Ming-Der Su

List of Publications by Year in Descending Order

134 papers	1,369 citations	20 h-index	30 g-index
143 ext. papers	1,581 ext. citations	4.3 avg, IF	5.14 L-index

#	Paper	IF	Citations
134	Amidinatoamidosilylene-Dibromodiborene. *Inorganic Chemistry*, **2021**, 60, 16065-16069	5.1	2
133	Diboron-Carbene Complexes Derived from a Geminal Dianion. *Organometallics*, **2021**, 40, 1848-1853	3.8	
132	Mechanistic insights into the insertion and addition reactions of group 13 analogues of the six-membered N-heterocyclic carbenes: interplay of electrophilicity, basicity, and aromaticity governing the reactivity.. *RSC Advances*, **2021**, 11, 20070-20080	3.7	
131	Reactivity of dicationic N-heterocyclic chalcogen carbene analogues with methane and ethene: a theoretical investigation. *Physical Chemistry Chemical Physics*, **2021**, 23, 2419-2429	3.6	0
130	Mechanistic Insight into Chemical Reactions of Acyclic Diboryloxy Carbenes: the Activation Strain Model Study. *European Journal of Inorganic Chemistry*, **2021**, 2021, 929-938	2.3	
129	Insights into the Factors Controlling the Origin of Activation Barriers in Group 13 Analogues of the Four-Membered N-Heterocyclic Carbenes. *ACS Omega*, **2021**, 6, 22272-22283	3.9	
128	Significant Insight into the Origin of Reaction Barriers Determining Dihydrogen Activation by G13-P-P (G13 = Group 13 Element) and G15-P-Ga (G15 = Group 15 Element) Frustrated Lewis Pairs. *Inorganic Chemistry*, **2021**, 60, 15253-15269	5.1	1
127	A -Phosphinoamidinato NHC-Diborene Catalyst for Hydroboration. *Journal of the American Chemical Society*, **2021**, 143, 4993-5002	16.4	10
126	Versatile Reaction Patterns of Phosphanylhydrosilylalkyne with B(C6F5)3: A Remarkable Group Substitution Effect. *European Journal of Inorganic Chemistry*, **2020**, 2020, 3496-3506	2.3	1
125	Formation of Alkynylgermyl-Substituted Germylenes via a Catenation of Ge Atoms. *Inorganic Chemistry*, **2020**, 59, 10123-10128	5.1	1
124	Understanding the reactivity of carbene-analogous phosphane complexes with group 13 elements as a central atom: a theoretical investigation. *New Journal of Chemistry*, **2020**, 44, 12815-12826	3.6	0
123	A mechanistic study of the activation of small molecules (H2 and C2H2) by group 14 analogues of selenophene. *New Journal of Chemistry*, **2020**, 44, 8922-8936	3.6	
122	A NHC-Silyliumylidene Cation for Catalytic N-Formylation of Amines Using Carbon Dioxide. *ACS Catalysis*, **2020**, 10, 14824-14833	13.1	16
121	A theoretical study of the reactivity of ethene and benzophenone with a hyper-coordinated alkene containing a so-called E=E (E = C, Si, Ge, Sn, and Pb) unit. *Dalton Transactions*, **2020**, 49, 12842-12853	4.3	1
120	The mechanistic investigations of photochemical decarbonylations and oxidative addition reactions for M(CO) (M = Fe, Ru, Os) complexes.. *RSC Advances*, **2019**, 9, 2626-2640	3.7	
119	Theoretical investigations of the reactivity of neutral molecules that feature an MM (M = B, Al, Ga, In, and Tl) double bond. *New Journal of Chemistry*, **2019**, 43, 9364-9375	3.6	3
118	A computational study to determine whether substituents make E[triple bond, length as m-dash]nitrogen (E = B, Al, Ga, In, and Tl) triple bonds synthetically accessible.. *RSC Advances*, **2019**, 9, 12195-12208	3.7	2

117	A Versatile NHC-Parent Silyliumylidene Cation for Catalytic Chemo- and Regioselective Hydroboration. *Journal of the American Chemical Society*, **2019**, 141, 17629-17636	16.4	33
116	A self-hydrosilylation of phosphanylhydrosilylalkynes promoted by B(CF)? An experimental and mechanistic study. *Chemical Communications*, **2019**, 55, 1494-1497	5.8	3
115	A Theoretical Study on the Stability of PtL Complexes of Endohedral Fullerenes: The Influence of Encapsulated Ions, Cage Sizes, and Ligands. *ACS Omega*, **2019**, 4, 3105-3113	3.9	
114	Photochemical isomerization reactions of acrylonitrile. A mechanistic study.. *RSC Advances*, **2018**, 8, 5647-5651	3.7	
113	Triple-Bonded Boron?Phosphorus Molecule: Is That Possible?. *ACS Omega*, **2018**, 3, 76-85	3.9	6
112	B-H Bond Activation by an Amidinate-Stabilized Amidosilylene: Non-Innocent Amidinate Ligand. *Inorganic Chemistry*, **2018**, 57, 5879-5887	5.1	17
111	A possible target: triple-bonded indiumantimony molecules with high stability. *New Journal of Chemistry*, **2018**, 42, 6932-6941	3.6	2
110	Mechanistic Investigations on the Photoisomerization Reactions of Five-Membered Ring Heterocyclic Molecules Containing Sulfur and Selenium Atoms. *ACS Omega*, **2018**, 3, 3482-3488	3.9	4
109	The mechanistic investigations of photochemical carbonyl elimination and oxidative addition reactions of (ECH)M(CO), (M = Mn and Re) complexes.. *RSC Advances*, **2018**, 8, 10987-10998	3.7	3
108	A model study on the photodecarbonyl reaction of (ECH)M(CO) (M = Co, Rh, Ir).. *RSC Advances*, **2018**, 8, 24641-24653	3.7	
107	Synthesis of a Dimeric Base-Stabilized Cobaltosilylene Complex for Catalytic C-H Bond Functionalization and C-C Bond Formation. *Chemistry - A European Journal*, **2018**, 24, 14329-14334	4.8	9
106	How Important is Metal-Carbon Back-Bonding for the Stability of Fullerene-Transition Metal Complexes? Role of Cage Sizes, Encapsulated Ions and Metal Ligands **2018**,		1
105	Is It Possible To Prepare and Stabilize Triple-Bonded Thallium?Antimony Molecules Using Substituents?. *ACS Omega*, **2018**, 3, 10163-10171	3.9	1
104	Photochemical rearrangement reactions of bicyclic molecules that contain a cyclopropane ring. *New Journal of Chemistry*, **2018**, 42, 11438-11449	3.6	3
103	The effect of substituents on triply bonded boron[triple bond, length as m-dash]antimony molecules: a theoretical approach. *Physical Chemistry Chemical Physics*, **2017**, 19, 8026-8033	3.6	4
102	Indium-Arsenic Molecules with an In?As Triple Bond: A Theoretical Approach. *ACS Omega*, **2017**, 2, 1172-1179	3.9	2
101	Mechanistic Study for the Photochemical Reactions of d M(CO)(CS) (M = Cr, Mo, and W) Complexes. *ACS Omega*, **2017**, 2, 2813-2826	3.9	4
100	Theoretical Study of Addition Reactions of LM(M = Rh, Ir) and LM(M = Pd, Pt) to Li@C. *Journal of Physical Chemistry A*, **2017**, 121, 2665-2673	2.8	5

99	The effect of substituents on the stability of triply bonded gallium[triple bond, length as m-dash]antimony molecules: a new target for synthesis. *Dalton Transactions*, **2017**, 46, 1848-1856	4.3	6
98	Total Synthesis of (+)-Antrocin and Its Diastereomer and Clarification of the Absolute Stereochemistry of (-)-Antrocin. *Journal of Organic Chemistry*, **2017**, 82, 9576-9584	4.2	1
97	Aluminum□phosphorus triple bonds: Do substituents make Al P synthetically accessible?. *Chemical Physics Letters*, **2017**, 686, 60-67	2.5	3
96	Mechanistic investigations and molecular properties of 1,2-bis(ferrocenyl)dimetallenes including group 14 elements. *RSC Advances*, **2017**, 7, 44724-44734	3.7	1
95	Mechanistic Investigations of the Photochemical Isomerizations of [(CO)MC(Me)(OMe)] (M = Cr, Mo, and W) Complexes. *ACS Omega*, **2017**, 2, 5395-5406	3.9	3
94	CASSCF and CASMP2 study on the photoisomerization mechanisms of [tris(trialkylsilyl)silyl]cyclotetrasilene and related cyclobutene molecules. *RSC Advances*, **2017**, 7, 9975-9980	3.7	
93	A Dimeric NHC□Silicon Monotelluride: Synthesis, Isomerization, and Reactivity. *Angewandte Chemie*, **2017**, 129, 11723-11727	3.6	4
92	A Dimeric NHC-Silicon Monotelluride: Synthesis, Isomerization, and Reactivity. *Angewandte Chemie - International Edition*, **2017**, 56, 11565-11569	16.4	10
91	Triply Bonded Gallium?Phosphorus Molecules: Theoretical Designs and Characterization. *Journal of Physical Chemistry A*, **2017**, 121, 6630-6637	2.8	2
90	Singlet oxygen-mediated selective C-H bond hydroperoxidation of ethereal hydrocarbons. *Nature Communications*, **2017**, 8, 1812	17.4	49
89	Substituent Effects on the Stability of Thallium and Phosphorus Triple Bonds: A Density Functional Study. *Molecules*, **2017**, 22,	4.8	2
88	Triply-bonded indiumphosphorus molecules: theoretical designs and characterization. *RSC Advances*, **2017**, 7, 20597-20603	3.7	1
87	A computational study of the mechanism of the photocyclization reaction of □-methylamino ketone. *RSC Advances*, **2016**, 6, 80712-80717	3.7	
86	Mechanistic Investigations on the Photorearrangement Reactions of M(CO)4(CS) (M = Group 6 Metal). *Inorganic Chemistry*, **2016**, 55, 9017-25	5.1	5
85	Substituent Effects on Boron□Bismuth Triple Bond: A New Target for Synthesis. *Organometallics*, **2016**, 35, 3924-3931	3.8	11
84	Mechanistic investigations of CO-photoextrusion and oxidative addition reactions of early transition-metal carbonyls: (□5)-C5H5)M(CO)4 (M = V, Nb, Ta). *Physical Chemistry Chemical Physics*, **2016**, 18, 16396-403	3.6	3
83	A mechanistic study of the addition of alcohol to a five-membered ring silene via a photochemical reaction. *Physical Chemistry Chemical Physics*, **2016**, 18, 8228-34	3.6	2
82	Mechanistic analysis of the photochemical carboxylation of o-alkylphenyl ketones with carbon dioxide. *RSC Advances*, **2016**, 6, 50825-50832	3.7	8

81	A model study on the photochemical isomerization of cyclic silenes. *Physical Chemistry Chemical Physics*, **2015**, 17, 5039-42	3.6	3
80	Doubly bonded E13?P and B?E15 molecules and their reactions with H2, acetonitrile, benzophenone, and 2,3-dimethylbutadiene. *Inorganic Chemistry*, **2015**, 54, 5154-61	5.1	11
79	The addition reactions between N-heterocyclic carbenes and fullerenes (C60 and C70): a density functional study. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	3
78	Theoretical Designs for Fullerene Carbenes, C60EC60 and C70EC70 (E = Group 14 Elements): A Target for Experimental Studies. *Journal of Physical Chemistry C*, **2015**, 119, 12668-12673	3.8	1
77	Excited-State Photolytic Mechanism of Cyclopentene Containing a Group 14 Element: An MP2-CAS//CASSCF Study. *Journal of Physical Chemistry A*, **2015**, 119, 8611-8	2.8	4
76	Theoretical study of the photo-isomerisation reactions of 1,2-dihydro-1,2-phosphaborine and 1,2-dihydro-1,2-alumazaine. *Molecular Physics*, **2015**, 113, 1590-1599	1.7	3
75	Mechanistic Analysis of an Isoxazole-Oxazole Photoisomerization Reaction Using a Conical Intersection. *Journal of Physical Chemistry A*, **2015**, 119, 9666-9	2.8	11
74	A Model Study on Molecular Properties and Mechanistic Investigations of P=C=E14 Molecules. *European Journal of Inorganic Chemistry*, **2015**, 2015, 1795-1803	2.3	
73	Relative Stability of Multiple Bonds between Germanium and Stibium. A Theoretical Study. *Journal of the Chinese Chemical Society*, **2015**, 62, 906-909	1.5	
72	A model study on the photochemical isomerization of isothiazoles and thiazoles. *Physical Chemistry Chemical Physics*, **2014**, 16, 17030-42	3.6	11
71	Mechanistic investigations on E-N bond-breaking and ring expansion for N-heterocyclic carbene analogues containing the group 14 elements (E). *Inorganic Chemistry*, **2014**, 53, 5080-7	5.1	24
70	A theoretical study of the photochemical isomerization reactions of (+)-2-carene-4-methanol from the triplet state. *Theoretical Chemistry Accounts*, **2014**, 133, 1	1.9	1
69	Substituent Effects on the Geometries and Energies of the Antimony–Silicon Multiple Bond. *Bulletin of the Chemical Society of Japan*, **2014**, 87, 816-818	5.1	2
68	Mechanistic Study of the Photochemical Isomerization Reactions of Silabenzene. *Organometallics*, **2014**, 33, 5231-5237	3.8	8
67	A theoretical investigation of photochemical reactions of an isolable silylene with benzene. *Chemistry - A European Journal*, **2014**, 20, 9419-23	4.8	4
66	Model study of the photochemical rearrangement pathways of 1,2,4-oxadiazole. *ChemPhysChem*, **2014**, 15, 2712-22	3.2	6
65	A mechanistic analysis of the tetrasilyl-substituted trimetallaallenes, >E=E=EDalton Transactions, **2013**, 42, 4873-84	4.3	
64	Theory predicts triplet ground-state carbene containing the N-heterocyclic carbenic unit. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	6

63	Mechanistic investigations on the photoisomerization reactions of 1,2-dihydro-1,2-azaborine. *Chemistry - A European Journal*, **2013**, 19, 9663-7	4.8	8
62	Theoretical Investigations of Mechanisms of Thermal Cleavage of E=E Bonds in Heavy Butadiene Systems (E = C, Si, Ge, Sn, and Pb). *European Journal of Inorganic Chemistry*, **2012**, 2012, 272-281	2.3	
61	Theoretical Study of the Mechanisms for the Reactions of the Ferrio-Substituted E(II) Compound Me5C5(CO)2FeEC5Me5(E = C, Si, Ge, Sn, and Pb). *Organometallics*, **2012**, 31, 3101-3112	3.8	7
60	Theoretical investigations of the reactions of phosphino disilenes and their derivatives with an E?E (E = C, Si, Ge, Sn, and Pb) double bond. *Journal of Physical Chemistry A*, **2012**, 116, 9412-20	2.8	5
59	Theoretical investigation of the mechanisms for the reaction of fused tricyclic dimetallenes containing highly strained E?E (E = C, Si, Ge, Sn, and Pb) double bonds. *Journal of Physical Chemistry A*, **2012**, 116, 4222-32	2.8	10
58	A computational study of the mechanisms of the photoisomerization reactions of monocyclic and bicyclic olefins. *Journal of Physical Chemistry A*, **2011**, 115, 5157-65	2.8	2
57	Triply bonded stannaacetylene (RC?SnR): theoretical designs and characterization. *Inorganic Chemistry*, **2011**, 50, 6814-22	5.1	14
56	Theoretical designs for germaacetylene (RC?GeR): a new target for synthesis. *Dalton Transactions*, **2011**, 40, 4253-9	4.3	17
55	Mechanisms for the Reaction of Water, Butadiene, and Palladium Complex with 1,2-Dimetallacyclohexene (R2M?MR2, M = C, Si, Ge, Sn, Pb). A Theoretical Study. *Organometallics*, **2011**, 30, 4862-4872	3.8	7
54	Reactivities of Adamantyl-Substituted Metallenes with a C?E (E = C, Si, Ge, Sn, and Pb) Double Bond. A Theoretical Study. *Organometallics*, **2011**, 30, 6189-6200	3.8	12
53	A New Target for Synthesis of Triply Bonded Plumbacetylene (RC?PbR): A Theoretical Design. *Organometallics*, **2011**, 30, 3293-3301	3.8	15
52	Diboration of the E?E Double Bond by [2]Metallocenophanes (E = N, P, As, Sb, and Bi): A Theoretical Study. *Organometallics*, **2010**, 29, 5812-5820	3.8	7
51	Computational study of the mechanisms of the photoisomerization reactions of bicycloalkene. *Journal of Physical Chemistry A*, **2010**, 114, 11656-62	2.8	
50	A computational study of photochemical isomerization reactions of thiophenes. *Journal of Computational Chemistry*, **2010**, 31, 43-56	3.5	9
49	Quantum mechanical study of the photoisomerizations of bicyclo[4,1,0]hept-2-ene (2-norcarene). *Journal of Physical Chemistry A*, **2009**, 113, 381-7	2.8	
48	Density Functional Theory Study of the Reactivities of Perimidine-Based Carbene Analogues of the Group 14 Elements. *Organometallics*, **2009**, 28, 4324-4334	3.8	8
47	Theoretical investigations of the photochemical isomerizations of indoxazene and isoxazole. *Journal of Organic Chemistry*, **2009**, 74, 6055-63	4.2	5
46	A theoretical study of the photochemical isomerization reactions of furans from the triplet state. *Journal of Physical Chemistry A*, **2008**, 112, 194-8	2.8	1

45	A theoretical insight into the reaction mechanism of photochemical transposition from pyrazole to imidazole. *Journal of Physical Chemistry A*, **2008**, 112, 10420-8	2.8	6
44	A mechanistic study on the photoisomerizations of spiro[2,4]hept-1-ene, vinylidenecyclopentane, and vinylidenecyclobutane hydrocarbons. *Journal of Physical Chemistry A*, **2008**, 112, 5527-37	2.8	2
43	Theoretical investigations of the reactivities of cationic six-membered carbene analogues of group 14 elements. *Journal of Physical Chemistry A*, **2008**, 112, 7689-98	2.8	20
42	Photoisomerization Reactions of Cyclopropene and 1,3,3-Trimethylcyclopropene: A Theoretical Study. *Journal of Chemical Theory and Computation*, **2008**, 4, 1263-73	6.4	5
41	A quantum mechanical study of the abstraction reactions of fused bicyclic dimetallenes. *Journal of Physical Chemistry A*, **2008**, 112, 10064-70	2.8	1
40	Theoretical Design of Silicon□Phosphorus Triple Bonds: A Density Functional Study. *European Journal of Inorganic Chemistry*, **2008**, 2008, 1241-1247	2.3	6
39	Model study on the pyridine-Dewar pyridine and some related photoisomerization reactions. *Journal of Physical Chemistry A*, **2007**, 111, 971-5	2.8	12
38	Theoretical studies of the [2 + 4] Diels-Alder cycloaddition reactions of alkene analogues of the group 13 elements with toluene. *Inorganic Chemistry*, **2007**, 46, 2028-34	5.1	8
37	Theoretical study of cycloaddition reactions of heavy carbenes with C60. *Journal of Physical Chemistry A*, **2007**, 111, 6232-40	2.8	17
36	The photochemical rearrangement pathways of imidazoles: a theoretical study. *Journal of Physical Chemistry A*, **2007**, 111, 1567-74	2.8	8
35	A theoretical characterization of the photoisomerization channels of 1,2-cyclononadienes on both singlet and triplet potential-energy surfaces. *Chemistry - A European Journal*, **2007**, 13, 9957-72	4.8	4
34	CASCSF study on the photochemical transposition reactions of pyrazines. *Journal of Physical Chemistry A*, **2006**, 110, 9420-8	2.8	15
33	Photochemical isomerization reactions of cyanopyrroles: a theoretical study. *Journal of Physical Chemistry A*, **2006**, 110, 12653-61	2.8	5
32	Theoretical Study of the Reactivities of Neutral Six-Membered Carbene Analogues of the Group 13 Elements. *Organometallics*, **2006**, 25, 2766-2773	3.8	26
31	Theoretical designs for planar tetracoordinated carbon in Cu, Ag, and Au organometallic chemistry: a new target for synthesis. *Inorganic Chemistry*, **2005**, 44, 4829-33	5.1	20
30	Theoretical study of addition reactions of heavy carbenes to carbon and boron nitride nanotubes. *Journal of Physical Chemistry B*, **2005**, 109, 21647-57	3.4	24
29	The Cycloaddition Reactions of Angle Strained Cycloalkynes. A Theoretical Study. *Journal of the Chinese Chemical Society*, **2005**, 52, 599-624	1.5	8
28	Theoretical examination of substituent effects on the stabilization of a Sn?Y (Y = Sb and Bi) multiple bond. *International Journal of Quantum Chemistry*, **2005**, 102, 72-79	2.1	4

27	Theoretical study on the reactivities of stannylene and plumbylene and the origin of their activation barriers. *Chemistry - A European Journal*, **2004**, 10, 6073-84	4.8	45
26	Theoretical Study of Intramolecular [4 + 2] Cycloadditions of Iminoacetonitriles: A New Class of Azadienophiles for Hetero Diels□Alder Reactions. *Organometallics*, **2004**, 23, 2507-2509	3.8	16
25	Theoretical Study of the Reaction Mechanism of Abstraction Reactions of Disilenes and Digermenes with Haloalkanes. *Journal of Physical Chemistry A*, **2004**, 108, 823-832	2.8	37
24	Mechanism of abstraction reactions of dimetallenes (R2X=XR2; X = C, Si, Ge, Sn, Pb) with halocarbons: a theoretical study. *Inorganic Chemistry*, **2004**, 43, 4846-61	5.1	29
23	Theoretical study of halophilic reactions of stable silylenes with chloro- and bromocarbons. *Journal of the American Chemical Society*, **2003**, 125, 1714-5	16.4	20
22	Dissociative photoionization of CH2Cl2 and enthalpy of formation of CHCl+: Experiments and calculations. *Journal of Chemical Physics*, **2003**, 118, 62-69	3.9	28
21	An examination of substituent effects on the stabilization of a silicon□selenium double bond. *International Journal of Quantum Chemistry*, **2002**, 90, 663-668	2.1	3
20	A Theoretical Study of Oxygen Atom Transfer Reactions from Oxiranes to Heavy Carbenes. *Journal of Physical Chemistry A*, **2002**, 106, 9563-9568	2.8	22
19	Theoretical study of silylene substituent effects on the abstraction reactions with oxirane and thiirane. *Journal of the American Chemical Society*, **2002**, 124, 12335-42	16.4	18
18	Density functional study of the relative reactivity in the concerted 1,3-dipolar cycloaddition of nitrile ylide to disubstituted ethylenes. *International Journal of Quantum Chemistry*, **2001**, 83, 318-323	2.1	9
17	A stable species with a formal Ge?C triple bond □a theoretical study. *Chemical Physics Letters*, **2001**, 341, 122-128	2.5	19
16	Theoretical study of triple bonds to germanium:relative stabilities of germanitriles and germaimines. *Chemical Communications*, **2001**, 1120-1121	5.8	7
15	Theoretical Study of the Germylene Insertion Reaction into the A-H Bond of First-Row and Second-Row AHn Hydrides. *Journal of the Chinese Chemical Society*, **2000**, 47, 135-139	1.5	6
14	Effects of substituents on the thermodynamic and kinetic stabilities of HCGeX (X = H, CH3, F, and Cl) isomers. A theoretical study. *Inorganic Chemistry*, **2000**, 39, 3522-5	5.1	15
13	Theoretical Studies of the Kinetic and Thermodynamic Stabilities of Isomers of HXGeS (X = H, F, Cl, and Br) in the Gas Phase. *Journal of Physical Chemistry A*, **2000**, 104, 9250-9259	2.8	9
12	Density functional theory of C?H bond activation by transition-metal complex: A (□5-C5H5)ML (M=Rh, Ir; L=CH2, CO, SH2, PH3)+CH4 case study. *International Journal of Quantum Chemistry*, **1999**, 72, 405-410	2.1	5
11	A Theoretical Model for the Orientation of 16-Electron [CpML] Insertion into the C□H Bond of Propane and Cyclopropane and Its Regio- and Stereoselectivity. *Chemistry - A European Journal*, **1999**, 5, 198-207	4.8	22
10	Density Functional Study of Some Germylene Insertion Reactions. *Journal of the American Chemical Society*, **1999**, 121, 4229-4237	16.4	69

9	Theoretical Study of Reactions of Arduengo-Type Carbene, Silylene, and Germylene with CH(4). *Inorganic Chemistry*, **1999**, 38, 4819-4823	5.1	30
8	Density Functional and MP2 Studies of Germylene Insertion into C–H, Si–H, N–H, P–H, O–H, S–H, F–H, and Cl–H Bonds. *Journal of Physical Chemistry A*, **1999**, 103, 11011-11019	2.8	31
7	Cycloadditions of 16-Electron 1,3-Dipoles with Ethylene. A Density Functional and CCSD(T) Study. *Journal of Organic Chemistry*, **1999**, 64, 6710-6716	4.2	67
6	A Correlation between C?H Bond Activation Barrier and Singlet-Tripet Energy Gap of Transition Metal Complex-Density Functional Study on CpML Insertion into CH4. *Journal of the Chinese Chemical Society*, **1999**, 46, 403-407	1.5	2
5	Substituent Effects on Oxidative Addition for Coordinatively Unsaturated d8ML3. Mechanistic and Thermodynamic Considerations. *Journal of Physical Chemistry A*, **1998**, 102, 10159-10166	2.8	11
4	Theoretical Study of Oxidative Addition and Reductive Elimination of 14-Electron d10 ML2 Complexes: A ML2 + CH4 (M = Pd, Pt; L = CO, PH3, L2 = PH2CH2CH2PH2) Case Study. *Inorganic Chemistry*, **1998**, 37, 3400-3406	5.1	57
3	A New Aspect for the Insertion of the 16-Electron Species (η5-C5H5)ML into Saturated Hydrocarbons. A (η5-C5H5)ML + CH4(M = Rh, Ir; L = CO, SH2, PH3) Case Study *Journal of Physical Chemistry A*, **1997**, 101, 6798-6806	2.8	20
2	An Energetically Feasible Mechanism for the Activation of the C–H Bond by the 16-Electron CpM(PH3)(CH3)+ (M = Rh, Ir) Complex. A Theoretical Study. *Journal of the American Chemical Society*, **1997**, 119, 5373-5383	16.4	81
1	Theoretical Model for Insertion of the 16-Electron Species (η5-C5H5)M(L) into Saturated Hydrocarbons. A (η5-C5H5)M(CO) + CH4 (M = Ru-, Os-, Rh, Ir, Pd+, Pt+) Case Study. *Organometallics*, **1997**, 16, 1621-1627	3.8	30