Li-Li Zhao

List of Publications by Year
in descending order

108 papers	3,694 citations	126907 33 h-index	149698 56 g-index
117 all docs	117 docs citations	117 times ranked	2275 citing authors

#	Article	IF	Citations
1	Dinitrogen Functionalization Affording Structurally Well-Defined Cobalt Diazenido Complexes. CCS Chemistry, 2022, 4, 532-539.	7.8	12
2	The strength of a chemical bond. International Journal of Quantum Chemistry, 2022, 122, e26773.	2.0	29
3	Complex Featuring Two Double Dative Bonds Between Carbon(0) and Uranium. CCS Chemistry, 2022, 4, 1921-1929.	7.8	9
4	Application of sugar-containing biomass: one-step synthesis of 2-furylglyoxylic acid and its derivatives from a vitamin C precursor. Green Chemistry, 2022, 24, 2000-2009.	9.0	2
5	A Bisâ€(carbone) Pincer Ligand and Its Coordinative Behavior toward Multiâ€Metallic Configurations. Angewandte Chemie - International Edition, 2022, 61, .	13.8	9
6	Mechanistic study of cobalt(I)â€catalyzed asymmetric coupling of ethylene and enynes to functionalized cyclobutanes. Journal of Computational Chemistry, 2022, 43, 440-447.	3.3	0
7	A multi-input/multi-output molecular system based on lanthanide(<scp>iii</scp>) complexes. Inorganic Chemistry Frontiers, 2022, 9, 2668-2675.	6.0	1
8	Carbodiphosphorane-Stabilized Parent Dioxophosphorane: A Valuable Synthetic HO₂P Source. Journal of the American Chemical Society, 2022, 144, 7357-7365.	13.7	7
9	Frontispiz: A Bisâ€(carbone) Pincer Ligand and Its Coordinative Behavior toward Multiâ€Metallic Configurations. Angewandte Chemie, 2022, 134, .	2.0	0
10	Frontispiece: A Bisâ€(carbone) Pincer Ligand and Its Coordinative Behavior toward Multiâ€Metallic Configurations. Angewandte Chemie - International Edition, 2022, 61, .	13.8	0
11	The nature of the polar covalent bond. Journal of Chemical Physics, 2022, 157, .	3.0	15
12	COâ€Induced Dinitrogen Fixation and Cleavage Mediated by Boron. Chemistry - A European Journal, 2021, 27, 2131-2137.	3.3	20
13	Isolable dicarbon stabilized by a single phosphine ligand. Nature Chemistry, 2021, 13, 89-93.	13.6	15
14	Generation and Identification of the Linear OCBNO and OBNCO Molecules with 24 Valence Electrons. Chemistry - A European Journal, 2021, 27, 412-418.	3.3	8
15	Donor-Stabilized Antimony(I) and Bismuth(I) Ions: Heavier Valence Isoelectronic Analogues of Carbones. Journal of the American Chemical Society, 2021, 143, 1301-1306.	13.7	40
16	Linear group 13 Eî€,E triple bonds. Physical Chemistry Chemical Physics, 2021, 23, 11611-11615.	2.8	2
17	Mechanistic study of the cooperative palladium/Lewis acid-catalyzed transfer hydrocyanation reaction: the origin of the regioselectivity. Dalton Transactions, 2021, 50, 1233-1238.	3.3	0
18	Photomediated core modification of organic photoredox catalysts in radical addition: mechanism and applications. Chemical Science, 2021, 12, 9432-9441.	7.4	13

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19	Copper-catalyzed regioselective [3+2] annulation of malonate-tethered acyl oximes with isatins. Chemical Communications, 2021, 57, 3379-3382.	4.1	12
20	CaCl₂ molten salt hydrate-promoted conversion of carbohydrates to 5-hydroxymethylfurfural: an experimental and theoretical study. Green Chemistry, 2021, 23, 2058-2068.	9.0	19
21	Dinitrogen complexation and reduction at low-valent calcium. Science, 2021, 371, 1125-1128.	12.6	131
22	Mechanistic Study of the N-Quaternized Pyridoxal-Catalyzed Biomimetic Asymmetric Mannich Reaction: Insights into the Origins of Enantioselectivity and Diastereoselectivity. Journal of Organic Chemistry, 2021, 86, 6592-6599.	3.2	3
23	Highly Coordinated Heteronuclear Calciumâ€“Iron Carbonyl Cation Complexes [CaFe(CO) n] + (n =5â€“12) with dâ^'d Bonding. Angewandte Chemie, 2021, 133, 13984-13989.	2.0	0
24	Bonding in M(NHBMe)2 and M[Mn(CO)5]2 complexes (M=Zn, Cd, Hg; NHBMe=(HCNMe)2B): divalent group 12 metals with zero oxidation state. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	4
25	Computational Mechanistic Study of BrÃ¸nsted Acid-Catalyzed Unsymmetrical 1,2,4,5-Tetrazines Synthesis. Journal of Physical Chemistry A, 2021, 125, 4715-4726.	2.5	2
26	Highly Coordinated Heteronuclear Calciumâ€“Iron Carbonyl Cation Complexes [CaFe(CO)_n]⁺(n=5â€“12) with dâ^'d Bonding. Angewandte Chemie - International Edition, 2021, 60, 13865-13870.	13.8	18
27	Isolation of a Uranium(III)â€Carbon Multiple Bond Complex. Chemistry - A European Journal, 2021, 27, 10006-10011.	3.3	12
28	An Isolable Mononuclear Palladium(I) Amido Complex. Journal of the American Chemical Society, 2021, 143, 10751-10759.	13.7	11
29	Divergent Metal-Free [4 + 2] Cascade Reaction of 1-Indanylidenemalononitrile with 3-Benzylidenebenzofuran-2(3H)-one: Access to Spiro-dihydrofluorene-benzofuranone and Axially Chiral Fluorenylamine-phenol Derivatives. Organic Letters, 2021, 23, 5611-5615.	4.6	4
30	Synergistic Catalysis by BrÃ¸nsted Acid/Carbodicarbene Mimicking Frustrated Lewis Pairâ€Like Reactivity. Angewandte Chemie, 2021, 133, 20102-20109.	2.0	6
31	Synergistic Catalysis by BrÃ¸nsted Acid/Carbodicarbene Mimicking Frustrated Lewis Pairâ€Like Reactivity. Angewandte Chemie - International Edition, 2021, 60, 19949-19956.	13.8	18
32	Covalent Bonding Between Be⁺and CO₂in BeOCO⁺with a Surprisingly High Antisymmetric OCO Stretching Vibration. Journal of the American Chemical Society, 2021, 143, 14300-14305.	13.7	10
33	Coinage metal aluminyl complexes: probing regiochemistry and mechanism in the insertion and reduction of carbon dioxide. Chemical Science, 2021, 12, 13458-13468.	7.4	42
34	A Strained Ion Pair Permits Carbon Dioxide Fixation at Atmospheric Pressure by Câ€“H H-Bonding Organocatalysis. Journal of Organic Chemistry, 2021, 86, 3422-3432.	3.2	22
35	Mechanistic insight into the organocalcium-mediated nucleophilic alkylation of benzene and further rational design. Catalysis Science and Technology, 2020, 10, 950-958.	4.1	4
36	Mechanistic Study of Unprecedented Highly Regioselective Hydrocyanation of Terminal Alkynes: Insight into the Origins of the Regioselectivity and Ligand Effects. Journal of Computational Chemistry, 2020, 41, 279-289.	3.3	4

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37	A diradical based on odd-electron ïƒ-bonds. Nature Communications, 2020, 11, 3441.	12.8	22
38	Visible-Light-Induced Regio- and Stereoselective C(sp²)â€“H Trifluoroethylation of Enamides with 2,2,2-Trifluoroethyl Iodide. Organic Letters, 2020, 22, 9029-9035.	4.6	34
39	Carbones and Carbon Atom as Ligands in Transition Metal Complexes. Molecules, 2020, 25, 4943.	3.8	43
40	Intriguing structural, bonding and reactivity features in some beryllium containing complexes. Physical Chemistry Chemical Physics, 2020, 22, 27476-27495.	2.8	10
41	Directing Groupâ€Promoted Inert Câˆ’O Bond Activation Using Versatile Boronic Acid as a Coupling Agent. Chemistry - A European Journal, 2020, 26, 17021-17026.	3.3	10
42	Inverse sandwich complexes of B₇M₂^{âˆ’}, B₈M₂, and B₉M₂⁺ (M = Zr, Hf): the nonclassical Mâ€“M bonds embedded in monocyclic boron rings. New Journal of Chemistry, 2020, 44, 17705-17713.	2.8	6
43	Beryllium Atom Mediated Dinitrogen Activation via Coupling with Carbon Monoxide. Angewandte Chemie, 2020, 132, 18358-18364.	2.0	3
44	Synthesis and characterization of heterometallic complexes involving coinage metals and isoelectronic Fe(CO)₅, [Mn(CO)₅]^{âˆ’}and [Fe(CO)₄CN]^{âˆ’}ligands. Dalton Transactions, 2020, 49, 8566-8581.	3.3	13
45	Carbodicarbene: geminal â€Bimetallic Coordination in Selective Manner. Chemistry - A European Journal, 2020, 26, 17350-17355.	3.3	10
46	Filling a Gap: The Coordinatively Saturated Groupâ€...4 Carbonyl Complexes TM(CO)₈ (TM=Zr,) Tj ETQq0 0 0 rgBT /Overloc	3.3	21
47	Sideâ€On Bonded Beryllium Dinitrogen Complexes. Angewandte Chemie - International Edition, 2020, 59, 10603-10609.	13.8	51
48	Monitoring the Hierarchical Evolution from a Double-Stranded Helix to a Well-Defined Microscopic Morphology Based on a Turbine-like Aromatic Molecule. ACS Omega, 2020, 5, 16612-16618.	3.5	0
49	Beryllium Atom Mediated Dinitrogen Activation via Coupling with Carbon Monoxide. Angewandte Chemie - International Edition, 2020, 59, 18201-18207.	13.8	29
50	Sideâ€On Bonded Beryllium Dinitrogen Complexes. Angewandte Chemie, 2020, 132, 10690-10696.	2.0	13
51	Double donation in trigonal planar ironâ€“carbodiphosphorane complexes â€“ a concise study on their spectroscopic and electronic properties. Dalton Transactions, 2020, 49, 2537-2546.	3.3	20
52	Isolable cyclic radical cations of heavy main-group elements. Chemical Communications, 2020, 56, 2167-2170.	4.1	21
53	Metal-free [3+3] benzannulation of 1-indanylidene-malononitrile with Moritaâ€“Baylisâ€“Hillman carbonates: direct access to functionalized fluorene and fluorenone derivatives. Chemical Communications, 2020, 56, 1948-1951.	4.1	15
54	Bonding Analysis of the Shortest Bond between Two Atoms Heavier than Hydrogen and Helium: O22+. Journal of Physical Chemistry A, 2020, 124, 1087-1092.	2.5	12

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55	Response to Comment on â€œObservation of alkaline earth complexes M(CO) ₈ (M = Ca, Sr,) Tj ETQq1 1 0.784314 rgBT /O	12.6	54
56	Octa-coordinated alkaline earth metalâ€“dinitrogen complexes M(N2)8 (M=Ca, Sr, Ba). Nature Communications, 2019, 10, 3375.	12.8	79
57	Chemical Bonding and Bonding Models of Main-Group Compounds. Chemical Reviews, 2019, 119, 8781-8845.	47.7	232
58	Octacarbonyl Ion Complexes of Actinides [An(CO)₈]^{+/â^'} (An=Th, U) and the Role of f Orbitals in Metalâ€“Ligand Bonding. Chemistry - A European Journal, 2019, 25, 11772-11784.	3.3	38
59	Transitionâ€Metal Chemistry of Alkalineâ€Earth Elements: The Trisbenzene Complexes M(Bz)₃(M=Sr, Ba). Angewandte Chemie - International Edition, 2019, 58, 17365-17374.	13.8	82
60	Transitionâ€Metal Chemistry of Alkalineâ€Earth Elements: The Trisbenzene Complexes M(Bz)₃(M=Sr, Ba). Angewandte Chemie, 2019, 131, 17526-17535.	2.0	28
61	Computational Insights into the Catalytic Mechanism of Bacterial Carboxylic Acid Reductase. Journal of Chemical Information and Modeling, 2019, 59, 832-841.	5.4	26
62	Alkali Metal Covalent Bonding in Nickel Carbonyl Complexes ENi(CO)₃^{â^'}. Angewandte Chemie, 2019, 131, 1746-1752.	2.0	53
63	Direct C(sp²)â€“H Arylsulfonylation of Enamides via Iridium(III)â€Catalyzed Insertion of Sulfur Dioxide with Aryldiazonium Tetrafluoroborates. Advanced Synthesis and Catalysis, 2019, 361, 3593-3598.	4.3	64
64	Synthesis of cAAC stabilized biradical of â€œMe₂Siâ€•and â€œMe₂SiClâ€•monoradical from Me₂SiCl₂ â€“ an important feedstock material. Chemical Communications, 2019, 55, 4534-4537.	4.1	9
65	Aluminum alkoxyâ€catalyzed biomass conversion of glucose to 5â€hydroxymethylfurfural: Mechanistic study of the cooperative bifunctional catalysis. Journal of Computational Chemistry, 2019, 40, 1599-1608.	3.3	12
66	Bent Phosphaallenes With â€œHiddenâ€•Lone Pairs as Ligands. Chemistry - A European Journal, 2019, 25, 7912-7920.	3.3	2
67	Mechanistic insight into the highly regioselective Ni(0)-catalyzed [2 + 2] self-cycloaddition of electron-deficient allenoates. Catalysis Science and Technology, 2019, 9, 1273-1278.	4.1	5
68	An Experimental and Theoretical Study of the Structures and Properties of [CDP^{Me}â€Ni(CO)₃] and [Ni₂(CO)₄(Âµ²â€CO)(Âµ²â€CDP^{Me})]. European Journal of Inorganic Chemistry, 2019, 2019, 4546-4554.	2.0	13
69	Ceriumâ€“carbon dative interactions supported by carbodiphosphorane. Dalton Transactions, 2019, 48, 16108-16114.	3.3	20
70	Octacarbonyl Anion Complexes of the Late Lanthanides Ln(CO)₈^{â^'} (Ln=Tm, Yb,) Tj ETQq0 0 0 rgBT /Overlock	3.3	38
71	The Lewis electron-pair bonding model: the physical background, one century later. Nature Reviews Chemistry, 2019, 3, 35-47.	30.2	52
72	The Lewis electron-pair bonding model: modern energy decomposition analysis. Nature Reviews Chemistry, 2019, 3, 48-63.	30.2	197

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73	Isolation of Transient Acyclic Germanium(I) Radicals Stabilized by Cyclic Alkyl(amino) Carbenes. Journal of the American Chemical Society, 2019, 141, 1908-1912.	13.7	27
74	Alkali Metal Covalent Bonding in Nickel Carbonyl Complexes ENi(CO)₃^{â^'}. Angewandte Chemie - International Edition, 2019, 58, 1732-1738.	13.8	62
75	Barium as Honorary Transition Metal in Action: Experimental and Theoretical Study of Ba(CO)⁺ and Ba(CO)^{â^'}. Angewandte Chemie, 2018, 130, 4038-4044.	2.0	16
76	Electronic Structure and Bonding Situation in M₂O₂ (M = Be, Mg, Ca) Rhombic Clusters. Journal of Physical Chemistry A, 2018, 122, 2816-2822.	2.5	34
77	Barium as Honorary Transition Metal in Action: Experimental and Theoretical Study of Ba(CO)⁺ and Ba(CO)^{â^'}. Angewandte Chemie - International Edition, 2018, 57, 3974-3980.	13.8	60
78	Boron Nanowheels with Axles Containing Noble Gas Atoms: Viable Noble Gas Bound MÂ©B₁₀^{â^'} Clusters (M=Nb, Ta). Chemistry - A European Journal, 2018, 24, 3590-3598.	3.3	19
79	Energy decomposition analysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1345.	14.6	369
80	Berichtigung: Barium as Honorary Transition Metal in Action: Experimental and Theoretical Study of Ba(CO)⁺ and Ba(CO)^{â^'}. Angewandte Chemie, 2018, 130, 15856-15857.	2.0	0
81	Double dative bond between divalent carbon(0) and uranium. Nature Communications, 2018, 9, 4997.	12.8	63
82	Improvement in hydrogen binding ability of closo-dicarboranes via functionalization and designing of extended frameworks. Journal of Molecular Modeling, 2018, 24, 307.	1.8	2
83	Nickel-Catalyzed Heteroarenes Cross Coupling via Tandem Câ€“H/Câ€“O Activation. ACS Catalysis, 2018, 8, 11368-11376.	11.2	37
84	Observation of alkaline earth complexes M(CO) ₈ (M = Ca, Sr, or Ba) that mimic transition metals. Science, 2018, 361, 912-916.	12.6	207
85	Cyanideâ€“isocyanide isomerization: stability and bonding in noble gas inserted metal cyanides (metal =) Tj ETQq1 1 0.784314 rgBT /	2.8	32
86	Bonding in Binuclear Carbonyl Complexes M₂(CO)₉ (M = Fe, Ru, Os). Inorganic Chemistry, 2018, 57, 7780-7791.	4.0	50
87	Aromaticity, the HÃ¼ckel 4â€‰n+2 Rule and Magnetic Current. ChemistrySelect, 2017, 2, 863-870.	1.5	66
88	Dative bonding in main group compounds. Coordination Chemistry Reviews, 2017, 344, 163-204.	18.8	174
89	A Very Short Beâ€“Be Distance but No Bond: Synthesis and Bonding Analysis of Ngâ€“Be₂O₂â€“Ngâ€² (Ng, Ngâ€²=Ne, Ar, Kr, Xe). Chemistry - A European Journal, 2017, 23, 2035-2039.	3.3	46
90	NHCâ€Stabilised Acetyleneâ€”How Far Can the Analogy Be Pushed?. Chemistry - A European Journal, 2017, 23, 2926-2934.	3.3	65

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91	Heterobimetallic Complexes Featuring Fe(CO)₅ as a Ligand on Gold. Chemistry - A European Journal, 2017, 23, 17222-17226.	3.3	18
92	Invisible Chelating Effect Exhibited between Carbodicarbene and Phosphine through Ï€â€“Ï€ Interaction and Implication in the Cross-Coupling Reaction. Organometallics, 2017, 36, 4287-4297.	2.3	21
93	Palladium-Catalyzed Hydroxycarbonylation of Pentenoic Acids. Computational and Experimental Studies on the Catalytic Selectivity. ACS Catalysis, 2017, 7, 7070-7080.	11.2	27
94	Parent Thioketene Sâ€Oxide H₂CCSO: Gasâ€Phase Generation, Structure, and Bonding Analysis. Chemistry - A European Journal, 2017, 23, 16566-16573.	3.3	39
95	Carbodicarbenes: Unexpected Ï€-Accepting Ability during Reactivity with Small Molecules. Journal of the American Chemical Society, 2017, 139, 12830-12836.	13.7	57
96	A C(sp²)â^'H Dehydrogenation of Heteroarenes and Arenes by a Functionalized Aluminum Hydride. Chemistry - A European Journal, 2017, 23, 13633-13637.	3.3	28
97	Highly responsive ethylenediamine vapor sensor based on a perylenediimideâ€“camphorsulfonic acid complex via ionic self-assembly. Journal of Materials Chemistry C, 2017, 5, 7644-7651.	5.5	26
98	Unusually Short Beâ^'Be Distances with and without a Bond in Be₂F₂ and in the Molecular Discuses Be₂B₈ and Be₂B₇^{â^'}. Angewandte Chemie - International Edition, 2016, 55, 7841-7846.	13.8	60
99	A computational experiment to study hydrogenations of various unsaturated compounds catalyzed by a rationally designed metal-free catalyst. Dalton Transactions, 2012, 41, 4674.	3.3	19
100	Reaction Mechanism of Phosphaneâ€Catalyzed [4+2] Annulations between Î±â€Alkylallenoates and Activated Alkenes: A Computational Study. European Journal of Organic Chemistry, 2012, 2012, 3587-3597.	2.4	45
101	Computational Mechanistic Study of PMe₃ and N-Heterocyclic Carbene Catalyzed Intramolecular Moritaâ^'Baylisâ^'Hillman-Like Cycloalkylations: The Origins of the Different Reactivity. Journal of Organic Chemistry, 2011, 76, 2733-2743.	3.2	34
102	Metal-free catalysts for hydrogenation of both small and large imines: a computational experiment. Dalton Transactions, 2011, 40, 1929.	3.3	25
103	Encumbering the intramolecular Ï€ donation by using a bridge: A strategy for designing metal-free compounds to hydrogen activation. Science Bulletin, 2010, 55, 239-245.	1.7	38
104	Reversible Heterolytic Methane Activation of Metalâ€Free Closedâ€Shell Molecules: A Computational Proofâ€ofâ€Principle Study. European Journal of Inorganic Chemistry, 2010, 2010, 2254-2260.	2.0	35
105	Computational design of metal-free catalysts for catalytic hydrogenation of imines. Dalton Transactions, 2010, 39, 4038.	3.3	45
106	Eî€,E triple bonds (E = Group 13) promoted by charge transfer from alkali metals. New Journal of Chemistry, 0, , .	2.8	0
107	A Bis â€(carbone) Pincer Ligand and Its Coordinative Behavior toward Multiâ€Metallic Configurations. Angewandte Chemie, 0, , .	2.0	1
108	How to capture C2O2: Structures and bonding of neutral and charged complexes [(NHC)-C2O2-(NHC)]q (NHC = N-heterocyclic carbene; q = 0, 1+, 2+). Physical Chemistry Chemical Physics, 0, , .	2.8	0