Odile Eisenstein

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/26858/publications.pdf

Version: 2024-02-01

330 papers	21,933 citations	6254 80 h-index	13771 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.	47.7	959
2	A New Intermolecular Interaction:â€‰ UnconventionalHydrogen Bonds with Elementâ€“Hydride Bonds as ProtonAcceptor. Accounts of Chemical Research, 1996, 29, 348-354.	15.6	639
3	Highly Active and Robust Cp* Iridium Complexes for Catalytic Water Oxidation. Journal of the American Chemical Society, 2009, 131, 8730-8731.	13.7	561
4	Half-Sandwich Iridium Complexes for Homogeneous Water-Oxidation Catalysis. Journal of the American Chemical Society, 2010, 132, 16017-16029.	13.7	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.	15.6	430
6	Transition Metal Polyhydrides:â€‰ From Qualitative Ideas to Reliable Computational Studies. Chemical Reviews, 2000, 100, 601-636.	47.7	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.	13.7	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.	2.5	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.	47.7	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.	13.7	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.	13.7	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.	2.4	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.	13.7	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.	4.0	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.	13.7	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.	13.7	213
17	Understanding d0-Olefin Metathesis Catalysts:Â Which Metal, Which Ligands?. Journal of the American Chemical Society, 2007, 129, 8207-8216.	13.7	210
18	Theoretical study of the structures of electron-deficient d6 ML5 complexes. Importance of a .pi.-donating ligand. Organometallics, 1992, 11, 729-737.	2.3	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.	13.7	190
21	Superjacent orbital control. Interpretation of the anomeric effect. Journal of the American Chemical Society, 1973, 95, 3806-3807.	13.7	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.	13.7	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.	13.7	172
24	Dinitrogen Dissociation on an Isolated Surface Tantalum Atom. Science, 2007, 317, 1056-1060.	12.6	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.	4.1	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.	2.3	161
27	Outer sphere hydrogenation catalysis. New Journal of Chemistry, 2013, 37, 21-27.	2.8	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.	13.7	158
29	A Well-Defined, Silica-Supported Tungsten Imido Alkylidene Olefin Metathesis Catalyst. Organometallics, 2006, 25, 3554-3557.	2.3	152
30	Catecholborane Bound to Titanocene. Unusual Coordination of Ligand Ïƒ-Bonds. Journal of the American Chemical Society, 1996, 118, 10936-10937.	13.7	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.	13.7	149
32	Mechanism of Homogeneous Iridium-Catalyzed Alkylation of Amines with Alcohols from a DFT Study. Organometallics, 2008, 27, 2529-2535.	2.3	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.	2.3	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.	7.4	132
36	.pi.-Stabilized, yet Reactive, Half-Sandwich Cp*Ru(PR3)X Compounds: Synthesis, Structure, and Bonding. Inorganic Chemistry, 1995, 34, 488-499.	4.0	130

#	Article	IF	Citations
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.	4.0	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.	13.7	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.	13.7	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.	13.7	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.	13.7	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.	13.7	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.	13.7	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.	2.3	111
45	Orbital factors and asymmetric induction. Journal of the American Chemical Society, 1973, 95, 6146-6147.	13.7	109
46	Lone pairs in organic molecules: Energetic and orientational non-equivalence. Tetrahedron, 1974, 30, 1717-1723.	1.9	109
47	Preferential C-Binding versus N-Binding in Imidazole Depends on the Metal Fragment Involved. Inorganic Chemistry, 2002, 41, 602-604.	4.0	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.	13.7	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.	13.7	104
50	Simple prediction of cycloaddition orientation IÃ¢Â€Â”diels-alder reactions. Tetrahedron, 1977, 33, 523-531.	1.9	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.	2.3	103
52	Single but Stronger UO, Double but Weaker UNMe Bonds:â€‰ The Tale Told by Cp₂UO and Cp₂UNR. Organometallics, 2007, 26, 5059-5065.	2.3	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.	13.7	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.	13.7	99

#	Article	IF	Citations
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.	13.7	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.	13.7	98
57	Entropy Explained: The Origin of Some Simple Trends. Journal of Chemical Education, 2002, 79, 1269.	2.3	96
58	Intermediate-Valence Tautomerism in Decamethylytterbocene Complexes of Methyl-Substituted Bipyridines. Journal of the American Chemical Society, 2010, 132, 17537-17549.	13.7	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.	13.7	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.	4.0	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.	13.7	90
62	Carbon Monoxide Activation via O-Bound CO Using Decamethylscandociniumâ€“Hydridoborate Ion Pairs. Journal of the American Chemical Society, 2012, 134, 10843-10851.	13.7	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.	4.1	89
64	From three- to four-coordination in copper(I) and silver(I). Inorganic Chemistry, 1992, 31, 1758-1762.	4.0	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.	2.8	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.	13.7	88
67	Coordinated carbenes from electron-rich olefins on RuHCl(PPr3i)2. New Journal of Chemistry, 2000, 24, 9-26.	2.8	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	4.0	87
69	Activation of a coordinated olefin toward nucleophilic attack. Journal of the American Chemical Society, 1980, 102, 6148-6149.	13.7	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.	13.7	86
71	New types of hydrogen bonds. Journal of Organometallic Chemistry, 1998, 567, 7-11.	1.8	86
72	Some geometrical and electronic features of the intermediate stages of olefin metathesis. Journal of the American Chemical Society, 1981, 103, 5582-5584.	13.7	85

#	Article	IF	Citations
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.	13.7	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.	2.3	84
75	DFT Study of Hâ^'H Activation by Cp2LnH d0Complexes. Journal of the American Chemical Society, 2001, 123, 1036-1039.	13.7	84
76	Outer sphere anion participation can modify the mechanism for conformer interconversion in Pd pincer complexes. Dalton Transactions, 2003, , 831-838.	3.3	84
77	Metathesis Activity Encoded in the Metallacyclobutane Carbon-13 NMR Chemical Shift Tensors. ACS Central Science, 2017, 3, 759-768.	11.3	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.	2.3	84
79	The Grignard Reaction â€“ Unraveling a Chemical Puzzle. Journal of the American Chemical Society, 2020, 142, 2984-2994.	13.7	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.	4.1	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.	11.2	82
82	New Access to Vinylidenes from Ruthenium Polyhydrides. Organometallics, 1997, 16, 2227-2229.	2.3	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.	2.3	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.	13.7	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.	15.6	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.	4.0	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.	13.7	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.	13.7	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.	13.7	78
90	An .eta.4-benzene species mediates acetylene cyclotrimerization. Journal of the American Chemical Society, 1991, 113, 5127-5129.	13.7	77

#	Article	IF	Citations
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.	13.7	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.	13.7	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.	2.8	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.	13.7	76
95	A DFT Study of SiH4 Activation by Cp2LnH. Inorganic Chemistry, 2002, 41, 4355-4362.	4.0	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.	2.3	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.	13.7	73
99	Geometrically Distorted and Redox-Active Organometallic Iridium Complexes Containing Biphenyl-2,2'-diyl. Organometallics, 1995, 14, 1168-1175.	2.3	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.	13.7	73
101	The structure of d0 ML6 complexes. Inorganic Chemistry, 1989, 28, 1611-1613.	4.0	71
102	DFT studies of some structures and reactions of lanthanides complexes. Journal of Organometallic Chemistry, 2002, 647, 190-197.	1.8	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.	13.7	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.	4.0	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.	13.7	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.	2.8	69
107	Heterolytic dihydrogen activation in an iridium complex with a pendant basic group. Chemical Communications, 1999, , 297-298.	4.1	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.	4.1	68

#	Article	IF	Citations
109	Deviation from the ideal octahedral field vs. alkyl distortion in d0 metal-alkyl complexes: a MO study. Organometallics, 1986, 5, 1457-1464.	2.3	67
110	Theoretical analysis of bonding in monomeric and polymeric C5H5M compounds. Organometallics, 1984, 3, 759-764.	2.3	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.	13.7	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,)	3.3	65
113	Remote functionalization of hydrocarbons with reversibility enhanced stereocontrol. Chemical Science, 2015, 6, 2770-2776.	7.4	65
114	Are Strong Gold-Gold Interactions Possible in Main Group XnA(AuPR3)m Molecules?. Inorganic Chemistry, 1994, 33, 3261-3268.	4.0	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.	13.7	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.	2.8	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.	2.6	63
118	The Mechanism of Acetylene Cyclotrimerization Catalyzed by the fac-IrP3+ Fragment: The Relationship between Fluxionality and Catalysis. Organometallics, 1994, 13, 2010-2023.	2.3	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.	4.1	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.	13.7	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.	13.7	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.	2.3	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.	13.7	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.	3.2	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.	2.3	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.	2.3	59

#	Article	IF	Citations
127	CO-Induced C(sp2)/C(sp) Coupling on Ru and Os:Â A Comparative Study. Organometallics, 1998, 17, 4700-4706.	2.3	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.	3.3	58
129	Generation and Structural Characterization of a Gold(III) Alkene Complex. Angewandte Chemie - International Edition, 2013, 52, 1660-1663.	13.8	58
130	Geminal dehydrogenation of ether and amine C(sp3)H2 groups by electron-rich Ru(ii) and OsElectronic supplementary information (ESI) available: crystallographic data, fractional coordinates and isotropic thermal parameters, anisotropic thermal parameters, and bond distances and angles. See http://www.rsc.org/suppdata/nj/b2/b200168n/. New Journal of Chemistry, 2002, 26, 687-700.	2.8	57
131	Orbital Analysis of Carbonâ€13 Chemical Shift Tensors Reveals Patterns to Distinguish Fischer and Schrock Carbenes. Angewandte Chemie - International Edition, 2017, 56, 10127-10131.	13.8	57
132	A comprehensive view of Mâ€“H addition across the RCî€,CH bond: frustration culminating in ultimate union. New Journal of Chemistry, 2001, 25, 1244-1255.	2.8	56
133	Metallacyclobutanes from Schrock-Type d⁰ Metal Alkylidene Catalysts: Structural Preferences and Consequences in Alkene Metathesis. Organometallics, 2015, 34, 1668-1680.	2.3	55
134	Importance of palladiumâ€“carbon bond energies in direct arylation of polyfluorinated benzenes. Dalton Transactions, 2010, 39, 10510.	3.3	54
135	cisâ€“trans Isomerisation of CpRe(CO)2(H)(ArF) (ArF= C6FnH5â^'n; n = 0â€“5) is the rate determining step in Câ€“H activation of fluoroarenes: a DFT study. Dalton Transactions, 2003, , 4065-4074.	3.3	53
136	The Key Role of the Hemiaminal Intermediate in the Iron-Catalyzed Deaminative Hydrogenation of Amides. ACS Catalysis, 2018, 8, 8751-8762.	11.2	53
137	Electronic origin of the thermochromic effect in 2,2',5,5'-tetramethylbistibole. Journal of the American Chemical Society, 1982, 104, 3876-3879.	13.7	51
138	Competition between Steric and Electronic Control of Structure in Ru(CO)2L2Lâ€˜ Complexes. Organometallics, 1997, 16, 1979-1993.	2.3	51
139	[Ru(Ph)(CO)(PtBu2Me)2]+: A Unique 14-Electron Ru11 Complex with Two Agostic Interactions. Angewandte Chemie International Edition in English, 1997, 36, 2004-2006.	4.4	51
140	Structural and Dynamic Properties of OsH2X2L2 (X = Cl, Br, I; L = PiPr3) Complexes: Interconversion between Remarkable Non-Octahedral Isomers. Journal of the American Chemical Society, 1995, 117, 281-292.	13.7	50
141	Multiple structural variants of LnCuI(.mu.-X)2CuILn (n = 1, 2). Influence of halide on a "soft" potential energy surface. Inorganic Chemistry, 1992, 31, 3306-3312.	4.0	49
142	Carbene Complexes from Olefins, Using RuHCl(PiPr3)2. Influence of the Olefin Substituent. Journal of the American Chemical Society, 1998, 120, 9388-9389.	13.7	49
143	Cationic Methyl Complexes of the Rare-Earth Metals: An Experimental and Computational Study on Synthesis, Structure, and Reactivity. Inorganic Chemistry, 2008, 47, 9265-9278.	4.0	49
144	Solid-State and Solution Structures of[{NW(OC(CH3)2CF3)3}3] and Factors Favoring the Metathesis of Cï£¿N and Wï£¿W Triple Bonds in Reactions Involving Organic Nitriles and Ditungsten Hexaalkoxides. Angewandte Chemie International Edition in English, 1995, 34, 110-112.	4.4	48

#	Article	IF	Citations
145	DFT studies of the methyl exchange reaction between Cp2Mâ€“CH3or Cp*2Mâ€“CH3(Cp = C5H5, Cp* = C5Me5,) Tj ETQq1 1 0.7843 3052-3057.	3.3	47
146	Metal alkyls programmed to generate metal alkylidenes by Î±-H abstraction: prognosis from NMR chemical shift. Chemical Science, 2018, 9, 1912-1918.	7.4	47
147	Dynamics on an ab Initio Surface for Calculating JHH NMR Exchange Coupling. The Case of OsH3X(PH3)2. Journal of the American Chemical Society, 1995, 117, 1797-1799.	13.7	46
148	DFT modeling of ligands in lanthanide chemistry: Is Ln[N(SiH3)2]3 a model for Ln[N(SiMe3)2]3?. New Journal of Chemistry, 2001, 25, 255-258.	2.8	46
149	Ï€-Bond Character in Metalâ€“Alkyl Compounds for Câ€“H Activation: How, When, and Why?. Journal of the American Chemical Society, 2019, 141, 648-656.	13.7	46
150	On coupling carbenes and carbynes. Journal of the American Chemical Society, 1982, 104, 632-634.	13.7	45
151	A novel coordination mode for oxygen: preparation and properties of (NBun4)2[V4O(edt)2Cl8] containing a square planar oxide bridge. Journal of the American Chemical Society, 1989, 111, 8027-8029.	13.7	45
152	Redox-active organometallic Ir complexes containing biphenyl-2,2â€²-diyl. Journal of the Chemical Society Chemical Communications, 1993, .	2.0	45
153	A theoretical study of [M(PH3)4] (Mâ€…=â€…Ru or Fe), models for the highly reactive d8 intermediates [M(dmpe)2] (dmpeâ€…=â€…Me2PCH2CH2PMe2). Zero activation energies for addition of CO and oxidative addition of H2â€Šâ€¡. Journal of the Chemical Society Dalton Transactions, 1998, , 291-300.	1.1	45
154	Câ€“H oxidation by hydroxo manganese(v) porphyrins: a DFT study. Chemical Communications, 2009, , 1772.	4.1	45
155	Structural Distortions in Six-Coordinate Adducts of Niobium(V) and Tantalum(V). Inorganic Chemistry, 1997, 36, 3623-3631.	4.0	44
156	Vinyl Câ^'F Cleavage by Os(H)3Cl(PiPr3)2. Inorganic Chemistry, 2002, 41, 6440-6449.	4.0	43
157	Are the Carbon Monoxide Complexes of Cp2M (M = Ca, Eu, or Yb) Carbon or Oxygen Bonded? An Answer from DFT Calculations. Journal of the American Chemical Society, 2002, 124, 5614-5615.	13.7	43
158	Hydrogen for X-Group Exchange in CH₃X (X = Cl, Br, I, OMe, and NMe₂) by Monomeric [1,2,4-(Me₃C)₃C₅H₂]₂CeH: Experimental and Computational Support for a Carbenoid Mechanism. Organometallics, 2009, 28, 3173-3185.	2.3	43
159	Why Is .beta.-Me Elimination Only Observed in d0 Early-Transition-Metal Complexes? An Organometallic Hyperconjugation Effect with Consequences for the Termination Step in Ziegler-Natta Catalysis. Organometallics, 1994, 13, 1049-1051.	2.3	42
160	Quantum Exchange Coupling:Â A Hypersensitive Indicator of Weak Interactions. Journal of the American Chemical Society, 1997, 119, 10153-10169.	13.7	42
161	Is Ï€-donation the only way? Unprecedented unsaturated Ru(II) species devoid of Ï€-donor ligands. Inorganica Chimica Acta, 1997, 259, 5-26.	2.4	42
162	Nitrido Dimers and Trimers of Tungsten Supported by tBuMe2SiO and CF3Me2CO Ligands, Respectively. Factors Influencing the Reductive Cleavage of Nitriles by Tungsten-Tungsten Triple Bonds and An Analysis of the Structure of the Cyclotrimer. Chemistry - A European Journal, 1999, 5, 2318-2326.	3.3	42

#	Article	IF	Citations
163	The reaction of the unsaturated rhenium fragment {Re(Î·5-C5Me5)(CO)2} with 1,4-difluorobenzene. Thermal intramolecular conversion of a rhenium (difluorophenyl)(hydride) to Re(Î·2-C6H4F2) and a [1,4]-metallotropic shift. Dalton Transactions RSC, 2001, , 1452-1461.	2.3	42
164	Mechanistic investigation of vinylic carbonâ€“fluorine bond activation of perfluorinated cycloalkenes using Cp*2ZrH2 and Cp*2ZrHF. Journal of Fluorine Chemistry, 2010, 131, 1122-1132.	1.7	42
165	Hypercoordinated XHn+1 radicals for first- and second-row atoms. A valence bond analysis. Journal of the American Chemical Society, 1989, 111, 5623-5631.	13.7	41
166	NMR chemical shift analysis decodes olefin oligo- and polymerization activity of d ⁰ group 4 metal complexes. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E5867-E5876.	7.1	40
167	Structural variants of tetranuclear L4Cu4X4. Influence of L on the coordination mode of copper(I). Inorganic Chemistry, 1992, 31, 5389-5394.	4.0	39
168	Characterization of PtH3(PtBu3)2+ as the First Dihydrogen Complex of d8, Pt(II). Journal of the American Chemical Society, 1994, 116, 7409-7410.	13.7	39
169	Interplay of Weak Interactions:Â An Iridium(III) System with an Agostictert-Butyl but a Nonagostic Isopropyl Group. Organometallics, 2002, 21, 575-580.	2.3	39
170	Computational Studies Explain the Importance of Two Different Substituents on the Chelating Bis(amido) Ligand for Transfer Hydrogenation by Bifunctional Cp*Rh(III) Catalysts. Organometallics, 2014, 33, 3433-3442.	2.3	39
171	Facile olefin hydrogenation with an osmium dihydrogen complex. Organometallics, 1989, 8, 2073-2074.	2.3	37
172	Chemoselectivity in Ïƒ bond activation by lanthanocene complexes from a DFT perspective: reactions of Cp2LnR (R = CH3, H, SiH3) with SiH4and CH3â€“SiH3. New Journal of Chemistry, 2007, 31, 549-555.	2.8	37
173	An Unusual Example of Hypervalent Silicon: A Fiveâ€Coordinate Silyl Group Bridging Two Palladium or Nickel Centers through a Nonsymmetrical Fourâ€Center Twoâ€Electron Bond. Angewandte Chemie - International Edition, 2014, 53, 1103-1108.	13.8	37
174	Atom economic synthesis of amides via transition metal catalyzed rearrangement of oxaziridines. Green Chemistry, 2007, 9, 976.	9.0	36
175	Simple prediction of regiospecificity in Dielsâ€“Alder reactions. Challenge, 1971, .	0.4	35
176	A comparative study of olefin or acetylene insertion into RuÃ¢â‚¬Å“H or OsÃ¢â‚¬Å“H of MHCl(CO)(phosphine)2. New Journal of Chemistry, 2001, 25, 1382-1388.	2.8	35
177	DFT calculations of NMR JCâ€“H coupling constants: An additional tool to characterize the Î±-agostic interaction in high oxidation state M-alkylidene complexes (M=Re, Mo and Ta). Polyhedron, 2006, 25, 339-348.	2.2	35
178	Synthesis and structure of â€œ16-electronâ€•rhodium(iii) catalysts for transfer hydrogenation of a cyclic imine: mechanistic implications. Chemical Communications, 2009, , 6801.	4.1	35
179	Synthesis, structure, and reductive elimination in the series Tpâ€²Rh(PR3)(ArF)H; Determination of rhodiumâ€“carbon bond energies of fluoroaryl substituents. Dalton Transactions, 2010, 39, 10495.	3.3	35
180	Successive Heterolytic Cleavages of H₂ Achieve N₂ Splitting on Silica-Supported Tantalum Hydrides: A DFT Proposed Mechanism. Inorganic Chemistry, 2012, 51, 7237-7249.	4.0	35

#	Article	IF	Citations
181	1,2-Hydrogen Migration to a Saturated Ruthenium Complex via Reversal of Electronic Properties for Tin in a Stannylene-to-Metallostannylene Conversion. Journal of the American Chemical Society, 2014, 136, 13991-13994.	13.7	35
182	A theoretical study of the formation and reactivity of substituted cyclohexadienyliron complexes. The structures and reactivities of tricarbonyl(2-methoxycyclohexadienyl)iron cation and tricarbonyl(1-methyl-4-methoxycyclohexadienyl)iron cation. Organometallics, 1984, 3, 1150-1157.	2.3	34
183	Site Preference Energetics, Fluxionality, and Intramolecular Mâ^'HÂ·Â·Â·Hâ^'N Hydrogen Bonding in a Dodecahedral Transition Metal Polyhydrideâ€. Inorganic Chemistry, 1997, 36, 5505-5511.	4.0	34
184	Different van der Waals radii for organic and inorganic halogen atoms: a significant improvement in IMOMM performance. Theoretical Chemistry Accounts, 1997, 96, 146-150.	1.4	34
185	Opposing steric and electronic contributions in OsCl2H2(PPr3i)2. A theoretical study of an unusual structure. New Journal of Chemistry, 1998, 22, 5-9.	2.8	34
186	DFT Investigation of the Catalytic Hydromethylation of Î±-Olefins by Metallocenes. 1. Differences between Scandium and Lutetium in Propene Hydromethylation. Organometallics, 2006, 25, 5699-5708.	2.3	34
187	The reaction of bis(1,2,4-tri-t-butylcyclopentadienyl)ceriumbenzyl, Cpâ€²2CeCH2Ph, with methylhalides: a metathesis reaction that does not proceed by a metathesis transition state. Dalton Transactions, 2010, 39, 6648.	3.3	34
188	Theoretical study of borohydride addition to formaldehyde. A one-step, nonsynchronous transition state. Journal of Organic Chemistry, 1982, 47, 2886-2891.	3.2	33
189	The origin of structural variety of alkyne complexes of d8 metals. An example of structural isomerism. Polyhedron, 1990, 9, 1867-1881.	2.2	33
190	Structural and dynamic properties of propane coordinated to TpRh(CNR) from a confrontation between theory and experiment. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 6939-6944.	7.1	33
191	Understanding reactivity trends by structural and theoretical studies of distortions in ground-state reagents. Organometallics, 1991, 10, 3062-3069.	2.3	32
192	Why Nickel(II) Binds CO Best in Trigonal Bipyramidal and Square Pyramidal Geometries and Possible Consequences for CO Dehydrogenase. Inorganic Chemistry, 1994, 33, 3616-3618.	4.0	32
193	Synthesis, Unusual Trigonal Prismatic Geometry, and Theoretical Study of the Homoleptic Tris-(2,2â€˜-biphosphinine) Complexes of Chromium, Molybdenum, and Tungsten. Inorganic Chemistry, 1998, 37, 3154-3158.	4.0	32
194	Bond Activations of PhSiH₃ by Cp₂SmH: A Mechanistic Investigation by the DFT Method. Organometallics, 2009, 28, 3767-3775.	2.3	32
195	Theoretical study of the conformation of cis carbene-olefin-transition metal complexes: back-donation vs. ligand-ligand interaction. Journal of the American Chemical Society, 1986, 108, 2173-2179.	13.7	31
196	Modeling C5H5with Atoms or Effective Group Potential in Lanthanide Complexes:Â Isolobality Not the Determining Factor. Journal of Physical Chemistry A, 2002, 106, 1797-1801.	2.5	31
197	Deciphering Selectivity in Organic Reactions: A Multifaceted Problem. Accounts of Chemical Research, 2016, 49, 1070-1078.	15.6	31
198	[Cp''Co(P4){(Cp''Co)2(.mu.-CO)}] (Cp'' = .eta.5-C5H3tBu2): A Complex with a P4 Unit on the Way to a P1 and a P3 Ligand. Inorganic Chemistry, 1995, 34, 3117-3119.	4.0	29

#	Article	IF	Citations
199	Observing and modelling energetically close Î±- and Î²-carbonâ€“hydrogen agostic interactions in an isopropyl tris(pyrazolyl)boratoniobium complex. Chemical Communications, 1998, , 2011-2012.	4.1	29
200	Cyclometalated N-Heterocyclic Carbene Complexes of Ruthenium for Access to Electron-Rich Silylene Complexes That Bind the Lewis Acids CuOTf and AgOTf. Journal of the American Chemical Society, 2014, 136, 11473-11482.	13.7	29
201	35Cl pure quadrupole resonance in acetylated glycopyranosyl chlorides. Relation between chlorine nuclear quadrupole coupling constant and molecular conformation. Journal of Chemical Physics, 1973, 58, 5579-5583.	3.0	28
202	Theoretical studies of SN2 transition states, the alpha effect. Tetrahedron Letters, 1982, 23, 615-618.	1.4	28
203	Theoretical analysis of radical reactions: on the anomalous behavior of methyl toward fluoro-substituted olefins. The Journal of Physical Chemistry, 1985, 89, 4856-4861.	2.9	28
204	An extremely low barrier to rotation of dihydrogen in the iridium complex IrClH2(.eta.2-H2)(PiPr3)2. Journal of the American Chemical Society, 1993, 115, 11056-11057.	13.7	28
205	16-Electron Ruthenium(0) Complexes Containing the Ru(NO)L2+Substructure:Â Planar RuCH3(NO)L2vs Sawhorse [Ru(NO)(CC(SiMe3)2)L2]+. Organometallics, 2000, 19, 1967-1972.	2.3	28
206	Silyl, Hydrido-Silylene, or Other Bonding Modes:Â Some Unusual Structures of [(dhpe)Pt(SiHR2)]+(dhpe) Tj ETQq0 0 0 rgBT /Overlock 10 Calculations. Inorganic Chemistry, 2002, 41, 7105-7112.	4.0	28
207	Bonding of H2, N2, Ethylene, and Acetylene to Bivalent Lanthanide Metallocenes:Â Trends from DFT Calculations on Cp2M and Cp*2M (M = Sm, Eu, Yb) and Experiments with Cp*2Yb. Organometallics, 2003, 22, 5447-5453.	2.3	28
208	CF4defluorination by Cp2Lnâ€“H: a DFT study. Dalton Transactions, 2003, , 4313-4318.	3.3	28
209	Theoretical analysis of the addition of nucleophiles to (.eta.4-diene)MLn complexes. Organometallics, 1987, 6, 1845-1849.	2.3	27
210	Isomeric Hydrido/Vinylidene, MH(halide)(CCH2)L2, and Ethylidyne, M(halide)(Câ’CH3)L2(M = Os, Ru; L =) Tj ETQq0 0 0 rgBT /Overlock 1	2.3	27
211	How hydrogen bonding affects ligand binding and fluxionality in transition metal complexes: a DFT study on interligand hydrogen bonds involving HF and H2O. New Journal of Chemistry, 2001, 25, 66-72.	2.8	27
212	Molecular recognition in Mn-catalyzed Câ€“H oxidation. Reaction mechanism and origin of selectivity from a DFT perspective. Dalton Transactions, 2009, , 5989.	3.3	27
213	Zirconocene-Mediated Selective Câ€“C Bond Cleavage of Strained Carbocycles: Scope and Mechanism. Journal of Organic Chemistry, 2018, 83, 3497-3515.	3.2	27
214	Thermochromic effect in distibines. The role of conjugation. Organometallics, 1987, 6, 1185-1188.	2.3	26
215	Ligand dependent nature of three possible shapes for a d6 pentacoordinated complex. Polyhedron, 1988, 7, 405-407.	2.2	26
216	Influence of a cis hydride on a coordinated molecular hydrogen ligand cis hydride, Ab initio calculations. Inorganic Chemistry, 1992, 31, 3344-3345.	4.0	26

#	Article	IF	Citations
217	Phosphine Dissociation Mediates Câˆ’H Cleavage of Fluoroarenes by OsH(C6H5)(CO)(PtBu2Me)2. Journal of the American Chemical Society, 1999, 121, 10895-10907.	13.7	26
218	Theoretical study of oxyhemocyanin active site: A possible insight on the first step of phenol oxidation by tyrosinase. Archives of Biochemistry and Biophysics, 1992, 296, 247-255.	3.0	25
219	Unifying the mechanisms for alkane dehydrogenation and alkene H/D exchange with [IrH2(O2CCF3)(PAr3)2]: the key role of CF3CO2 in the â€œstickyâ€™ alkane route. New Journal of Chemistry, 2001, 25, 1121-1131.	2.8	25
220	Electronic control of the stereochemistry of electrophilic and nucleophilic attack on double bonds in 6-membered rings. Tetrahedron, 1979, 35, 225-228.	1.9	24
221	Five-coordinate bent metallocenes. Structure and dynamics of bis(.eta.-cyclopentadienyl)chloro(N,N-dialkyldithiocarbamato)zirconium(IV) complexes. Inorganic Chemistry, 1983, 22, 759-770.	4.0	24
222	A double ionic mechanism for the Chapman-like rearrangement of imino-ethers to N-alkylmides, in the solid state or in the melt. Theoretical and experimental evidence. Journal of the Chemical Society Chemical Communications, 1992, .	2.0	24
223	Modelling Me5C5for reactivity studies in (Î·5-C5Me5)2Lnâ€“R: full DFT and QM/MM approaches. New Journal of Chemistry, 2004, 28, 1255-1259.	2.8	24
224	Bridging Silyl Groups in Ïƒ-Bond Metathesis and [1,2]-Shifts. Experimental and Computational Study of the Reaction between Cerium Metallocenes and MeOSiMe₃. Organometallics, 2010, 29, 5103-5110.	2.3	24
225	Three- and four-co-ordinate copper(I) complexes: 1:1 and 1:2 1-cyanoguanidineâ€“copper(I) halide adducts. Journal of the Chemical Society Dalton Transactions, 1994, , 1935-1942.	1.1	23
226	Facile C(sp2)/OR Bond Cleavage by Ru or Os. Inorganic Chemistry, 2001, 40, 6610-6621.	4.0	23
227	Alkyne hydrogenation by a dihydrogen complex: synthesis and structure of an unusual iridium-butyne complex. Journal of the American Chemical Society, 1989, 111, 2346-2347.	13.7	22
228	Eine ungewÃ¶hnliche intermolekulare Dreizentrenâ€Nâ€H âƒ›H₂Reâ€Wasserstoffbrücke zwischen [ReH₅(PPh₃)₃] und Indol im Kristall. Angewandte Chemie, 1995, 107, 2711-2713.	2.0	22
229	Breaking an electronically preferred symmetry by steric effects in a series of [Ir(biph)X(QR3)2] compounds (X=Cl or I, Q=P or As). New Journal of Chemistry, 1998, 22, 1493-1498.	2.8	22
230	Facile C(sp2)/O2CR bond cleavage by Ru or Os. New Journal of Chemistry, 2003, 27, 1451-1462.	2.8	22
231	A theoretical study of models for X2Y2 Zintl ions. Journal of the American Chemical Society, 1989, 111, 8105-8111.	13.7	21
232	[K([18]crown-6)]+[Mo4(Î¼4-H)(OCH2tBu)12]âˆ’, the First Alkoxidohydrido Cluster of Molybdenum, Evidence for a Rare, if not the First, Example of aÎ¼4-Hydride. Angewandte Chemie International Edition in English, 1994, 33, 191-193.	4.4	21
233	Tungsten(6+) Tris(pinacolate): Structure and Comments on the Preference for an Octahedral Geometry Relative to Trigonal Prismatic (D3h) for a d0 Complex in the Presence of Strong .pi.-Donor Ligands. Inorganic Chemistry, 1994, 33, 812-815.	4.0	21
234	Four-Electron Reduction of Diazo Compounds at a Single Tungsten Metal Center:Â A Theoretical Study of the Mechanism. Journal of the American Chemical Society, 1998, 120, 6598-6602.	13.7	21

#	Article	IF	Citations
235	Comparison of Î± CH and CF activation in alkyl transition metal complexes: a DFT and CASSCF study. Molecular Physics, 2002, 100, 533-540.	1.7	21
236	Reduction of ketones by sodium borohydride in the absence of protic solvents. Inter versus intramolecular mechanism. Tetrahedron Letters, 1983, 24, 1015-1018.	1.4	20
237	Theoretical study of the reactivity of phosphonium and sulfonium ylides with carbonyl groups. Journal of the American Chemical Society, 1984, 106, 6117-6119.	13.7	20
238	Long-range interaction between nonbonded hydrides. Attractive in the case of transition metals?. Journal of the American Chemical Society, 1990, 112, 7203-7207.	13.7	20
239	16-Electron, non-Ï€-stabilized Ir(H)2(H2)(PBu2tPh)2+ and 18-electron Ir(H)2(H2)2(PBu2tPh)2+: fluxionality and H/D exchange as independent processes. New Journal of Chemistry, 1998, 22, 307-310.	2.8	20
240	Influence of Ancillary Ligands on the Kinetics and the Thermodynamics of H2Addition to IrXH2(PR3)2(X) Tj ETQq0 0 0 rgBT /Overlock 10 Journal of Physical Chemistry A, 1998, 102, 3592-3598.	2.5	20
241	Solution and Solid-State Structure of Ru(CO)2(Bu2PtC2H4PtBu2):Â Square Planar and Monomeric?. Journal of the American Chemical Society, 1999, 121, 3242-3243.	13.7	20
242	Stereochemical Nonrigidity of a Chiral Rhodium Boryl Hydride Complex:Â A Ïƒ-Borane Complex as Transition State for Isomerization. Journal of the American Chemical Society, 2008, 130, 4375-4385.	13.7	20
243	Coordination and insertion of alkenes and alkynes in Au^{III}complexes: nature of the intermediates from a computational perspective. Dalton Transactions, 2016, 45, 5504-5513.	3.3	20
244	An oscillating C22? unit inside a copper rectangleElectronic supplementary information (ESI) available: NMR spectra and computational details. See http://www.rsc.org/suppdata/cc/b3/b301842c/. Chemical Communications, 2003, , 1260.	4.1	19
245	Two [1,2,4-(Me₃C)₃C₅H₂]₂CeH Molecules are Involved in Hydrogenation of Pyridine to Piperidine as Shown by Experiments and Computations. Inorganic Chemistry, 2014, 53, 6361-6373.	4.0	19
246	Metal alkoxides. Models for metal oxides. 18. Structure, bonding and dynamic behavior of bis(.eta.2-ethylene)hexakis(neopentoxy)ditungsten. Studies of the reversible addition of carbon-carbon double bonds to a tungsten-tungsten triple bond. Journal of the American Chemical Society, 1992, 114, 8497-8509.	13.7	18
247	DFT Investigation of the Catalytic Hydromethylation of Olefins by Scandocenes. 2. Influence of the Ansa Ligand on Propene and Isobutene Hydromethylation. Organometallics, 2008, 27, 2252-2257.	2.3	18
248	Mechanistic Insights on the Stereoselective Nucleophilic 1,2-Addition to Sulfinyl Imines. Journal of Organic Chemistry, 2014, 79, 2514-2521.	3.2	18
249	Does the Mode of Dioxygen Binding to Dinuclear Copper Complexes Depend on the Spectator Nitrogen-Containing Ligands? An ab Initio Theoretical Study. Inorganic Chemistry, 1997, 36, 3455-3460.	4.0	17
250	Fate of CH2CHE (E = H, OMe) in the Presence of Unsaturated Ru(X)(H)L2q+(X = Cl,q= 0; X = CO,q= 1):Â Highly Sensitive to X and E. Organometallics, 2000, 19, 2291-2298.	2.3	17
251	Unsaturated Ru(0) Species with a Constrained Bis-Phosphine Ligand:â€‰ [Ru(CO)2(tBu2PCH2CH2PtBu2)]2. Comparison to [Ru(CO)2(PtBu2Me)2]. Inorganic Chemistry, 2000, 39, 3957-3962.	4.0	17
252	Intermolecular Câˆ’HÂ·Â·Â·O and Câˆ’HÂ·Â·Â·Ï€ Interactions in the Chloroform Solvate (CH3)3Siâˆ’Câ‹®Câˆ’Câ‹®Câˆ’Si(OCH2CH2)3NÂ·2CHCl3:Â Crystallographic, Spectroscopic, and DFT Studies. Organometallics, 2001, 20, 47-54.	2.3	17

#	Article	IF	Citations
253	A NMR, X-ray, and DFT combined study on the regio-chemistry of nucleophilic addition to platinum(II) coordinated terminal olefins. Journal of Organometallic Chemistry, 2008, 693, 2819-2827.	1.8	17
254	Symmetrical Hydrogen Bonds in Iridium(III) Alkoxides with Relevance to Outer Sphere Hydrogen Transfer. Inorganic Chemistry, 2012, 51, 12313-12323.	4.0	17
255	Borate anion (B11H14-): a nido cage with no hydrogen...hydrogen interaction. Journal of the American Chemical Society, 1993, 115, 7747-7751.	13.7	16
256	Unexpected Coexistence of Isomeric Forms and Unusual Structures of Ru(CO)2L3â€–. Inorganic Chemistry, 1996, 35, 7468-7469.	4.0	16
257	18-Electron Os(X)(CHR)(Cl)(CO)L2 (X=H, Cl): not octahedral and metastable?. New Journal of Chemistry, 1999, 23, 495-498.	2.8	16
258	Lanthanide Complexes: Electronic Structure and Hâ€”H, Câ€”H, and Siâ€”H Bond Activation from a DFT Perspective. ACS Symposium Series, 2004, , 116-133.	0.5	16
259	Metal fragment isomerisation upon grafting a d2 ML4 perhydrocarbyl Os complex on a silica surface: origin and consequence. Dalton Transactions, 2009, , 5879.	3.3	16
260	An ab initio SCF + CI study of the SH3 and SF3 radicals. Chemical Physics Letters, 1986, 130, 419-422.	2.6	15
261	Conformation of hydrogen molecule on dinuclear complexes: attractive effect of a cis hydride. Inorganic Chemistry, 1990, 29, 3910-3914.	4.0	15
262	When Do Close B-B Contacts Imply a Bond, and When Not: The Case of Five-Vertex Boron-Containing Deltahedra?. Journal of the American Chemical Society, 1995, 117, 11939-11945.	13.7	15
263	Intermolecular Reî—¸HÂ·Hî—¸X hydrogen bonding (X î—» N, C) involving ReH5(PPh3)3. Inorganica Chimica Acta, 1998, 280, 26-29.	2.4	15
264	Functionalization vs. Î²-elimination in alkane activation: a key role for 16-electron ML5 intermediates. New Journal of Chemistry, 2001, 25, 665-666.	2.8	15
265	Catalytic hydrosilylation of olefins with organolanthanides: a DFT study. Part I: Hydrosilylation of propene by SiH4. Dalton Transactions, 2010, 39, 10749.	3.3	15
266	What Makes a Good (Computed) Energy Profile?. Topics in Organometallic Chemistry, 2020, , 1-38.	0.7	15
267	Theoretical study of regioselectivity in nucleophilic addition to unsymmetrical cyclic anhydrides. Intrinsic reactivity and influence of the cation. Canadian Journal of Chemistry, 1981, 59, 2457-2462.	1.1	14
268	H/D Exchange on Silica-Grafted Tantalum(V) Imido Amido [(â‰¡SiO)2Ta(V)(NH)(NH2)] Synthesized from Either Ammonia or Dinitrogen: IR and DFT Evidence for Heterolytic Splitting of D2. Topics in Catalysis, 2009, 52, 1482-1491.	2.8	14
269	Facile Interconversion of [Cp₂(Cl)Hf(SnH₃)] and [Cp₂(Cl)Hf(Î¼â€H)SnH₂]: DFT Investigations of Hafnocene Stannyl Complexes as Masked Stannylenes. Angewandte Chemie - International Edition, 2010, 49, 1816-1819.	13.8	14
270	Selectivity in the Câ€“H Activation Reaction of CH₃OSO₂CH₃ with [1,2,4-(Me₃C)₃C₅H₂]₂CeH or [1,2,4-(Me₃C)₃C₅H₂][1,2-(Me₃C)₂-4-(Me₂ To Choose or Not To Choose. Organometallics, 2012, 31, 870-881.	2.3	14

#	Article	IF	Citations
271	Cleaving bonds in CH₃OSO₂CF₃with [1,2,4-(Me₃C)₃C₅H₂]₂CeH; an experimental and computational study. New Journal of Chemistry, 2013, 37, 132-142.	2.8	14
272	Donor-Promoted 1,2-Hydrogen Migration from Silicon to a Saturated Ruthenium Center and Access to Silaoxiranyl and Silaiminyl Complexes. Journal of the American Chemical Society, 2015, 137, 9186-9194.	13.7	14
273	Hypothetical strain-free oligoradicals. Proceedings of the National Academy of Sciences of the United States of America, 1980, 77, 5588-5592.	7.1	13
274	Preparation, X-ray crystal and electronic structure of the novel raft cluster [NbAuH2{C5H4(SiMe3)}2]3. Journal of the Chemical Society Chemical Communications, 1990, , 17.	2.0	13
275	Lâ€˜ = CO vs Cl- Transposition:â€‰ Remarkable Consequences for the Product of (Lâ€˜)â^'Ru(L)2â^'(H) and Vinyl Ether. Organometallics, 1999, 18, 5441-5443.	2.3	13
276	Nonclassical CHâ^'Ï€ Supramolecular Interactions in Artemisinic Acid Favor a Single Conformation, Yielding High Diastereoselectivity in the Reduction with Diazene. Journal of Organic Chemistry, 2014, 79, 5939-5947.	3.2	13
277	Modelling and Rationalizing Organometallic Chemistry with Computation: Where Are We?. Structure and Bonding, 2015, , 1-37.	1.0	13
278	Orbital Analysis of Carbonâ€13 Chemical Shift Tensors Reveals Patterns to Distinguish Fischer and Schrock Carbenes. Angewandte Chemie, 2017, 129, 10261-10265.	2.0	13
279	Regio- and stereoselectivity of chiral binaphthyl reductive aminoalkylation. Rotational conformation and electron distribution of alkali-metal biarylides. Journal of the American Chemical Society, 1977, 99, 2230-2235.	13.7	12
280	A mechanistic approach to MgCl₂ supported stereospecific propene polymerization: A new model of active sites. Macromolecular Symposia, 1995, 89, 39-54.	0.7	12
281	DFT calculations of 29Si-NMR chemical shifts in Ru(ii) silyl complexes: Searching for trends and accurate values. Dalton Transactions, 2011, 40, 11321.	3.3	12
282	Catalytic Olefin Hydrosilations Mediated by Ruthenium Î·3-H2Si Ïƒ Complexes of Primary and Secondary Silanes. ACS Catalysis, 2018, 8, 11513-11523.	11.2	12
283	³¹P Chemical Shifts in Ru(II) Phosphine Complexes. A Computational Study of the Influence of the Coordination Sphere. Inorganic Chemistry, 2020, 59, 17038-17048.	4.0	12
284	Synthesis, Xâ€ray and Electronic Structure of Trinickel Tetradecker Sandwich Complexes {(Î·⁵â€C₅H₅)Ni[Î¼,Î·⁵â€(CR¹)₂(BR²)₂)<sub> Chemische Berichte, 1993, 126, 1587-1592.	1.2	11
285	Silyl, Hydrido Silylene or Alternative Bonding Modes:Â The Many Possible Structures of [(C5H5)(PH3)IrX]+(X = SiHR2and SiR3; R = H, CH3, SiH3, and Cl). Organometallics, 2006, 25, 4748-4755.	2.3	11
286	Splitting a Câ€“O bond in dialkylethers with bis(1,2,4-tri-tert-butylcyclopentadienyl)cerium hydride does not occur by a Ïƒ-bond metathesis pathway: a combined experimental and DFT computational study. New Journal of Chemistry, 2010, 34, 2189.	2.8	11
287	Catalytic hydrosilylation of olefins with organolanthanide complexes: A DFT study. Part II: Influence of the substitution on olefin and silane. Dalton Transactions, 2010, 39, 10757.	3.3	11
288	Heterolytic cleavage of ammonia Nâ€“H bond by bifunctional activation in silica-grafted single site Ta(V) imido amido surface complex. Importance of the outer sphere NH3 assistance. New Journal of Chemistry, 2011, 35, 1011.	2.8	11

#	Article	IF	Citations
289	Experimental and DFT Computational Study of Î²-Me and Î²-H Elimination Coupled with Proton Transfer: From Amides to Enamides in Cp*₂MX (M = La, Ce). Organometallics, 2017, 36, 97-108.	2.3	11
290	Modelling the surface of amorphous dehydroxylated silica: the influence of the potential on the nature and density of defects. New Journal of Chemistry, 2018, 42, 1356-1367.	2.8	11
291	6-Methyl-6-boraspiro[2.5]octa-4,7-diene, a boron analog of the phenonium ion. Journal of Organic Chemistry, 1983, 48, 901-903.	3.2	10
292	Polymeric one-dimensional [CoXL2]n vs. dimeric [CoXL2]2. Theoretical analysis of the factors favoring each form. Inorganic Chemistry, 1983, 22, 2398-2401.	4.0	10
293	Molecular graphics investigation of the addition of nucleophiles to (Î·4-butadiene) M(CO)3 complexes (M = Fe, Co+). Computational and Theoretical Chemistry, 1992, 254, 343-357.	1.5	10
294	Struktur von [{NW(OC(CH₃)₂CF₃)₃}₃] im Kristall und in LÃ¶sung; Faktoren, die die Metathese von Câ€Nâ€•und Wâ€Wâ€Dreifachbindungen bei Reaktionen mit organischen Nitrilen und Diwolframhexaalkoxiden begÃ¼nstigen. Angewandte Chemie, 1995, 107, 61-63.	2.0	10
295	Selectivity in Câ€“Cl bond activation of dichloroarenes by photogenerated Cp*Re(CO)2: combined experimental and DFT studies. New Journal of Chemistry, 2005, 29, 226-231.	2.8	10
296	The mechanism of N-vinylindole formation via tandem imine formation and cycloisomerisation of o-ethynylanilines. Dalton Transactions, 2009, , 10296.	3.3	10
297	Electronic switching of ring orientation in cyclopentadienyl-bridged polymers. Inorganic Chemistry, 1984, 23, 2435-2440.	4.0	9
298	Valence bond analysis of hypervalent sulphur compounds. Journal of the Chemical Society Chemical Communications, 1986, , 301.	2.0	9
299	Polynuclear metal hydrido alkoxides. Preparation and characterization of Mo4(Î¼-H)3(OBut)7(HNMe2) and [K(18-crown-6)][Mo4(Î¼4-H)(OR)12] (Râ€…=â€…Pri or CH2But). Journal of the Chemical Society Dalton Transactions, 1998, , 2563-2568.	1.1	9
300	Structure and stability of one-dimensional (MX2)n polymers. A band structure analysis. Inorganic Chemistry, 1983, 22, 3856-3861.	4.0	8
301	Synthesis, Structure, and Bonding of [CpCoW2(OCH2tBu)6], and Comments on the Combining Properties of CO and CpCo. Angewandte Chemie International Edition in English, 1992, 31, 896-898.	4.4	8
302	Olefin insertion in the Ruâ€“H and Ruâ€“F bonds of pentacoordinated d6 Ru(ii) species: a DFT study. Dalton Transactions, 2003, , 839.	3.3	8
303	Theoretical Studies on the Reaction Mechanism of Metal-Assisted CH Activation. , 2013, , 695-726.		8
304	Hydrazine Nâ€“N Bond Cleavage over Silica-Supported Tantalum-Hydrides. Inorganic Chemistry, 2015, 54, 11648-11659.	4.0	8
305	Mechanistic insight into organic and industrial transformations: general discussion. Faraday Discussions, 2019, 220, 282-316.	3.2	8
306	Is the Allylpalladium Structure Altered between Solid and Solutions?. Journal of the American Chemical Society, 2004, 126, 9079-9084.	13.7	7

#	Article	IF	Citations
307	Efficient alkene hydrosilation with bis(8-quinolyl)phosphine (NPN) nickel catalysts. The dominant role of silyl-over hydrido-nickel catalytic intermediates. Chemical Science, 2020, 11, 5043-5051.	7.4	7
308	Theoretical study of the conformation of cis-bis(carbene) complexes. Organometallics, 1988, 7, 829-835.	2.3	5
309	Hydrides and Hydrogen Bonding. , 2001, , 75-88.		5
310	Self-Consistency versus â€œBest-Fitâ€•Approaches in Understanding the Structure of Metal Nitrosyl Complexes. Organometallics, 2004, 23, 6008-6014.	2.3	5
311	Stereoselectivity through a network of non-classical CH weak interactions: a prospective study of a bicyclic organocatalytic scaffold. New Journal of Chemistry, 2014, 38, 5975-5982.	2.8	5
312	Potential Energy Surface of BH₄^{â¯} and Molecular Deformations Induced by an External Cation. Israel Journal of Chemistry, 1980, 19, 292-298.	2.3	4
313	Isomerization of Double and Triple C-C Bonds at a Metal Center. Catalysis By Metal Complexes, 2002, , 137-160.	0.6	4
314	Concluding remarks for â€œMechanistic Processes in Organometallic Chemistryâ€• the importance of a multidisciplinary approach. Faraday Discussions, 2019, 220, 489-495.	3.2	4
315	X-Ray and Theoretical Study of Cyclophane-tetracyanoethylene Charge Transfer Complexes. Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1988, 164, 179-195.	0.3	3
316	FemExâ€”female excellence in theoretical and computational chemistry. International Journal of Quantum Chemistry, 2015, 115, 1195-1196.	2.0	3
317	Computational and theoretical approaches for mechanistic understanding: general discussion. Faraday Discussions, 2019, 220, 464-488.	3.2	3
318	Computational Catalysis: A Land of Opportunities. Topics in Catalysis, 2022, 65, 1-5.	2.8	3
319	Conformational complexity of morphine and morphinum in the gas phase and in water. A DFT and MP2 study. RSC Advances, 2014, 4, 24729-24735.	3.6	2
320	From the Felkinâ€Anh Rule to the Grignard Reaction: an Almost Circular 50â€…Year Adventure in the World of Molecular Structures and Reaction Mechanisms with Computational Chemistry**. Israel Journal of Chemistry, 2022, 62, .	2.3	2
321	Agostic Interactions from a Computational Perspective: One Name, Many Interpretations. ChemInform, 2005, 36, no.	0.0	1
322	Nitrido Dimers and Trimers of Tungsten Supported by tBuMe2SiO and CF3Me2CO Ligands, Respectively. Factors Influencing the Reductive Cleavage of Nitriles by Tungstenâ€“Tungsten Triple Bonds and An Analysis of the Structure of the Cyclotrimer. Chemistry - A European Journal, 1999, 5, 2318-2326.	3.3	1
323	Perspective on â€œIntermolecular orbital theory of the interactions between conjugated systems.â€• I General theory; II Thermal and photochemical cycloadditions. , 2000, , 289-291.		1
324	Theoretical study of the conformations of cis carbene-acetylene transition metal complexes. Computational and Theoretical Chemistry, 1988, 166, 475-480.	1.5	0

#	Article	IF	Citations
325	Tungsten (6+) tris(pinacolate) : structure and comments on the preference for an octahedral geometry relative to trigonal prismatic (D3h) for a d0 complex in the presence of strong .pi.-donor ligands. [Erratum to document cited in CA120:123521]. Inorganic Chemistry, 1994, 33, 3204-3204.	4.0	0
326	Biscarbeneâ€"Ruthenium Complexes in Catalysis: Novel Stereoselective Synthesis of (1E,3E)-1,4-Disubstituted-1,3-dienes via Head-to-Head Coupling of Terminal Alkynes and Addition of Carboxylic Acids.. ChemInform, 2004, 35, no.	0.0	0
327	Reflections on 30 years in the life of a journal. New Journal of Chemistry, 2007, 31, 1995.	2.8	0
328	Structures of d4MH3X: a Computational Study of the Influence of the Metal and the Ligands. Inorganic Chemistry, 2012, 51, 5705-5715.	4.0	0
329	Understanding unusual element-element bond formation and activation: general discussion. Faraday Discussions, 2019, 220, 376-385.	3.2	0
330	Physical methods for mechanistic understanding: general discussion. Faraday Discussions, 2019, 220, 144-178.	3.2	0