

Odile Eisenstein

List of Publications by Year in descending order

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330
papers

21,933
citations

7251

80
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15698

129
g-index

385
all docs

385
docs citations

385
times ranked

12809
citing authors

#	ARTICLE	IF	CITATIONS
1	C–H Bond Activation in Transition Metal Species from a Computational Perspective. <i>Chemical Reviews</i> , 2010, 110, 749-823.	23.0	959
2	A New Intermolecular Interaction: Unconventional Hydrogen Bonds with Element–Hydride Bonds as Proton Acceptor. <i>Accounts of Chemical Research</i> , 1996, 29, 348-354.	7.6	639
3	Highly Active and Robust Cp* Iridium Complexes for Catalytic Water Oxidation. <i>Journal of the American Chemical Society</i> , 2009, 131, 8730-8731.	6.6	561
4	Half-Sandwich Iridium Complexes for Homogeneous Water-Oxidation Catalysis. <i>Journal of the American Chemical Society</i> , 2010, 132, 16017-16029.	6.6	507
5	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, 333-348.	7.6	430
6	Transition Metal Polyhydrides: From Qualitative Ideas to Reliable Computational Studies. <i>Chemical Reviews</i> , 2000, 100, 601-636.	23.0	341
7	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, 7547-7562.	6.6	296
8	Do f Electrons Play a Role in the Lanthanide–Ligand Bonds? A DFT Study of Ln(NR ₂) ₃ ; R = H, SiH ₃ . <i>Journal of Physical Chemistry A</i> , 2000, 104, 7140-7143.	1.1	292
9	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.	23.0	265
10	Linear-Selective Hydroarylation of Unactivated Terminal and Internal Olefins with Trifluoromethyl-Substituted Arenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 13098-13101.	6.6	263
11	Transition-metal complexed olefins: how their reactivity toward a nucleophile relates to their electronic structure. <i>Journal of the American Chemical Society</i> , 1981, 103, 4308-4320.	6.6	254
12	Interactions between C–H and Ni–H bonds and d ₈ square planar metal complexes: hydrogen bonded or agostic?. <i>Inorganica Chimica Acta</i> , 1997, 254, 105-111.	1.2	248
13	Factors Affecting the Strength of N–H...H–Ir Hydrogen Bonds. <i>Journal of the American Chemical Society</i> , 1995, 117, 3485-3491.	6.6	244
14	Computed Ligand Electronic Parameters from Quantum Chemistry and Their Relation to Tolman Parameters, Lever Parameters, and Hammett Constants. <i>Inorganic Chemistry</i> , 2001, 40, 5806-5811.	1.9	233
15	An attractive cis-effect of hydride on neighbor ligands: experimental and theoretical studies on the structure and intramolecular rearrangements of Fe(H) ₂ (η ² -H ₂)(PEtPh ₂) ₃ . <i>Journal of the American Chemical Society</i> , 1990, 112, 4831-4841.	6.6	226
16	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, 12834-12846.	6.6	213
17	Understanding d ₀ -Olefin Metathesis Catalysts: Which Metal, Which Ligands?. <i>Journal of the American Chemical Society</i> , 2007, 129, 8207-8216.	6.6	210
18	Theoretical study of the structures of electron-deficient d ₆ ML ₅ complexes. Importance of a π-donating ligand. <i>Organometallics</i> , 1992, 11, 729-737.	1.1	204

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19	An Unconventional Intermolecular Three-Center $\text{H}\cdots\text{H}\cdots\text{Re}$ Hydrogen Bond in Crystalline $[\text{ReH}_5(\text{PPh}_3)_3]\cdot\text{indole}\cdot\text{C}_6\text{H}_6$. <i>Angewandte Chemie International Edition in English</i> , 1995, 34, 2507-2509.	4.4	195
20	Hydrogen for Fluorine Exchange in C_6F_6 and $\text{C}_6\text{F}_5\text{H}$ by Monomeric $[\text{1,3,4-(Me}_3\text{C)}_3\text{C}_5\text{H}_2]_2\text{CeH}$: Experimental and Computational Studies. <i>Journal of the American Chemical Society</i> , 2005, 127, 279-292.	6.6	190
21	Superjacent orbital control. Interpretation of the anomeric effect. <i>Journal of the American Chemical Society</i> , 1973, 95, 3806-3807.	6.6	186
22	An Anion-Dependent Switch in Selectivity Results from a Change of $\text{C}\cdots\text{H}$ Activation Mechanism in the Reaction of an Imidazolium Salt with $\text{IrH}_5(\text{PPh}_3)_2$. <i>Journal of the American Chemical Society</i> , 2005, 127, 16299-16311.	6.6	172
23	Exceptional Sensitivity of Metal-Aryl Bond Energies to <i>ortho</i> -Fluorine Substituents: Influence of the Metal, the Coordination Sphere, and the Spectator Ligands on $\text{M}\cdots\text{C}/\text{H}\cdots\text{C}$ Bond Energy Correlations. <i>Journal of the American Chemical Society</i> , 2009, 131, 7817-7827.	6.6	172
24	Dinitrogen Dissociation on an Isolated Surface Tantalum Atom. <i>Science</i> , 2007, 317, 1056-1060.	6.0	163
25	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, , 2231-2233.	2.2	163
26	Hydrofluoroarylation of Alkynes with Ni Catalysts. $\text{C}\cdots\text{H}$ Activation via Ligand-to-Ligand Hydrogen Transfer, an Alternative to Oxidative Addition. <i>Organometallics</i> , 2012, 31, 1300-1314.	1.1	161
27	Outer sphere hydrogenation catalysis. <i>New Journal of Chemistry</i> , 2013, 37, 21-27.	1.4	161
28	d^0Re -Based Olefin Metathesis Catalysts, $\text{Re}(\text{CR})(\text{CHR})(\text{X})(\text{Y})$: The Key Role of X and Y Ligands for Efficient Active Sites. <i>Journal of the American Chemical Society</i> , 2005, 127, 14015-14025.	6.6	158
29	A Well-Defined, Silica-Supported Tungsten Imido Alkylidene Olefin Metathesis Catalyst. <i>Organometallics</i> , 2006, 25, 3554-3557.	1.1	152
30	Catecholborane Bound to Titanocene. Unusual Coordination of Ligand σ -Bonds. <i>Journal of the American Chemical Society</i> , 1996, 118, 10936-10937.	6.6	151
31	Wittig versus Corey-Chaykovsky Reaction. Theoretical study of the reactivity of phosphonium methylide and sulfonium methylide with formaldehyde. <i>Journal of the American Chemical Society</i> , 1987, 109, 1-14.	6.6	149
32	Mechanism of Homogeneous Iridium-Catalyzed Alkylation of Amines with Alcohols from a DFT Study. <i>Organometallics</i> , 2008, 27, 2529-2535.	1.1	149
33	A molecular orbital analysis of the regioselectivity of nucleophilic addition to η^3 -allyl complexes and the conformation of the η^3 -allyl ligand in $\text{L}_3(\text{CO})_2(\eta^3\text{-C}_3\text{H}_5)\text{Mo}(\text{II})$ complexes. <i>Organometallics</i> , 1984, 3, 887-895.	1.1	141
34	Agostic Interactions from a Computational Perspective: One Name, Many Interpretations. <i>Structure and Bonding</i> , 2004, , 1-36.	1.0	132
35	Decamethylscandocinium-hydrido-(perfluorophenyl)borate: fixation and tandem tris(perfluorophenyl)borane catalysed deoxygenative hydrosilation of carbon dioxide. <i>Chemical Science</i> , 2013, 4, 2152.	3.7	132
36	π -Stabilized, yet Reactive, Half-Sandwich $\text{Cp}^*\text{Ru}(\text{PR}_3)_3\text{X}$ Compounds: Synthesis, Structure, and Bonding. <i>Inorganic Chemistry</i> , 1995, 34, 488-499.	1.9	130

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37	RuHX(CO)(PR ₃) ₂ : Can ν .CO Be a Probe for the Nature of the Ru-X Bond?. <i>Inorganic Chemistry</i> , 1994, 33, 1476-1485.	1.9	122
38	Computational Evidence of the Importance of Substituent Bulk on Agostic Interactions in Ir(H) ₂ (PtBu ₂ Ph) ₂ ⁺ . <i>Journal of the American Chemical Society</i> , 1998, 120, 361-365.	6.6	121
39	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, 7750-7757.	6.6	121
40	Neutron structure and inelastic-neutron-scattering and theoretical studies of molybdenum complex Mo(CO)(H ₂)[(C ₆ D ₅) ₂ PC ₂ H ₄ P(C ₆ D ₅) ₂] ₂ . A complex with an extremely low barrier to hydrogen rotation. Implications on the reaction coordinate for H-H cleavage to dihydride. <i>Journal of the American Chemical Society</i> , 1993, 115, 569-581.	6.6	117
41	Energetics of C-H Bond Activation of Fluorinated Aromatic Hydrocarbons Using a [Tp ² Rh(CNneopentyl)] Complex. <i>Journal of the American Chemical Society</i> , 2009, 131, 13464-13473.	6.6	117
42	Reaction of molecular hydrogen (H ₂) with chlorohydroiridium phosphines IrHCl ₂ P ₂ (P = PPr-iso ₃ or Tj ETQq ₀ O ₀ rgBT /Overlock 10 TF). <i>Journal of the American Chemical Society</i> , 1993, 115, 7300-7312.	6.6	116
43	Decamethyltetracyclopentadiene Complexes of Bipyridines and Diazabutadienes: Multiconfigurational Ground States and Open-Shell Singlet Formation. <i>Journal of the American Chemical Society</i> , 2009, 131, 6480-6491.	6.6	112
44	Hydride Is Not a Spectator Ligand in the Formation of Hydrido Vinylidene from Terminal Alkyne and Ruthenium and Osmium Hydrides: A Mechanistic Differences. <i>Organometallics</i> , 1998, 17, 3091-3100.	1.1	111
45	Orbital factors and asymmetric induction. <i>Journal of the American Chemical Society</i> , 1973, 95, 6146-6147.	6.6	109
46	Lone pairs in organic molecules: Energetic and orientational non-equivalence. <i>Tetrahedron</i> , 1974, 30, 1717-1723.	1.0	109
47	Preferential C-Binding versus N-Binding in Imidazole Depends on the Metal Fragment Involved. <i>Inorganic Chemistry</i> , 2002, 41, 602-604.	1.9	107
48	Computational and Experimental Test of Steric Influence on Agostic Interactions: A Homologous Series for Ir(III). <i>Journal of the American Chemical Society</i> , 1999, 121, 97-106.	6.6	105
49	Factors favoring an M...H-C interaction in metal-methyl complexes. An MO analysis. <i>Journal of the American Chemical Society</i> , 1985, 107, 1177-1186.	6.6	104
50	Simple prediction of cycloaddition orientation in diels-alder reactions. <i>Tetrahedron</i> , 1977, 33, 523-531.	1.0	104
51	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.	1.1	103
52	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.	1.1	102
53	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, 7605-7616.	6.6	100
54	Biscarbene 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. <i>Journal of the American Chemical Society</i> , 2003, 125, 11964-11975.	6.6	99

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55	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, 2261-2272.	6.6	99
56	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, 5886-5900.	6.6	98
57	Entropy Explained: The Origin of Some Simple Trends. <i>Journal of Chemical Education</i> , 2002, 79, 1269.	1.1	96
58	Intermediate-Valence Tautomerism in Decamethyltetracyclophane Complexes of Methyl-Substituted Bipyridines. <i>Journal of the American Chemical Society</i> , 2010, 132, 17537-17549.	6.6	92
59	Hydrogen for Fluorine Exchange in CH_4 - CF_4 Monomeric $[1,2,4-(Me_3C)_3C_5H_2]_2CeH$: Experimental and Computational Studies. <i>Journal of the American Chemical Society</i> , 2005, 127, 7781-7795.	6.6	91
60	Structure and H ₂ -Loss Energies of $OsHX(H_2)(CO)_2L_2$ Complexes (L = P(<i>t</i> -Bu) ₂ Me, P(<i>i</i> -Pr) ₃ ; X = Cl, I, H): Attempted Correlation of $1J(H\hat{=}D)$, T ₁ min, and ρ^{GASS} . <i>Inorganic Chemistry</i> , 1996, 35, 6775-6783.	1.9	90
61	Inertness of the Aryl-F Bond toward Oxidative Addition to Osmium and Rhodium Complexes: Thermodynamic or Kinetic Origin?. <i>Journal of the American Chemical Society</i> , 1998, 120, 12634-12640.	6.6	90
62	Carbon Monoxide Activation via O-Bound CO Using Decamethylscandocinium-Hydridoborate Ion Pairs. <i>Journal of the American Chemical Society</i> , 2012, 134, 10843-10851.	6.6	90
63	Bond energy, M $\hat{=}C/H\hat{=}C$ correlations: dual theoretical and experimental approach to the sensitivity of M $\hat{=}C$ bond strength to substituents Electronic supplementary information (ESI) available: methods of calculation; Fig. S1: Comparison of calculated and experimental C $\hat{=}H$ bond dissociation energies for organic molecules; Table S1, comparison of calculated and experimental CO-stretching frequencies; Table S2, total energies, BDE for Re $\hat{=}C$ and H $\hat{=}C$; Table S3, NPA charges $q(C)$ and $q(aryl)$ for the organic fragments C ₆ H ₆ . <i>Chemical Communications</i> , 2003, , 490-491.	2.2	89
64	From three- to four-coordination in copper(I) and silver(I). <i>Inorganic Chemistry</i> , 1992, 31, 1758-1762.	1.9	88
65	$\hat{3}$ Agostic C $\hat{=}H$ or $\hat{2}$ agostic Si $\hat{=}C$ bonds in $La\{CH(SiMe_3)_2\}_3$? A DFT study of the role of the ligand. <i>New Journal of Chemistry</i> , 2003, 27, 121-127.	1.4	88
66	$\hat{2}$ -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, 6288-6297.	6.6	88
67	Coordinated carbenes from electron-rich olefins on $RuHCl(PPr_3)_2$. <i>New Journal of Chemistry</i> , 2000, 24, 9-26.	1.4	87
68	A Rational Basis for the Axial Ligand Effect in C $\hat{=}H$ Oxidation by $[MnO(\text{porphyrin})(X)]^+$ (X = H ₂ O, OH $\hat{=}$), Tj ETQq0,0,0 rgBT (Overlock 1	1.9	87
69	Activation of a coordinated olefin toward nucleophilic attack. <i>Journal of the American Chemical Society</i> , 1980, 102, 6148-6149.	6.6	86
70	The First $\hat{2}$ -CH ₂ Cl ₂ Adduct of Ru(II): $[RuH(\hat{2}\text{-CH}_2\text{Cl}_2)(CO)(PtBu_2Me)_2][BAr^{\text{F}}_4]$ ($Ar^{\text{F}} = 3,5\text{-C}_6\text{H}_3(\text{CF}_3)_2$) and Its $RuH(CO)(PtBu_2Me)_2^+$ Precursor. <i>Journal of the American Chemical Society</i> , 1997, 119, 7398-7399.	6.6	86
71	New types of hydrogen bonds. <i>Journal of Organometallic Chemistry</i> , 1998, 567, 7-11.	0.8	86
72	Some geometrical and electronic features of the intermediate stages of olefin metathesis. <i>Journal of the American Chemical Society</i> , 1981, 103, 5582-5584.	6.6	85

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73	Defluorination of Perfluoropropene Using Cp* ₂ ZrH ₂ and Cp* ₂ ZrHF: A Mechanism Investigation from a Joint Experimental/Theoretical Perspective. <i>Journal of the American Chemical Society</i> , 2004, 126, 5647-5653.	6.6	85
74	Osmium Converts Terminal Olefins to Carbynes: σ -Hydrogen Migration Redox Isomers with Reversed Stability for Ruthenium and for Osmium. <i>Organometallics</i> , 1998, 17, 999-1001.	1.1	84
75	DFT Study of H α -H Activation by Cp ₂ LnH ₂ d ⁰ Complexes. <i>Journal of the American Chemical Society</i> , 2001, 123, 1036-1039.	6.6	84
76	Outer sphere anion participation can modify the mechanism for conformer interconversion in Pd pincer complexes. <i>Dalton Transactions</i> , 2003, , 831-838.	1.6	84
77	Metathesis Activity Encoded in the Metallacyclobutane Carbon-13 NMR Chemical Shift Tensors. <i>ACS Central Science</i> , 2017, 3, 759-768.	5.3	84
78	Aromatic C-H σ -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.	1.1	84
79	The Grignard Reaction "Unraveling a Chemical Puzzle. <i>Journal of the American Chemical Society</i> , 2020, 142, 2984-2994.	6.6	84
80	Counter-ion effects switch ligand binding from C-2 to C-5 in kinetic carbenes formed from an imidazolium salt and IrH ₅ (PPh ₃) ₂ . <i>Chemical Communications</i> , 2002, , 2580-2581.	2.2	82
81	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.	5.5	82
82	New Access to Vinylidenes from Ruthenium Polyhydrides. <i>Organometallics</i> , 1997, 16, 2227-2229.	1.1	81
83	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.	1.1	81
84	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.	6.6	80
85	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.	7.6	80
86	OsH ₅ (PMe ₂ Ph) ₃ ⁺ : Structure, Reactivity, and Its Use as a Catalyst Precursor for Olefin Hydrogenation and Hydroformylation. <i>Inorganic Chemistry</i> , 1994, 33, 4966-4976.	1.9	79
87	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, 2529-2541.	6.6	79
88	Synthesis and properties of [(η -C ₅ H ₅)Re(NO)(PPh ₃)(σ -C ₆ H ₅)] ⁺ PF ₆ ⁻ : a benzylidene complex that is formed by a stereospecific α -hydride abstraction, exists as two geometric isomers, and undergoes stereospecific nucleophilic attack. <i>Journal of the American Chemical Society</i> , 1982, 104, 4865-4878.	6.6	78
89	Distinct structures for ruthenium and osmium hydrido halides: Os(H) ₃ X(PiPr ₃) ₂ (X = Cl, Br, I) are nonoctahedral classical trihydrides with exchange coupling. <i>Journal of the American Chemical Society</i> , 1994, 116, 2685-2686.	6.6	78
90	An η -4-benzene species mediates acetylene cyclotrimerization. <i>Journal of the American Chemical Society</i> , 1991, 113, 5127-5129.	6.6	77

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91	RuX(CO)(NO)L ₂ and Ru(CO)(NO)L ₂ : Ru(0) or Ru(II) or In Between?. Journal of the American Chemical Society, 1997, 119, 8642-8651.	6.6	77
92	Double Geminal C-H Activation and Reversible H ₂ -Elimination in 2-Aminopyridine Iridium(III) Complexes: The Role of Hydrides and Solvent in Flattening the Free Energy Surface. Journal of the American Chemical Society, 2004, 126, 8795-8804.	6.6	77
93	Structure, spectroscopic and electronic properties of a well defined silica supported olefin metathesis catalyst, [(tBuSiO)Re(tBuCR)(CHR)(CH ₂ R)], through DFT periodic calculations: silica is just a large siloxy ligand. New Journal of Chemistry, 2006, 30, 842-850.	1.4	77
94	Preparation, x-ray molecular structure, and electronic structure of the first 16-electron ruthenium dihydrogen complexes RuH(H ₂)X(PCy ₃) ₂ . Journal of the American Chemical Society, 1991, 113, 2314-2316.	6.6	76
95	A DFT Study of SiH ₄ Activation by Cp ₂ LnH. Inorganic Chemistry, 2002, 41, 4355-4362.	1.9	75
96	Reactions of New Osmium(II) Dihydride Complexes with Terminal Alkynes: Metallacyclopropene versus Metal-Carbyne. Influence of the Alkyne Substituent. Organometallics, 1999, 18, 4949-4959.	1.1	74
97	DFT study of CH ₄ activation by d ⁰ Cl ₂ LnZ (Z = H, CH ₃) complexes. Dalton Transactions RSC, 2002, , 534-539.	2.3	74
98	Reactivity of the molecular hydrogen complex [IrH ₄ (PMe ₂ Ph) ₃]BF ₄ towards olefins. The origin of stereochemical rigidity of M(PR ₃) ₃ (olefin) ₂ species. Journal of the American Chemical Society, 1990, 112, 855-863.	6.6	73
99	Geometrically Distorted and Redox-Active Organometallic Iridium Complexes Containing Biphenyl-2,2'-diyl. Organometallics, 1995, 14, 1168-1175.	1.1	73
100	Validation of the M-C/H-C Bond Enthalpy Relationship through Application of Density Functional Theory. Journal of the American Chemical Society, 2006, 128, 8350-8357.	6.6	73
101	The structure of d ⁰ ML ₆ complexes. Inorganic Chemistry, 1989, 28, 1611-1613.	1.9	71
102	DFT studies of some structures and reactions of lanthanides complexes. Journal of Organometallic Chemistry, 2002, 647, 190-197.	0.8	71
103	Mono-, Di-, and Trianionic η^2 -Diketiminato Ligands: A Computational Study and the Synthesis and Structure of [(YbL) ₃ (THF)], L = [{N(SiMe ₃)C(Ph)} ₂ CH]. Journal of the American Chemical Society, 2003, 125, 10790-10791.	6.6	71
104	Modulation of reactivity and stereochemistry of substrate binding by the group X in RuHX(CO)(P-tert-Bu ₂ Me) ₂ . Inorganic Chemistry, 1993, 32, 5490-5501.	1.9	69
105	Characterization and Reactivity of an Unprecedented Unsaturated Zero-Valent Ruthenium Species: Isolable, Yet Highly Reactive. Journal of the American Chemical Society, 1996, 118, 10189-10199.	6.6	69
106	Ion pairing effects in intramolecular heterolytic H ₂ activation in an Ir(III) complex: a combined theoretical/experimental study. New Journal of Chemistry, 2003, 27, 80-87.	1.4	69
107	Heterolytic dihydrogen activation in an iridium complex with a pendant basic group. Chemical Communications, 1999, , 297-298.	2.2	68
108	The rebound mechanism in catalytic C-H oxidation by MnO(tpp)Cl from DFT studies: electronic nature of the active species. Chemical Communications, 2008, , 744-746.	2.2	68

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109	Deviation from the ideal octahedral field vs. alkyl distortion in d0 metal-alkyl complexes: a MO study. <i>Organometallics</i> , 1986, 5, 1457-1464.	1.1	67
110	Theoretical analysis of bonding in monomeric and polymeric C ₅ H ₅ M compounds. <i>Organometallics</i> , 1984, 3, 759-764.	1.1	66
111	Interaction between d ₆ ML ₅ metal fragments and hydrogen: η ² -H ₂ vs. dihydride structure. <i>Journal of the American Chemical Society</i> , 1986, 108, 6587-6592.	6.6	65
112	Theoretical Studies on the Metathesis Processes, [Tp(PH ₃)MR(2-Hiξ _i CH ₃)] ⁺ [Tp(PH ₃)M(CH ₃)(2-Hiξ _i R)] ⁻ (M=Fe, Ti) <i>ETQqO</i>	1.7	65
113	Remote functionalization of hydrocarbons with reversibility enhanced stereocontrol. <i>Chemical Science</i> , 2015, 6, 2770-2776.	3.7	65
114	Are Strong Gold-Gold Interactions Possible in Main Group X _n A(AuPR ₃) _m Molecules?. <i>Inorganic Chemistry</i> , 1994, 33, 3261-3268.	1.9	63
115	Mechanistic Studies of the Facile Four-Electron Reduction of Azobenzene at a Single Tungsten Metal Center. <i>Journal of the American Chemical Society</i> , 1996, 118, 2762-2763.	6.6	63
116	R-Group reversal of isomer stability for RuH(X)L ₂ (CCHR) vs. Ru(X)L ₂ (CCH ₂ R): access to four-coordinate ruthenium carbenes and carbynes. <i>New Journal of Chemistry</i> , 2000, 24, 925-927.	1.4	63
117	How Solvent Dynamics Controls the Schlenk Equilibrium of Grignard Reagents: A Computational Study of CH ₃ ⁺ MgCl in Tetrahydrofuran. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4226-4237.	1.2	63
118	The Mechanism of Acetylene Cyclotrimerization Catalyzed by the fac-IrP ₃ ⁺ Fragment: The Relationship between Fluxionality and Catalysis. <i>Organometallics</i> , 1994, 13, 2010-2023.	1.1	62
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