New Journal of Chemistry</i> , 2005 , 29, 226-231	3.6	10
218	Hydrogen for fluorine exchange in C ₆ F ₆ and C ₆ F ₅ H by monomeric [1,3,4-(Me ₃ C) ₃ C ₅ H ₂] ₂ CeH: experimental and computational studies. <i>Journal of the American Chemical Society</i> , 2005 , 127, 279-92	16.4	178
217	An anion-dependent switch in selectivity results from a change of C-H activation mechanism in the reaction of an imidazolium salt with IrH ₅ (PPh ₃) ₂ . <i>Journal of the American Chemical Society</i> , 2005 , 127, 16299-311	16.4	160
216	Hydrogen for fluorine exchange in CH ₄ -xFx by monomeric [1,2,4-(Me ₃ C) ₃ C ₅ H ₂] ₂ CeH: experimental and computational studies. <i>Journal of the American Chemical Society</i> , 2005 , 127, 7781-95	16.4	86
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