

Ming-Der Su

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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	An Energetically Feasible Mechanism for the Activation of the C≡H Bond by the 16-Electron CpM(PH ₃)(CH ₃) ⁺ (M = Rh, Ir) Complex. A Theoretical Study. <i>Journal of the American Chemical Society</i> , 1997 , 119, 5373-5383	16.4	81
133	Density Functional Study of Some Germylene Insertion Reactions. <i>Journal of the American Chemical Society</i> , 1999 , 121, 4229-4237	16.4	69
132	Cycloadditions of 16-Electron 1,3-Dipoles with Ethylene. A Density Functional and CCSD(T) Study. <i>Journal of Organic Chemistry</i> , 1999 , 64, 6710-6716	4.2	67
131	Theoretical Study of Oxidative Addition and Reductive Elimination of 14-Electron d ¹⁰ ML ₂ Complexes: A ML ₂ + CH ₄ (M = Pd, Pt; L = CO, PH ₃ , L ₂ = PH ₂ CH ₂ CH ₂ PH ₂) Case Study. <i>Inorganic Chemistry</i> , 1998 , 37, 3400-3406	5.1	57
130	Singlet oxygen-mediated selective C-H bond hydroperoxidation of ethereal hydrocarbons. <i>Nature Communications</i> , 2017 , 8, 1812	17.4	49
129	Theoretical study on the reactivities of stannylene and plumbylene and the origin of their activation barriers. <i>Chemistry - A European Journal</i> , 2004 , 10, 6073-84	4.8	45
128	Theoretical Study of the Reaction Mechanism of Abstraction Reactions of Disilenes and Digermenes with Haloalkanes. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 823-832	2.8	37
127	A Versatile NHC-Parent Silyliumylidene Cation for Catalytic Chemo- and Regioselective Hydroboration. <i>Journal of the American Chemical Society</i> , 2019 , 141, 17629-17636	16.4	33
126	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. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 11011-11019	2.8	31
125	Theoretical Model for Insertion of the 16-Electron Species (≡-C ₅ H ₅)M(L) into Saturated Hydrocarbons. A (≡-C ₅ H ₅)M(CO) + CH ₄ (M = Ru-, Os-, Rh, Ir, Pd+, Pt+) Case Study. <i>Organometallics</i> , 1997 , 16, 1621-1627	3.8	30
124	Theoretical Study of Reactions of Arduengo-Type Carbene, Silylene, and Germylene with CH ₄ . <i>Inorganic Chemistry</i> , 1999 , 38, 4819-4823	5.1	30
123	Mechanism of abstraction reactions of dimetallenes (R ₂ X=XR ₂ ; X = C, Si, Ge, Sn, Pb) with halocarbons: a theoretical study. <i>Inorganic Chemistry</i> , 2004 , 43, 4846-61	5.1	29
122	Dissociative photoionization of CH ₂ Cl ₂ and enthalpy of formation of CHCl ₂ ⁺ : Experiments and calculations. <i>Journal of Chemical Physics</i> , 2003 , 118, 62-69	3.9	28
121	Theoretical Study of the Reactivities of Neutral Six-Membered Carbene Analogues of the Group 13 Elements. <i>Organometallics</i> , 2006 , 25, 2766-2773	3.8	26
120	Mechanistic investigations on E-N bond-breaking and ring expansion for N-heterocyclic carbene analogues containing the group 14 elements (E). <i>Inorganic Chemistry</i> , 2014 , 53, 5080-7	5.1	24
119	Theoretical study of addition reactions of heavy carbenes to carbon and boron nitride nanotubes. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 21647-57	3.4	24
118	A Theoretical Study of Oxygen Atom Transfer Reactions from Oxiranes to Heavy Carbenes. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 9563-9568	2.8	22

117	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. <i>Chemistry - A European Journal</i> , 1999 , 5, 198-207	4.8	22
116	A New Aspect for the Insertion of the 16-Electron Species (B-C5H5)ML into Saturated Hydrocarbons. A (B-C5H5)ML + CH4(M = Rh, Ir; L = CO, SH2, PH3) Case Study. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 6798-6806	2.8	20
115	Theoretical investigations of the reactivities of cationic six-membered carbene analogues of group 14 elements. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 7689-98	2.8	20
114	Theoretical designs for planar tetracoordinated carbon in Cu, Ag, and Au organometallic chemistry: a new target for synthesis. <i>Inorganic Chemistry</i> , 2005 , 44, 4829-33	5.1	20
113	Theoretical study of halophilic reactions of stable silylenes with chloro- and bromocarbons. <i>Journal of the American Chemical Society</i> , 2003 , 125, 1714-5	16.4	20
112	A stable species with a formal Ge-C triple bond: a theoretical study. <i>Chemical Physics Letters</i> , 2001 , 341, 122-128	2.5	19
111	Theoretical study of silylene substituent effects on the abstraction reactions with oxirane and thiirane. <i>Journal of the American Chemical Society</i> , 2002 , 124, 12335-42	16.4	18
110	B-H Bond Activation by an Amidinate-Stabilized Amidosilylene: Non-Innocent Amidinate Ligand. <i>Inorganic Chemistry</i> , 2018 , 57, 5879-5887	5.1	17
109	Theoretical designs for germaacetylene (RC=GeR) a new target for synthesis. <i>Dalton Transactions</i> , 2011 , 40, 4253-9	4.3	17
108	Theoretical study of cycloaddition reactions of heavy carbenes with C60. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 6232-40	2.8	17
107	Theoretical Study of Intramolecular [4 + 2] Cycloadditions of Iminoacetonitriles: A New Class of Azadienophiles for Hetero Diels-Alder Reactions. <i>Organometallics</i> , 2004 , 23, 2507-2509	3.8	16
106	A NHC-Silyliumylidene Cation for Catalytic N-Formylation of Amines Using Carbon Dioxide. <i>ACS Catalysis</i> , 2020 , 10, 14824-14833	13.1	16
105	A New Target for Synthesis of Triply Bonded Plumbacetylene (RC=PbR): A Theoretical Design. <i>Organometallics</i> , 2011 , 30, 3293-3301	3.8	15
104	CASCSF study on the photochemical transposition reactions of pyrazines. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 9420-8	2.8	15
103	Effects of substituents on the thermodynamic and kinetic stabilities of HCGeX (X = H, CH3, F, and Cl) isomers. A theoretical study. <i>Inorganic Chemistry</i> , 2000 , 39, 3522-5	5.1	15
102	Triply bonded stannaacetylene (RC=SnR): theoretical designs and characterization. <i>Inorganic Chemistry</i> , 2011 , 50, 6814-22	5.1	14
101	Reactivities of Adamantyl-Substituted Metallenes with a C=E (E = C, Si, Ge, Sn, and Pb) Double Bond. A Theoretical Study. <i>Organometallics</i> , 2011 , 30, 6189-6200	3.8	12
100	Model study on the pyridine-Dewar pyridine and some related photoisomerization reactions. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 971-5	2.8	12

99	Doubly bonded E13?P and B?E15 molecules and their reactions with H2, acetonitrile, benzophenone, and 2,3-dimethylbutadiene. <i>Inorganic Chemistry</i> , 2015 , 54, 5154-61	5.1	11
98	Mechanistic Analysis of an Isoxazole-Oxazole Photoisomerization Reaction Using a Conical Intersection. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 9666-9	2.8	11
97	Substituent Effects on BoronBismuth Triple Bond: A New Target for Synthesis. <i>Organometallics</i> , 2016 , 35, 3924-3931	3.8	11
96	A model study on the photochemical isomerization of isothiazoles and thiazoles. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 17030-42	3.6	11
95	Substituent Effects on Oxidative Addition for Coordinatively Unsaturated d8ML3. Mechanistic and Thermodynamic Considerations. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 10159-10166	2.8	11
94	A Dimeric NHC-Silicon Monotelluride: Synthesis, Isomerization, and Reactivity. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 11565-11569	16.4	10
93	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. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 4222-32	2.8	10
92	A -Phosphinoamidinato NHC-Diborene Catalyst for Hydroboration. <i>Journal of the American Chemical Society</i> , 2021 , 143, 4993-5002	16.4	10
91	Synthesis of a Dimeric Base-Stabilized Cobaltosilylene Complex for Catalytic C-H Bond Functionalization and C-C Bond Formation. <i>Chemistry - A European Journal</i> , 2018 , 24, 14329-14334	4.8	9
90	A computational study of photochemical isomerization reactions of thiophenes. <i>Journal of Computational Chemistry</i> , 2010 , 31, 43-56	3.5	9
89	Density functional study of the relative reactivity in the concerted 1,3-dipolar cycloaddition of nitrile ylide to disubstituted ethylenes. <i>International Journal of Quantum Chemistry</i> , 2001 , 83, 318-323	2.1	9
88	Theoretical Studies of the Kinetic and Thermodynamic Stabilities of Isomers of HXGeS (X = H, F, Cl, and Br) in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2000 , 104, 9250-9259	2.8	9
87	Mechanistic Study of the Photochemical Isomerization Reactions of Silabenzene. <i>Organometallics</i> , 2014 , 33, 5231-5237	3.8	8
86	Mechanistic investigations on the photoisomerization reactions of 1,2-dihydro-1,2-azaborine. <i>Chemistry - A European Journal</i> , 2013 , 19, 9663-7	4.8	8
85	Density Functional Theory Study of the Reactivities of Perimidine-Based Carbene Analogues of the Group 14 Elements. <i>Organometallics</i> , 2009 , 28, 4324-4334	3.8	8
84	Theoretical studies of the [2 + 4] Diels-Alder cycloaddition reactions of alkene analogues of the group 13 elements with toluene. <i>Inorganic Chemistry</i> , 2007 , 46, 2028-34	5.1	8
83	The photochemical rearrangement pathways of imidazoles: a theoretical study. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 1567-74	2.8	8
82	The Cycloaddition Reactions of Angle Strained Cycloalkynes. A Theoretical Study. <i>Journal of the Chinese Chemical Society</i> , 2005 , 52, 599-624	1.5	8

81	Mechanistic analysis of the photochemical carboxylation of o-alkylphenyl ketones with carbon dioxide. <i>RSC Advances</i> , 2016 , 6, 50825-50832	3.7	8
80	Theoretical Study of the Mechanisms for the Reactions of the Ferric-Substituted E(II) Compound Me ₅ C ₅ (CO) ₂ FeEC ₅ Me ₅ (E = C, Si, Ge, Sn, and Pb). <i>Organometallics</i> , 2012 , 31, 3101-3112	3.8	7
79	Diboration of the E?E Double Bond by [2]Metalocenophanes (E = N, P, As, Sb, and Bi): A Theoretical Study. <i>Organometallics</i> , 2010 , 29, 5812-5820	3.8	7
78	Mechanisms for the Reaction of Water, Butadiene, and Palladium Complex with 1,2-Dimetallacyclohexene (R ₂ M?MR ₂ , M = C, Si, Ge, Sn, Pb). A Theoretical Study. <i>Organometallics</i> , 2011 , 30, 4862-4872	3.8	7
77	Theoretical study of triple bonds to germanium: relative stabilities of germanitriles and germainines. <i>Chemical Communications</i> , 2001 , 1120-1121	5.8	7
76	The effect of substituents on the stability of triply bonded gallium[triple bond, length as m-dash]antimony molecules: a new target for synthesis. <i>Dalton Transactions</i> , 2017 , 46, 1848-1856	4.3	6
75	Triple-Bonded Boron?Phosphorus Molecule: Is That Possible?. <i>ACS Omega</i> , 2018 , 3, 76-85	3.9	6
74	Model study of the photochemical rearrangement pathways of 1,2,4-oxadiazole. <i>ChemPhysChem</i> , 2014 , 15, 2712-22	3.2	6
73	Theory predicts triplet ground-state carbene containing the N-heterocyclic carbenic unit. <i>Theoretical Chemistry Accounts</i> , 2013 , 132, 1	1.9	6
72	A theoretical insight into the reaction mechanism of photochemical transposition from pyrazole to imidazole. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 10420-8	2.8	6
71	Theoretical Design of Silicon?Phosphorus Triple Bonds: A Density Functional Study. <i>European Journal of Inorganic Chemistry</i> , 2008 , 2008, 1241-1247	2.3	6
70	Theoretical Study of the Germylene Insertion Reaction into the A-H Bond of First-Row and Second-Row AH _n Hydrides. <i>Journal of the Chinese Chemical Society</i> , 2000 , 47, 135-139	1.5	6
69	Theoretical Study of Addition Reactions of LM (M = Rh, Ir) and LM (M = Pd, Pt) to Li@C. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 2665-2673	2.8	5
68	Mechanistic Investigations on the Photorearrangement Reactions of M(CO) ₄ (CS) (M = Group 6 Metal). <i>Inorganic Chemistry</i> , 2016 , 55, 9017-25	5.1	5
67	Theoretical investigations of the reactions of phosphino disilenes and their derivatives with an E?E (E = C, Si, Ge, Sn, and Pb) double bond. <i>Journal of Physical Chemistry A</i> , 2012 , 116, 9412-20	2.8	5
66	Theoretical investigations of the photochemical isomerizations of indoxazene and isoxazole. <i>Journal of Organic Chemistry</i> , 2009 , 74, 6055-63	4.2	5
65	Photoisomerization Reactions of Cyclopropene and 1,3,3-Trimethylcyclopropene: A Theoretical Study. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 1263-73	6.4	5
64	Photochemical isomerization reactions of cyanopyrroles: a theoretical study. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 12653-61	2.8	5

63	Density functional theory of C-H bond activation by transition-metal complex: A (η-C ₅ H ₅)ML (M=Rh, Ir; L=CH ₂ , CO, SH ₂ , PH ₃)+CH ₄ case study. <i>International Journal of Quantum Chemistry</i> , 1999 , 72, 405-410	2.1	5
62	The effect of substituents on triply bonded boron [triple bond, length as m-dash]antimony molecules: a theoretical approach. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 8026-8033	3.6	4
61	Mechanistic Study for the Photochemical Reactions of d M(CO)(CS) (M = Cr, Mo, and W) Complexes. <i>ACS Omega</i> , 2017 , 2, 2813-2826	3.9	4
60	Excited-State Photolytic Mechanism of Cyclopentene Containing a Group 14 Element: An MP2-CAS//CASSCF Study. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 8611-8	2.8	4
59	Mechanistic Investigations on the Photoisomerization Reactions of Five-Membered Ring Heterocyclic Molecules Containing Sulfur and Selenium Atoms. <i>ACS Omega</i> , 2018 , 3, 3482-3488	3.9	4
58	A Dimeric NHC-Silicon Monotelluride: Synthesis, Isomerization, and Reactivity. <i>Angewandte Chemie</i> , 2017 , 129, 11723-11727	3.6	4
57	A theoretical investigation of photochemical reactions of an isolable silylene with benzene. <i>Chemistry - A European Journal</i> , 2014 , 20, 9419-23	4.8	4
56	A theoretical characterization of the photoisomerization channels of 1,2-cyclononadienes on both singlet and triplet potential-energy surfaces. <i>Chemistry - A European Journal</i> , 2007 , 13, 9957-72	4.8	4
55	Theoretical examination of substituent effects on the stabilization of a Sn-Y (Y = Sb and Bi) multiple bond. <i>International Journal of Quantum Chemistry</i> , 2005 , 102, 72-79	2.1	4
54	Theoretical investigations of the reactivity of neutral molecules that feature an MM (M = B, Al, Ga, In, and Tl) double bond. <i>New Journal of Chemistry</i> , 2019 , 43, 9364-9375	3.6	3
53	A model study on the photochemical isomerization of cyclic silenes. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 5039-42	3.6	3
52	The addition reactions between N-heterocyclic carbenes and fullerenes (C ₆₀ and C ₇₀): a density functional study. <i>Theoretical Chemistry Accounts</i> , 2015 , 134, 1	1.9	3
51	Theoretical study of the photo-isomerisation reactions of 1,2-dihydro-1,2-phosphaborine and 1,2-dihydro-1,2-alumazaine. <i>Molecular Physics</i> , 2015 , 113, 1590-1599	1.7	3
50	The mechanistic investigations of photochemical carbonyl elimination and oxidative addition reactions of (η-C ₅ H ₅)M(CO), (M = Mn and Re) complexes.. <i>RSC Advances</i> , 2018 , 8, 10987-10998	3.7	3
49	Mechanistic investigations of CO-photoextrusion and oxidative addition reactions of early transition-metal carbonyls: (η-C ₅ H ₅)M(CO) ₄ (M = V, Nb, Ta). <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 16396-403	3.6	3
48	A self-hydrosilylation of phosphanylhydrosilylalkynes promoted by B(CF ₃) ₃ : An experimental and mechanistic study. <i>Chemical Communications</i> , 2019 , 55, 1494-1497	5.8	3
47	Aluminum-Phosphorus triple bonds: Do substituents make Al-P synthetically accessible?. <i>Chemical Physics Letters</i> , 2017 , 686, 60-67	2.5	3
46	Mechanistic Investigations of the Photochemical Isomerizations of [(CO)M(CMe)(OMe)] (M = Cr, Mo, and W) Complexes. <i>ACS Omega</i> , 2017 , 2, 5395-5406	3.9	3

45	An examination of substituent effects on the stabilization of a silicon-bismuth double bond. <i>International Journal of Quantum Chemistry</i> , 2002 , 90, 663-668	2.1	3
44	Photochemical rearrangement reactions of bicyclic molecules that contain a cyclopropane ring. <i>New Journal of Chemistry</i> , 2018 , 42, 11438-11449	3.6	3
43	Indium-Arsenic Molecules with an In-As Triple Bond: A Theoretical Approach. <i>ACS Omega</i> , 2017 , 2, 1172-1179	3.7	2
42	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.. <i>RSC Advances</i> , 2019 , 9, 12195-12208	3.7	2
41	A possible target: triple-bonded indium-antimony molecules with high stability. <i>New Journal of Chemistry</i> , 2018 , 42, 6932-6941	3.6	2
40	A mechanistic study of the addition of alcohol to a five-membered ring silene via a photochemical reaction. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 8228-34	3.6	2
39	Substituent Effects on the Geometries and Energies of the Antimony-Silicon Multiple Bond. <i>Bulletin of the Chemical Society of Japan</i> , 2014 , 87, 816-818	5.1	2
38	Triply Bonded Gallium-Phosphorus Molecules: Theoretical Designs and Characterization. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 6630-6637	2.8	2
37	Substituent Effects on the Stability of Thallium and Phosphorus Triple Bonds: A Density Functional Study. <i>Molecules</i> , 2017 , 22,	4.8	2
36	A computational study of the mechanisms of the photoisomerization reactions of monocyclic and bicyclic olefins. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 5157-65	2.8	2
35	A mechanistic study on the photoisomerizations of spiro[2,4]hept-1-ene, vinylidenecyclopentane, and vinylidenecyclobutane hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 5527-37	2.8	2
34	A Correlation between C-H Bond Activation Barrier and Singlet-Triplet Energy Gap of Transition Metal Complex-Density Functional Study on CpML Insertion into CH ₄ . <i>Journal of the Chinese Chemical Society</i> , 1999 , 46, 403-407	1.5	2
33	Amidinatoamidosilylene-Dibromodiborene. <i>Inorganic Chemistry</i> , 2021 , 60, 16065-16069	5.1	2
32	Theoretical Designs for Fullerene Carbenes, C ₆₀ H ₂ C ₆₀ and C ₇₀ H ₂ C ₇₀ (E = Group 14 Elements): A Target for Experimental Studies. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 12668-12673	3.8	1
31	Versatile Reaction Patterns of Phosphanylhydrosilylalkyne with B(C ₆ F ₅) ₃ : A Remarkable Group Substitution Effect. <i>European Journal of Inorganic Chemistry</i> , 2020 , 2020, 3496-3506	2.3	1
30	Formation of Alkynylgermyl-Substituted Germylenes via a Catenation of Ge Atoms. <i>Inorganic Chemistry</i> , 2020 , 59, 10123-10128	5.1	1
29	A theoretical study of the photochemical isomerization reactions of (+)-2-carene-4H-methanol from the triplet state. <i>Theoretical Chemistry Accounts</i> , 2014 , 133, 1	1.9	1
28	Total Synthesis of (+)-Antrocin and Its Diastereomer and Clarification of the Absolute Stereochemistry of (-)-Antrocin. <i>Journal of Organic Chemistry</i> , 2017 , 82, 9576-9584	4.2	1

27	Mechanistic investigations and molecular properties of 1,2-bis(ferrocenyl)dimetallenes including group 14 elements. <i>RSC Advances</i> , 2017 , 7, 44724-44734	3.7	1
26	A theoretical study of the photochemical isomerization reactions of furans from the triplet state. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 194-8	2.8	1
25	A quantum mechanical study of the abstraction reactions of fused bicyclic dimetallenes. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 10064-70	2.8	1
24	Triply-bonded indiumphosphorus molecules: theoretical designs and characterization. <i>RSC Advances</i> , 2017 , 7, 20597-20603	3.7	1
23	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. <i>Dalton Transactions</i> , 2020 , 49, 12842-12853	4.3	1
22	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
21	Is It Possible To Prepare and Stabilize Triple-Bonded Thallium?Antimony Molecules Using Substituents?. <i>ACS Omega</i> , 2018 , 3, 10163-10171	3.9	1
20	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. <i>Inorganic Chemistry</i> , 2021 , 60, 15253-15269	5.1	1
19	Understanding the reactivity of carbene-analogous phosphane complexes with group 13 elements as a central atom: a theoretical investigation. <i>New Journal of Chemistry</i> , 2020 , 44, 12815-12826	3.6	0
18	Reactivity of dicationic N-heterocyclic chalcogen carbene analogues with methane and ethene: a theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 2419-2429	3.6	0
17	The mechanistic investigations of photochemical decarbonylations and oxidative addition reactions for M(CO) (M = Fe, Ru, Os) complexes.. <i>RSC Advances</i> , 2019 , 9, 2626-2640	3.7	
16	A mechanistic study of the activation of small molecules (H ₂ and C ₂ H ₂) by group 14 analogues of selenophene. <i>New Journal of Chemistry</i> , 2020 , 44, 8922-8936	3.6	
15	Photochemical isomerization reactions of acrylonitrile. A mechanistic study.. <i>RSC Advances</i> , 2018 , 8, 5647-5651	3.7	
14	A computational study of the mechanism of the photocyclization reaction of N-methylamino ketone. <i>RSC Advances</i> , 2016 , 6, 80712-80717	3.7	
13	A model study on the photodecarbonyl reaction of (ECH)M(CO) (M = Co, Rh, Ir).. <i>RSC Advances</i> , 2018 , 8, 24641-24653	3.7	
12	Theoretical Investigations of Mechanisms of Thermal Cleavage of E=E Bonds in Heavy Butadiene Systems (E = C, Si, Ge, Sn, and Pb). <i>European Journal of Inorganic Chemistry</i> , 2012 , 2012, 272-281	2.3	
11	A mechanistic analysis of the tetrasilyl-substituted trimetallaallenes, >E=E=EDalton Transactions, 2013 , 42, 4873-84	4.3	
10	CASSCF and CASMP2 study on the photoisomerization mechanisms of [tris(trialkylsilyl)silyl]cyclobutene and related cyclobutene molecules. <i>RSC Advances</i> , 2017 , 7, 9975-9980	3.7	

- 9 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
- 8 Relative Stability of Multiple Bonds between Germanium and Stibium. A Theoretical Study. *Journal of the Chinese Chemical Society*, **2015**, 62, 906-909 1.5
- 7 Computational study of the mechanisms of the photoisomerization reactions of bicycloalkene. *Journal of Physical Chemistry A*, **2010**, 114, 11656-62 2.8
- 6 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
- 5 Diboron-Carbene Complexes Derived from a Geminal Dianion. *Organometallics*, **2021**, 40, 1848-1853 3.8
- 4 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
- 3 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
- 2 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
- 1 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