Ming Lei

List of Publications by Year
in descending order

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120	2,258	201674	289244
papers	citations	27 h-index	40 g-index

123	123	123	2467
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Targeting MLL1 H3K4 Methyltransferase Activity in Mixed-Lineage Leukemia. Molecular Cell, 2014, 53, 247-261.	9.7	252
2	Structural basis for protein-RNA recognition in telomerase. Nature Structural and Molecular Biology, 2014, 21, 507-512.	8.2	71
3	Transitionâ€Metalâ€Free Hydrogen Autotransfer: Diastereoselective Nâ€Alkylation of Amines with Racemic Alcohols. Angewandte Chemie - International Edition, 2019, 58, 10528-10536.	13.8	65
4	Study of the properties of molecularly imprinted polymers by computational and conformational analysis. Analytica Chimica Acta, 2007, 581, 137-146.	5.4	64
5	Asymmetric Guerbet Reaction to Access Chiral Alcohols. Angewandte Chemie - International Edition, 2020, 59, 11408-11415.	13.8	60
6	The Nature of Hydrogen Production from Aqueousâ€Phase Methanol Dehydrogenation with Ruthenium Pincer Complexes Under Mild Conditions. European Journal of Inorganic Chemistry, 2015, 2015, 794-803.	2.0	56
7	Transition-metal-free synthesis of pyrimidines from lignin Î²-O-4 segments via a one-pot multi-component reaction. Nature Communications, 2022, 13, .	12.8	52
8	Why is Leu55â†'Pro55 transthyretin variant the most amyloidogenic: Insights from molecular dynamics simulations of transthyretin monomers. Protein Science, 2003, 12, 1222-1231.	7.6	43
9	Toward Understanding Metal-Binding Specificity of Porphyrin: A Conceptual Density Functional Theory Study. Journal of Physical Chemistry B, 2009, 113, 13381-13389.	2.6	42
10	Theoretical Studies on the Stability and Reactivity of the Metal-Doped CeO₂(100) Surface: Toward H₂ Dissociation and Oxygen Vacancy Formation. Langmuir, 2020, 36, 5891-5901.	3.5	42
11	Low-cost synthesis of small molecule acceptors makes polymer solar cells commercially viable. Nature Communications, 2022, 13, .	12.8	38
12	A comparative study on the hydrogenation of ketones catalyzed by diphosphineâ€“diamine transition metal complexes using DFT method. Dalton Transactions, 2009, , 2359.	3.3	36
13	Palladium-Catalyzed Highly Regioselective Hydrocarboxylation of Alkynes with Carbon Dioxide. ACS Catalysis, 2020, 10, 7968-7978.	11.2	36
14	Mechanistic Insights into the Directed Hydrogenation of Hydroxylated Alkene Catalyzed by Bis(phosphine)cobalt Dialkyl Complexes. Journal of Organic Chemistry, 2017, 82, 2703-2712.	3.2	35
15	Mechanistic Investigations on Thermal Hydrogenation of CO₂ to Methanol by Nanostructured CeO₂(100): The Crystal-Plane Effect on Catalytic Reactivity. Journal of Physical Chemistry C, 2019, 123, 11763-11771.	3.1	35
16	Preference of H₂ as Hydrogen Source in Hydrogenation of Ketones Catalyzed by Late Transition Metal Complexes. A DFT Study. Organometallics, 2010, 29, 543-548.	2.3	34
17	Mechanisms of Ketone/Imine Hydrogenation Catalyzed by Transitionâ€Metal Complexes. Energy and Environmental Materials, 2019, 2, 292-312.	12.8	34
18	Synthesis of Alkenylboronates from N-Tosylhydrazones through Palladium-Catalyzed Carbene Migratory Insertion. Journal of the American Chemical Society, 2021, 143, 9769-9780.	13.7	34

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19	The role of interfacial modifier in toughening of nylon 6 with a core-shell toughener. Journal of Polymer Science, Part B: Polymer Physics, 1999, 37, 2664-2672.	2.1	33
20	Origins of enantioselectivity in asymmetric ketone hydrogenation catalyzed by a RuH₂(binap)(cydn) complex: insights from a computational study. Dalton Transactions, 2013, 42, 2130-2145.	3.3	32
21	Cobalt(III)-Catalyzed Regioselective C6 Olefination of 2-Pyridones Using Alkynes: Olefination/Directing Group Migration and Olefination. Organic Letters, 2021, 23, 4624-4629.	4.6	31
22	Mechanism investigation of ketone hydrogenation catalyzed by ruthenium bifunctional catalysts: insights from a DFT study. Physical Chemistry Chemical Physics, 2012, 14, 6003.	2.8	30
23	A Hydride-Shuttle Mechanism for the Catalytic Hydroboration of CO₂. Inorganic Chemistry, 2018, 57, 3054-3060.	4.0	30
24	Dynamics and cooperativity of Trp-cage folding. Archives of Biochemistry and Biophysics, 2008, 475, 140-147.	3.0	29
25	Nature of Asynchronous Hydrogen Transfer in Ketone Hydrogenation Catalyzed by Ru Complex. Journal of Physical Chemistry C, 2008, 112, 13524-13527.	3.1	28
26	A theoretical study of X ligand effect on catalytic activity of complexes RuHX(diamine)(PPh3)2 (X =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 2036.	3.3	28
27	DFT Study on the Mechanism of Tandem Oxidative Acetoxylation/Ortho Câ€“H Activation/Carbocyclization Catalyzed by Pd(OAc)₂. Organometallics, 2016, 35, 3301-3310.	2.3	27
28	The enantioselectivity in asymmetric ketone hydrogenation catalyzed by RuH₂(diphosphine)(diamine) complexes: insights from a 3D-QSSR and DFT study. Catalysis Science and Technology, 2016, 6, 4450-4457.	4.1	27
29	Access to Polycyclic Sulfonyl Indolines via Fe(II)-Catalyzed or UV-Driven Formal [2 + 2 + 1] Cyclization Reactions of N-((1H-indol-3-yl)methyl)propiolamides with NaHSO₃. Organic Letters, 2019, 21, 2602-2605.	4.6	27
30	Initial Conformational Changes of Human Transthyretin under Partially Denaturing Conditions. Biophysical Journal, 2005, 89, 433-443.	0.5	26
31	Mechanism and Influence of Acid in Hydrogenation of Ketones by Î·⁶-Arene/N-Tosylethylenediamine Ruthenium(II). Organometallics, 2009, 28, 2078-2084.	2.3	26
32	Stabilizing a different cyclooctatetraene stereoisomer. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9803-9808.	7.1	26
33	Substituent effects and chemoselectivity of the intramolecular Buchner reaction of diazoacetamide derivatives catalyzed by the di-Rh(<scp>II</scp>)-complex. Dalton Transactions, 2016, 45, 8506-8512.	3.3	25
34	Metalâ€“Substrate Cooperation Mechanism for Dehydrogenative Amidation Catalyzed by a PNN-Ru Catalyst. Inorganic Chemistry, 2018, 57, 8778-8787.	4.0	24
35	Ditantalum Dinitrogen Complex: Reaction of H₂ Molecule with â€œEnd-on-Bridgedâ€• [Ta^{IV}]₂(Î¼-Î·¹:Î·¹-N₂) and Bis(Î¼-nitrido) [Ta^V]₂(Î¼-N)₂ Complexes. Inorganic Chemistry, 2011, 50, 9481-9490.	4.0	23
36	Intrinsic versus mutation dependent instability/flexibility: a comparative analysis of the structure and dynamics of wild-type transthyretin and its pathogenic variants. Journal of Structural Biology, 2004, 148, 153-168.	2.8	20

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37	Molecular modeling and docking study on dopamine D2-like and serotonin 5-HT2A receptors. Journal of Molecular Graphics and Modelling, 2015, 57, 143-155.	2.4	20
38	Asymmetric Guerbet Reaction to Access Chiral Alcohols. Angewandte Chemie, 2020, 132, 11505-11512.	2.0	20
39	Toughening of a copolyester with a maleated core-shell toughener. Journal of Polymer Science, Part B: Polymer Physics, 2000, 38, 2801-2809.	2.1	19
40	Borneol Is a TRPM8 Agonist that Increases Ocular Surface Wetness. PLoS ONE, 2016, 11, e0158868.	2.5	19
41	Hydrogenation of CO₂to methanol catalyzed by a manganese pincer complex: insights into the mechanism and solvent effect. Dalton Transactions, 2021, 50, 7348-7355.	3.3	19
42	Peptide Plane Can Flip in Two Opposite Directions:Â Implication in Amyloid Formation of Transthyretin. Journal of Physical Chemistry B, 2006, 110, 5829-5833.	2.6	18
43	Why Iron? A Spin-Polarized Conceptual Density Functional Theory Study on Metal-Binding Specificity of Porphyrin. Journal of Physical Chemistry A, 2010, 114, 6342-6349.	2.5	18
44	Concerted or Stepwise Hydrogen Transfer in the Transfer Hydrogenation of Acetophenone Catalyzed by Rutheniumâ€“Acetamido Complex: A Theoretical Mechanistic Investigation. Journal of Physical Chemistry A, 2011, 115, 12321-12330.	2.5	18
45	Guest-modulation of the mechanical properties of flexible porous metalâ€“organic frameworks. Journal of Materials Chemistry A, 2014, 2, 9691-9698.	10.3	18
46	DFT Mechanistic Study on Alkene Hydrogenation Catalysis of Iron Metallaboratrane: Characteristic Features of Iron Species. Organometallics, 2017, 36, 3530-3538.	2.3	18
47	Rhodium(III)â€Catalyzed Câ^'H Bond Functionalization of 2â€Pyridones with Alkynes: Switchable Alkenylation, Alkenylation/Directing Group Migration and Rollover Annulation. Chemistry - A European Journal, 2021, 27, 8811-8821.	3.3	17
48	Toughening of polyethylene terephthalate/amorphous copolyester blends with a maleated thermoplastic elastomer. Journal of Applied Polymer Science, 2003, 89, 797-805.	2.6	16
49	Rational Design and Study on Recognition Property of Paracetamol-Imprinted Polymer. Applied Biochemistry and Biotechnology, 2010, 160, 328-342.	2.9	16
50	Fission yeast telomere-binding protein Taz1 is a functional but not a structural counterpart of human TRF1 and TRF2. Cell Research, 2015, 25, 881-884.	12.0	16
51	Experimental and Theoretical Study on the Stability of CL-20-Based Hostâ€“Guest Energetic Materials. Journal of Physical Chemistry A, 2020, 124, 6389-6398.	2.5	16
52	Mechanism of the Zinc Dithiocarbamate-Activated Rubber Vulcanization Process: A Density Functional Theory Study. ACS Applied Polymer Materials, 2021, 3, 5188-5196.	4.4	16
53	Hydroboration of CO₂ to Methyl Boronate Catalyzed by a Manganese Pincer Complex: Insights into the Reaction Mechanism and Ligand Effect. Inorganic Chemistry, 2022, 61, 5616-5625.	4.0	16
54	First-Principles Study on the Mechanism of Nitrobenzene Reduction to Aniline Catalyzed by a N-Doped Carbon-Supported Cobalt Single-Atom Catalyst. Journal of Physical Chemistry C, 2021, 125, 19171-19182.	3.1	15

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55	Models for binding cooperativities of inhibitors with transthyretin. Archives of Biochemistry and Biophysics, 2007, 466, 85-97.	3.0	14
56	Dimerization of SLX4 contributes to functioning of the SLX4-nuclease complex. Nucleic Acids Research, 2016, 44, 4871-4880.	14.5	14
57	Methanol oxidation over rutile Au1@TiO2 catalyst: Importance of facets and oxygen vacancy. Applied Surface Science, 2021, 542, 148541.	6.1	14
58	Molecular dynamics studies of the antimicrobial peptides piscidin 1 and its mutants with a DOPC lipid bilayer. Biopolymers, 2012, 97, 998-1009.	2.4	13
59	CO assisted N₂functionalization activated by a dinuclear hafnium complex: a DFT mechanistic exploration. Physical Chemistry Chemical Physics, 2013, 15, 901-910.	2.8	13
60	Mechanistic Studies on the Carboxylation of Hafnocene and ansa-Zirconocene Dinitrogen Complexes with CO2. Organometallics, 2013, 32, 7077-7082.	2.3	13
61	Enhancement of methanol resistance of Yarrowia lipolytica lipase 2 using Î²-cyclodextrin as an additive: Insights from experiments and molecular dynamics simulation. Enzyme and Microbial Technology, 2017, 96, 157-162.	3.2	13
62	Asymmetric Induction with a Chiral Amine Catalyzed by a Ru-PNP Pincer Complex: Insight from Theoretical Investigation. Inorganic Chemistry, 2020, 59, 8404-8411.	4.0	13
63	Asymmetric Hydroformylation Catalyzed by RhH(CO)2[(R,S)-Yanphos]: Mechanism and Origin of Enantioselectivity. Journal of Physical Chemistry A, 2014, 118, 8960-8970.	2.5	12
64	A DFT study on ring-opening polymerization of Îµ-caprolactone initiated by Mg and Al complexes. Inorganica Chimica Acta, 2018, 477, 34-39.	2.4	12
65	Transitionâ€Metalâ€Free Hydrogen Autotransfer: Diastereoselective Nâ€Alkylation of Amines with Racemic Alcohols. Angewandte Chemie, 2019, 131, 10638-10646.	2.0	12
66	A theoretical study on the mechanisms of intermolecular hydroacylation of aldehyde catalyzed by neutral and cationic rhodium complexes. Science China Chemistry, 2014, 57, 1264-1275.	8.2	11
67	An experimental and theoretical study on the growth of plate-like Î²-HMX crystals in the hydroxylated interlayer space. Physical Chemistry Chemical Physics, 2021, 23, 12340-12349.	2.8	11
68	Homogeneous and Heterogeneous Pd-Catalyzed Selective Câ€“P Activation and Transfer Hydrogenation for â€œGroup-Substitutionâ€•Synthesis of Trivalent Phosphines. Organic Letters, 2022, 24, 2868-2872.	4.6	11
69	A theoretical study on the hydrogenation of CO₂to methanol catalyzed by ruthenium pincer complexes. Dalton Transactions, 2022, 51, 10020-10028.	3.3	10
70	Theoretical calculation of rate constants for the thermal isomerization from 1, 2-butadiene to 1, 3-butadiene. Science in China Series B: Chemistry, 1998, 41, 60-64.	0.8	9
71	The role of temperature and solvent microenvironment on the activity of Yarrowia lipolytica Lipase 2: Insights from molecular dynamics simulation. Journal of Molecular Catalysis B: Enzymatic, 2014, 109, 101-108.	1.8	9
72	Quinolylâ€Amidinates Chelating Bimetallic Magnesium and Mononuclear Aluminum Complexes for Îµâ€Caprolactone Polymerization. ChemistrySelect, 2016, 1, 5660-5665.	1.5	9

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73	Homolytic or Heterolytic Dihydrogen Splitting with Ditantalum/Dizirconium Dinitrogen Complexes? A Computational Study. Organometallics, 2015, 34, 1255-1263.	2.3	8
74	Rutile TiO2 supported single atom Au catalyst: A facile approach to enhance methanol dehydrogenation. Molecular Catalysis, 2020, 482, 110670.	2.0	8
75	Theoretical Design of a Catalyst with Both High Activity and Selectivity in Câ€“H Borylation. Journal of Organic Chemistry, 2021, 86, 16858-16866.	3.2	8
76	A theoretical study of asymmetric ketone hydrogenation catalyzed by Mn complexes: from the catalytic mechanism to the catalyst design. Physical Chemistry Chemical Physics, 2022, 24, 13365-13375.	2.8	8
77	A theoretical study on the alkene insertion step in Rh-Yanphos catalyzed hydroformylation. Chinese Chemical Letters, 2013, 24, 1083-1086.	9.0	7
78	3D-QSAR and docking studies on 2-arylbenzoxazole and linker-Y transthyretin amyloidogenesis inhibitors. Science China Chemistry, 2013, 56, 1550-1563.	8.2	7
79	Î²-cyclodextrin as an additive to improve the thermostability of Yarrowia lipolytica Lipase 2: Experimental and simulation insights. Journal of the Taiwan Institute of Chemical Engineers, 2017, 70, 49-55.	5.3	7
80	HCl and O₂ co-activated bis(8-quinolinolato) oxovanadium(<scp>iv</scp>) complexes as efficient photoactive species for visible light-driven oxidation of cyclohexane to KA oil. Catalysis Science and Technology, 2019, 9, 275-285.	4.1	7
81	A Computational Study on Iridiumâ€Catalyzed Production of Acetic Acid from Ethanol and Water Solution. Chinese Journal of Chemistry, 2019, 37, 883-886.	4.9	7
82	pH-Dependent transfer hydrogenation or dihydrogen release catalyzed by a [(Î·6-arene)RuCl(Î²2-N,N-dmobpy)]+ complex: a DFT mechanistic understanding. RSC Advances, 2020, 10, 10411-10419.	3.6	7
83	Mechanistic Understanding of Baseâ€Catalyzed Aldimine/Ketoamine Condensations: An Old Story and A New Model. Asian Journal of Organic Chemistry, 2021, 10, 634-641.	2.7	7
84	A phosphine-free Mn(<scp>i</scp>)-NNS catalyst for asymmetric transfer hydrogenation of acetophenone: a theoretical prediction. Dalton Transactions, 2021, 50, 14738-14744.	3.3	7
85	Theoretical Study on Nitrogenous Heterocyclic Assisted Aldimine Condensation. Acta Chimica Sinica, 2020, 78, 437.	1.4	7
86	The Role of AQ in the Regioselectivity of Strong Alkyl Câ€“O Bond Activation Catalyzed by Pd(OAc)₂: A Density Functional Theory Mechanistic Study. Inorganic Chemistry, 2021, 60, 17555-17564.	4.0	7
87	Elastic Image Pair Method for Finding Transition States on Potential Energy Surfaces Using Only First Derivatives. Journal of Chemical Theory and Computation, 2022, 18, 5108-5115.	5.3	7
88	Bent and planar structures of Î¼â€Î·2:Î·2-N2dinuclear early transition metal complexes. Dalton Transactions, 2014, 43, 11658.	3.3	6
89	Computational Study and Modified Design of Selective Dopamine <scp>D</scp>₃ Receptor Agonists. Chemical Biology and Drug Design, 2016, 88, 142-154.	3.2	6
90	Investigation on terpolymer of ethylene/propylene/Î‰-bromo-Î±-olefins catalyzed by titanium complexes. Journal of Materials Science, 2017, 52, 5981-5991.	3.7	6

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91	3D-QSAR studies of D3R antagonists and 5-HT1AR agonists. Journal of Molecular Graphics and Modelling, 2019, 86, 132-141.	2.4	6
92	Ab initio MO study of reaction mechanism for carbonyl migration of Co complex. Science Bulletin, 2000, 45, 1176-1178.	1.7	5
93	Molecular Dynamics Simulations on the Stability and Assembly Mechanisms of Quadruple and Double Helical Aromatic Amide Foldamers. Journal of Physical Chemistry B, 2009, 113, 10934-10941.	2.6	5
94	Ruthenium-catalyzed deoxygenative hydroboration of carboxylic acids: a DFT mechanistic study. New Journal of Chemistry, 2019, 43, 11493-11496.	2.8	5
95	Rapid screening of the hydrogen bonding strength of radicals by electrochemiluminescent probes. Chemical Communications, 2019, 55, 5563-5566.	4.1	5
96	Theoretical investigation on regioselectivity of aromatic ketones in the addition with olefin catalyzed by RuH2(CO)(PPh3)3. Science in China Series B: Chemistry, 2000, 43, 412-420.	0.8	4
97	Theoretical Study of the Histidine-catalyzed Asymmetric Aldol Reaction of Acetone and Benzaldehyde. Journal of Physical Chemistry A, 2018, 122, 7842-7851.	2.5	4
98	Structure Simulation and Hostâ€“Guest Interaction of Histidine-Intercalated Hydrotalciteâ€“Montmorillonite Complex. Minerals (Basel, Switzerland), 2018, 8, 198.	2.0	4
99	The reaction paths of CH₂O decomposition on CuO(111) surface: A DFT study. Journal of Physical Organic Chemistry, 2020, 33, e4017.	1.9	4
100	Theoretical study on the mechanism of C N and C C coupling to form indole catalyzed by Pd(OAc)2. Molecular Catalysis, 2021, 515, 111895.	2.0	4
101	Theoretical Study on N-N Activation by Thiolate-bridged Dinuclear Dinitrogen Transition-metal Complexes. Acta Chimica Sinica, 2016, 74, 340.	1.4	4
102	Ab initio study on the mechanism of reaction HNCO+NH2. Science in China Series B: Chemistry, 2002, 45, 365-372.	0.8	3
103	A novel algorithm for a rotation invariant template matching. Optoelectronics Letters, 2008, 4, 379-383.	0.8	3
104	A DFT Study on Formation of Bisaryl Oxime Ether from Benzaldehyde and Phenoxyamine. Chemistry Letters, 2008, 37, 656-657.	1.3	3
105	Quantitative Theoretical Predictions and Qualitative Bonding Analysis of the Divinylborinium System and Its Al, Ga, In, and Tl Congeners. Inorganic Chemistry, 2018, 57, 7851-7859.	4.0	3
106	Transition-metal-free polycyclic indoline formation via a free radical pathway: a computational mechanistic study. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	3
107	A theoretical study of the hydroboration of Î±,Î²-unsaturated carbonyl compounds catalyzed by a metal-free complex and subsequent Câ€“C coupling with acetonitrile. New Journal of Chemistry, 2021, 45, 14134-14140.	2.8	3
108	Mechanistic Investigation of H₂O₂â€dependent Chemiluminescence from Tetrabromoâ€1,4â€Benzoquinone. ChemPhysChem, 2022, 23, e202100885.	2.1	3

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109	Poly(Amino Acid) Coordination Nanoparticle as a Potent Sonosensitizer for Cancer Therapy. ACS Applied Bio Materials, 2021, 4, 881-889.	4.6	2
110	Ab initio study on the mechanism of rhodium-complexcatalyzed carbonylation of methanol to acetic acid. Science in China Series B: Chemistry, 2001, 44, 465-472.	0.8	1
111	UNDERSTANDING THE ROLE OF WATER IN PROMOTING E-ISOMER PRODUCTION AND PHOTOCHROMISM OF SOLID SCHIFF BASE: A DFT AND TD-DFT STUDY. Journal of Theoretical and Computational Chemistry, 2008, 07, 1071-1084.	1.8	1
112	How Does Methanol Assist the Hydrogen Transfer in Pd-catalyzed Cyclocarbonylation of Allylic Alcohols? Insights from a DFT Study. Chemistry Letters, 2012, 41, 693-695.	1.3	1
113	WHICH IS THE PROTON-SHUTTLE IN ISOXANTHOPTERIN DEAMINASE? QM/MM MD UNDERSTANDING. Journal of Theoretical and Computational Chemistry, 2013, 12, 1341002.	1.8	1
114	1,2 addition or cycloaddition of allenes by a dihafnium Î¼â^'Nitrido complex? A DFT study. Journal of Organometallic Chemistry, 2018, 874, 101-105.	1.8	1
115	Using Bases as Initiators to Isomerize Allylic Alcohols: Insights from Density Functional Theory Studies. Journal of Physical Chemistry A, 2021, 125, 2316-2323.	2.5	1
116	Theoretical Study on the Mechanism of the Benzaldehydes Deoxyfluorination by Sulfuryl Fluoride and Tetramethylammonium Fluoride. Journal of Physical Organic Chemistry, 0, , .	1.9	1
117	RÃ¼cktitelbild: Transitionâ€Metalâ€Free Hydrogen Autotransfer: Diastereoselective Nâ€Alkylation of Amines with Racemic Alcohols (Angew. Chem. 31/2019). Angewandte Chemie, 2019, 131, 10876-10876.	2.0	0
118	Inside Cover: A Computational Study on Iridiumâ€Catalyzed Production of Acetic Acid from Ethanol and Water Solution (Chin. J. Chem. 9/2019). Chinese Journal of Chemistry, 2019, 37, 862-862.	4.9	0
119	RÃ¼cktitelbild: Asymmetric Guerbet Reaction to Access Chiral Alcohols (Angew. Chem. 28/2020). Angewandte Chemie, 2020, 132, 11768-11768.	2.0	0
120	Theoretical investigation of Prolylâ€Histidineâ€catalyzed intermolecular aldol reaction. Journal of Physical Organic Chemistry, 2021, 34, e4203.	1.9	0