Odile Eisenstein

List of Publications by Year
in descending order

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330 papers	21,933 citations	6233 80 h-index	13727 129 g-index
385 all docs	385 docs citations	385 times ranked	11524 citing authors

#	Article	IF	Citations
1	Câ€”H Bond Activation in Transition Metal Species from a Computational Perspective. Chemical Reviews, 2010, 110, 749-823.	23.0	959
2	A New Intermolecular Interaction:â€‰ UnconventionalHydrogen Bonds with Elementâ^'Hydride Bonds as ProtonAcceptor. Accounts of Chemical Research, 1996, 29, 348-354.	7.6	639
3	Highly Active and Robust Cp* Iridium Complexes for Catalytic Water Oxidation. Journal of the American Chemical Society, 2009, 131, 8730-8731.	6.6	561
4	Half-Sandwich Iridium Complexes for Homogeneous Water-Oxidation Catalysis. Journal of the American Chemical Society, 2010, 132, 16017-16029.	6.6	507
5	Câ^'F and Câ^'H Bond Activation of Fluorobenzenes and Fluoropyridines at Transition Metal Centers: How Fluorine Tips the Scales. Accounts of Chemical Research, 2011, 44, 333-348.	7.6	430
6	Transition Metal Polyhydrides:â€‰ From Qualitative Ideas to Reliable Computational Studies. Chemical Reviews, 2000, 100, 601-636.	23.0	341
7	Iridium-Catalyzed Hydrogenation of N-Heterocyclic Compounds under Mild Conditions by an Outer-Sphere Pathway. Journal of the American Chemical Society, 2011, 133, 7547-7562.	6.6	296
8	Do f Electrons Play a Role in the Lanthanideâ^'Ligand Bonds? A DFT Study of Ln(NR2)3; R = H, SiH3. Journal of Physical Chemistry A, 2000, 104, 7140-7143.	1.1	292
9	Selectivity of Câ€“H Activation and Competition between Câ€“H and Câ€“F Bond Activation at Fluorocarbons. Chemical Reviews, 2017, 117, 8710-8753.	23.0	265
10	Linear-Selective Hydroarylation of Unactivated Terminal and Internal Olefins with Trifluoromethyl-Substituted Arenes. Journal of the American Chemical Society, 2014, 136, 13098-13101.	6.6	263
11	Transition-metal complexed olefins: how their reactivity toward a nucleophile relates to their electronic structure. Journal of the American Chemical Society, 1981, 103, 4308-4320.	6.6	254
12	Interactions between Cî—¸H and Nî—¸H bonds and d8 square planar metal complexes: hydrogen bonded or agostic?. Inorganica Chimica Acta, 1997, 254, 105-111.	1.2	248
13	Factors Affecting the Strength of N-H.cntdot..cntdot..cntdot.H-Ir Hydrogen Bonds. Journal of the American Chemical Society, 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. Inorganic Chemistry, 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(.eta.2-H2)(PEtPh2)3. Journal of the American Chemical Society, 1990, 112, 4831-4841.	6.6	226
16	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.	6.6	213
17	Understanding d0-Olefin Metathesis Catalysts:Â Which Metal, Which Ligands?. Journal of the American Chemical Society, 2007, 129, 8207-8216.	6.6	210
18	Theoretical study of the structures of electron-deficient d6 ML5 complexes. Importance of a .pi.-donating ligand. Organometallics, 1992, 11, 729-737.	1.1	204

#	Article	IF	Citations
19	An Unconventional Intermolecular Three-Center Nâ€“Hâ€¦ H2Re Hydrogen Bond in Crystalline[ReH5(PPh3)3]Â·indoleÂ·C6H6. Angewandte Chemie International Edition in English, 1995, 34, 2507-2509.	4.4	195
20	Hydrogen for Fluorine Exchange in C6F6and C6F5H by Monomeric [1,3,4-(Me3C)3C5H2]2CeH:Â Experimental and Computational Studies. Journal of the American Chemical Society, 2005, 127, 279-292.	6.6	190
21	Superjacent orbital control. Interpretation of the anomeric effect. Journal of the American Chemical Society, 1973, 95, 3806-3807.	6.6	186
22	An Anion-Dependent Switch in Selectivity Results from a Change of Câ^'H Activation Mechanism in the Reaction of an Imidazolium Salt with IrH5(PPh3)2. Journal of the American Chemical Society, 2005, 127, 16299-16311.	6.6	172
23	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.	6.6	172
24	Dinitrogen Dissociation on an Isolated Surface Tantalum Atom. Science, 2007, 317, 1056-1060.	6.0	163
25	Computational structureâ€“activity relationships in H2storage: how placement of N atoms affects release temperatures in organic liquid storage materials. Chemical Communications, 2007, , 2231-2233.	2.2	163
26	Hydrofluoroarylation of Alkynes with Ni Catalysts. Câ€“H Activation via Ligand-to-Ligand Hydrogen Transfer, an Alternative to Oxidative Addition. Organometallics, 2012, 31, 1300-1314.	1.1	161
27	Outer sphere hydrogenation catalysis. New Journal of Chemistry, 2013, 37, 21-27.	1.4	161
28	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.	6.6	158
29	A Well-Defined, Silica-Supported Tungsten Imido Alkylidene Olefin Metathesis Catalyst. Organometallics, 2006, 25, 3554-3557.	1.1	152
30	Catecholborane Bound to Titanocene. Unusual Coordination of Ligand Ïƒ-Bonds. Journal of the American Chemical Society, 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. Journal of the American Chemical Society, 1987, 109, 1-14.	6.6	149
32	Mechanism of Homogeneous Iridium-Catalyzed Alkylation of Amines with Alcohols from a DFT Study. Organometallics, 2008, 27, 2529-2535.	1.1	149
33	A molecular orbital analysis of the regioselectivity of nucleophilic addition to .eta.3-allyl complexes and the conformation of the .eta.3-allyl ligand in L3(CO)2(.eta.3-C3H5)Mo(II) complexes. Organometallics, 1984, 3, 887-895.	1.1	141
34	Agostic Interactions from a Computational Perspective: One Name, Many Interpretations. Structure and Bonding, 2004, , 1-36.	1.0	132
35	Decamethylscandocinium-hydrido-(perfluorophenyl)borate: fixation and tandem tris(perfluorophenyl)borane catalysed deoxygenative hydrosilation of carbon dioxide. Chemical Science, 2013, 4, 2152.	3.7	132
36	.pi.-Stabilized, yet Reactive, Half-Sandwich Cp*Ru(PR3)X Compounds: Synthesis, Structure, and Bonding. Inorganic Chemistry, 1995, 34, 488-499.	1.9	130

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37	RuHX(CO)(PR3)2: Can .nu.CO Be a Probe for the Nature of the Ru-X Bond?. Inorganic Chemistry, 1994, 33, 1476-1485.	1.9	122
38	Computational Evidence of the Importance of Substituent Bulk on Agostic Interactions in Ir(H)2(PtBu2Ph)2+. Journal of the American Chemical Society, 1998, 120, 361-365.	6.6	121
39	Shutting Down Secondary Reaction Pathways: The Essential Role of the Pyrrolyl Ligand in Improving Silica Supported d⁰-ML₄ Alkene Metathesis Catalysts from DFT Calculations. Journal of the American Chemical Society, 2010, 132, 7750-7757.	6.6	121
40	Neutron structure and inelastic-neutron-scattering and theoretical studies of molybdenum complex Mo(CO)(H2)[(C6D5)2PC2H4P(C6D5)2]2.cntdot.4.5C6D6, a complex with an extremely low barrier to hydrogen rotation. Implications on the reaction coordinate for H-H cleavage to dihydride. Journal of the American Chemical Society, 1993, 115, 569-581.	6.6	117
41	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.	6.6	117
42	Reaction of molecular hydrogen (H2) with chlorohydridoiridium phosphines IrHCl2P2 (P = PPr-iso3 or) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Journal of the American Chemical Society, 1993, 115, 7300-7312.	6.6	116
43	Decamethylytterbocene Complexes of Bipyridines and Diazabutadienes: Multiconfigurational Ground States and Open-Shell Singlet Formation. Journal of the American Chemical Society, 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:Â Mechanistic Differences. Organometallics, 1998, 17, 3091-3100.	1.1	111
45	Orbital factors and asymmetric induction. Journal of the American Chemical Society, 1973, 95, 6146-6147.	6.6	109
46	Lone pairs in organic molecules: Energetic and orientational non-equivalence. Tetrahedron, 1974, 30, 1717-1723.	1.0	109
47	Preferential C-Binding versus N-Binding in Imidazole Depends on the Metal Fragment Involved. Inorganic Chemistry, 2002, 41, 602-604.	1.9	107
48	Computational and Experimental Test of Steric Influence on Agostic Interactions:Â A Homologous Series for Ir(III). Journal of the American Chemical Society, 1999, 121, 97-106.	6.6	105
49	Factors favoring an M...H-C interaction in metal-methyl complexes. An MO analysis. Journal of the American Chemical Society, 1985, 107, 1177-1186.	6.6	104
50	Simple prediction of cycloaddition orientation IÃ¢Â€Â”diels-alder reactions. Tetrahedron, 1977, 33, 523-531.	1.0	104
51	An Experimentalâ^'Theoretical Study of the Factors That Affect the Switch between Ruthenium-Catalyzed Dehydrogenative Amide Formation versus Amine Alkylation. Organometallics, 2010, 29, 6548-6558.	1.1	103
52	Single but Stronger UO, Double but Weaker UNMe Bonds:â€‰ The Tale Told by Cp₂UO and Cp₂UNR. Organometallics, 2007, 26, 5059-5065.	1.1	102
53	Manganese Catalysts for Câ^'H Activation: An Experimental/Theoretical Study Identifies the Stereoelectronic Factor That Controls the Switch between Hydroxylation and Desaturation Pathways. Journal of the American Chemical Society, 2010, 132, 7605-7616.	6.6	100
54	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.	6.6	99

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55	Elucidating the Link between NMR Chemical Shifts and Electronic Structure in d⁰ Olefin Metathesis Catalysts. Journal of the American Chemical Society, 2016, 138, 2261-2272.	6.6	99
56	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.	6.6	98
57	Entropy Explained: The Origin of Some Simple Trends. Journal of Chemical Education, 2002, 79, 1269.	1.1	96
58	Intermediate-Valence Tautomerism in Decamethylytterbocene Complexes of Methyl-Substituted Bipyridines. Journal of the American Chemical Society, 2010, 132, 17537-17549.	6.6	92
59	Hydrogen for Fluorine Exchange in CH4-xFxby Monomeric [1,2,4-(Me3C)3C5H2]2CeH:Â Experimental and Computational Studies. Journal of the American Chemical Society, 2005, 127, 7781-7795.	6.6	91
60	Structure and H2-Loss Energies of OsHX(H2)(CO)L2Complexes (L = P(t-Bu)2Me, P(i-Pr)3; X = Cl, I, H):Â Attempted Correlation of1J(Hâ^D),T1min, and Î”Gâ§§. Inorganic Chemistry, 1996, 35, 6775-6783.	1.9	90
61	Inertness of the Arylâ^F Bond toward Oxidative Addition to Osmium and Rhodium Complexes:â€‰ Thermodynamic or Kinetic Origin?. Journal of the American Chemical Society, 1998, 120, 12634-12640.	6.6	90
62	Carbon Monoxide Activation via O-Bound CO Using Decamethylscandociniumâ€“Hydridoborate Ion Pairs. Journal of the American Chemical Society, 2012, 134, 10843-10851.	6.6	90
63	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.	2.2	89
64	From three- to four-coordination in copper(I) and silver(I). Inorganic Chemistry, 1992, 31, 1758-1762.	1.9	88
65	Î³ Agostic Câ€“H or Î² agostic Siâ€“C bonds in La{CH(SiMe3)2}3? A DFT study of the role of the ligand. New Journal of Chemistry, 2003, 27, 121-127.	1.4	88
66	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.	6.6	88
67	Coordinated carbenes from electron-rich olefins on RuHCl(PPr3i)2. New Journal of Chemistry, 2000, 24, 9-26.	1.4	87
68	A Rational Basis for the Axial Ligand Effect in Câ^H Oxidation by [MnO(porphyrin)(X)]+ (X = H2O, OHâ^,) Tj ETQq0 0 0 rgBT /Overlock 1	1.9	87
69	Activation of a coordinated olefin toward nucleophilic attack. Journal of the American Chemical Society, 1980, 102, 6148-6149.	6.6	86
70	The First Î·2-CH2Cl2 Adduct of Ru(II):[RuH(Î·2-CH2Cl2)(CO)(PtBu2Me)2][BArâ€˜4] (Arâ€˜ = 3,5-C6H3(CF3)2) and Its RuH(CO)(PtBu2Me)2+ Precursor. Journal of the American Chemical Society, 1997, 119, 7398-7399.	6.6	86
71	New types of hydrogen bonds. Journal of Organometallic Chemistry, 1998, 567, 7-11.	0.8	86
72	Some geometrical and electronic features of the intermediate stages of olefin metathesis. Journal of the American Chemical Society, 1981, 103, 5582-5584.	6.6	85

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73	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.	6.6	85
74	Osmium Converts Terminal Olefins to Carbynes:Â Î±-Hydrogen Migration Redox Isomers with Reversed Stability for Ruthenium and for Osmium. Organometallics, 1998, 17, 999-1001.	1.1	84
75	DFT Study of Hâ^'H Activation by Cp2LnH d0Complexes. Journal of the American Chemical Society, 2001, 123, 1036-1039.	6.6	84
76	Outer sphere anion participation can modify the mechanism for conformer interconversion in Pd pincer complexes. Dalton Transactions, 2003, , 831-838.	1.6	84
77	Metathesis Activity Encoded in the Metallacyclobutane Carbon-13 NMR Chemical Shift Tensors. ACS Central Science, 2017, 3, 759-768.	5.3	84
78	Aromatic Câ€“H Ïƒ-Bond Activation by Ni⁰, Pd⁰, and Pt⁰ Alkene Complexes: Concerted Oxidative Addition to Metal vs Ligand-to-Ligand H Transfer Mechanism. Organometallics, 2017, 36, 2761-2771.	1.1	84
79	The Grignard Reaction â€“ Unraveling a Chemical Puzzle. Journal of the American Chemical Society, 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 IrH5(PPh3)2. Chemical Communications, 2002, , 2580-2581.	2.2	82
81	Cp* Iridium Precatalysts for Selective Câ€“H Oxidation via Direct Oxygen Insertion: A Joint Experimental/Computational Study. ACS Catalysis, 2012, 2, 208-218.	5.5	82
82	New Access to Vinylidenes from Ruthenium Polyhydrides. Organometallics, 1997, 16, 2227-2229.	1.1	81
83	Oxo vs Imido Alkylidene d⁰-Metal Species: How and Why Do They Differ in Structure, Activity, and Efficiency in Alkene Metathesis?. Organometallics, 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. Journal of the American Chemical Society, 2017, 139, 17597-17607.	6.6	80
85	Carbon-13 NMR Chemical Shift: A Descriptor for Electronic Structure and Reactivity of Organometallic Compounds. Accounts of Chemical Research, 2019, 52, 2278-2289.	7.6	80
86	OsH5(PMe2Ph)3+: Structure, Reactivity, and Its Use as a Catalyst Precursor for Olefin Hydrogenation and Hydroformylation. Inorganic Chemistry, 1994, 33, 4966-4976.	1.9	79
87	Reactions of Monomeric [1,2,4-(Me3C)3C5H2]2CeH and CO with or without H2:Â An Experimental and Computational Study. Journal of the American Chemical Society, 2007, 129, 2529-2541.	6.6	79
88	Synthesis and properties of [(.eta.-C5H5)Re(NO)(PPh3)(:CHC6H5)]+PF6-: a benzylidene complex that is formed by a stereospecific .alpha.-hydride abstraction, exists as two geometric isomers, and undergoes stereospecific nucleophilic attack. Journal of the American Chemical Society, 1982, 104, 4865-4878.	6.6	78
89	Distinct structures for ruthenium and osmium hydrido halides: Os(H)3X(PiPr3)2 (X = Cl, Br, I) are nonoctahedral classical trihydrides with exchange coupling. Journal of the American Chemical Society, 1994, 116, 2685-2686.	6.6	78
90	An .eta.4-benzene species mediates acetylene cyclotrimerization. Journal of the American Chemical Society, 1991, 113, 5127-5129.	6.6	77

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91	RuX(CO)(NO)L2and Ru(CO)(NO)L2+:Â Ru(0) or Ru(II) or In Between?. Journal of the American Chemical Society, 1997, 119, 8642-8651.	6.6	77
92	Double Geminal Câˆ'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.	6.6	77
93	Structure, spectroscopic and electronic properties of a well defined silica supported olefin metathesis catalyst, [(î€,SiO)Re(î€,CR)(î€CHR)(CH2R)], 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(H2)X(PCy3)2. Journal of the American Chemical Society, 1991, 113, 2314-2316.	6.6	76
95	A DFT Study of SiH4 Activation by Cp2LnH. Inorganic Chemistry, 2002, 41, 4355-4362.	1.9	75
96	Reactions of New Osmiumâˆ'Dihydride Complexes with Terminal Alkynes:Â Metallacyclopropene versus Metalâˆ'Carbyne. Influence of the Alkyne Substituent. Organometallics, 1999, 18, 4949-4959.	1.1	74
97	DFT study of CH4 activation by d0 Cl2LnZ (Z = H, CH3) complexes. Dalton Transactions RSC, 2002, , 534-539.	2.3	74
98	Reactivity of the molecular hydrogen complex [IrH4(PMe2Ph)3]BF4 towards olefins. The origin of stereochemical rigidity of M(PR3)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 Mâˆ'C/Hâˆ'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 d0 ML6 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 Î²-Diketiminato Ligands:Â A Computational Study and the Synthesis and Structure of [(YbL)3(THF)], L = [{N(SiMe3)C(Ph)}2CH]. 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-Bu2Me)2. Inorganic Chemistry, 1993, 32, 5490-5501.	1.9	69
105	Characterization and Reactivity of an Unprecedented Unsaturated Zero-Valent Ruthenium Species:Â Isolable, Yet Highly Reactive. Journal of the American Chemical Society, 1996, 118, 10189-10199.	6.6	69
106	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.	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 Câ€"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. Organometallics, 1986, 5, 1457-1464.	1.1	67
110	Theoretical analysis of bonding in monomeric and polymeric C5H5M compounds. Organometallics, 1984, 3, 759-764.	1.1	66
111	Interaction between d6 ML5 metal fragments and hydrogen: .eta.2-H2 vs. dihydride structure. Journal of the American Chemical Society, 1986, 108, 6587-6592.	6.6	65
112	Theoretical Studies on the Metathesis Processes, [Tp(PH3)MR(2-Hï£¿CH3)]â€‰â†'â€‰[Tp(PH3)M(CH3)(2-Hï£¿R)] (M=Fe,) Tj ETQq0 0	1.7	65
113	Remote functionalization of hydrocarbons with reversibility enhanced stereocontrol. Chemical Science, 2015, 6, 2770-2776.	3.7	65
114	Are Strong Gold-Gold Interactions Possible in Main Group XnA(AuPR3)m Molecules?. Inorganic Chemistry, 1994, 33, 3261-3268.	1.9	63
115	Mechanistic Studies of the Facile Four-Electron Reduction of Azobenzene at a Single Tungsten Metal Center. Journal of the American Chemical Society, 1996, 118, 2762-2763.	6.6	63
116	R-Group reversal of isomer stability for RuH(X)L2(CCHR) vs. Ru(X)L2(CCH2R): access to four-coordinate ruthenium carbenes and carbynes. New Journal of Chemistry, 2000, 24, 925-927.	1.4	63
117	How Solvent Dynamics Controls the Schlenk Equilibrium of Grignard Reagents: A Computational Study of CH₃MgCl in Tetrahydrofuran. Journal of Physical Chemistry B, 2017, 121, 4226-4237.	1.2	63
118	The Mechanism of Acetylene Cyclotrimerization Catalyzed by the fac-IrP3+ Fragment: The Relationship between Fluxionality and Catalysis. Organometallics, 1994, 13, 2010-2023.	1.1	62
119	Cerium masquerading as a Group 4 element: synthesis, structure and computational characterisation of [CeCl{N(SiMe3)2}3]. Chemical Communications, 2001, , 1560-1561.	2.2	62
120	tert-Butyl Is Superior to Phenyl as an Agostic Donor to 14-Electron Ir(III). Journal of the American Chemical Society, 1997, 119, 9069-9070.	6.6	61
121	Isolable, Unsaturated Ru(0) in Ru(CO)2(PtBu2Me)2: Not Isostructural with Rh(I) in Rh(CO)2(PR3)2+. Journal of the American Chemical Society, 1995, 117, 8869-8870.	6.6	59
122	A 14-Electron Ruthenium(II) Hydride, [RuH(CO)(PtBu2Me)2]BArâ€˜4(Arâ€˜ = 3,5-(C6H3)(CF3)2):Â Synthesis, Structure, and Reactivity toward Alkenes and Oxygen Ligands. Organometallics, 2000, 19, 2281-2290.	1.1	59
123	Equilibria between Î±- and Î²-Agostic Stabilized Rotamers of Secondary Alkyl Niobium Complexes. Journal of the American Chemical Society, 2001, 123, 6000-6013.	6.6	59
124	Some structural and electronic properties of MX3(Mâ€‰=â€‰Ln, Sc, Y, Ti+, Zr+, Hf+; Xâ€‰=â€‰H, Me, Hal, NH2) from DFT calculations. Faraday Discussions, 2003, 124, 25-39.	1.6	59
125	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.	1.1	59
126	The Bond between CO and Cpâ€²₃U in Cpâ€²₃U(CO) Involves Back-bonding from the Cpâ€²₃U Ligand-Based Orbitals of Ï€-Symmetry, where Cpâ€² Represents a Substituted Cyclopentadienyl Ligand. Organometallics, 2009, 28, 3629-3635.	1.1	59

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127	CO-Induced C(sp2)/C(sp) Coupling on Ru and Os:Â A Comparative Study. Organometallics, 1998, 17, 4700-4706.	1.1	58
128	DFT calculations of d0M(NR)(CHtBu)(X)(Y) (M = Mo, W; R = CPh3, 2,6-iPrâ€“C6H3; X and Y = CH2tBu, OtBu,) Tj ETQq0 0 0 rgBT /Overlo Transactions, 2006, , 3077-3087.	1.6	58
129	Generation and Structural Characterization of a Gold(III) Alkene Complex. Angewandte Chemie - International Edition, 2013, 52, 1660-1663.	7.2	58
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