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	Mechanistic Investigation of H₂O₂â€dependent Chemiluminescence from Tetrabromoâ€1,4â€Benzoquinone. ChemPhysChem, 2022, 23, e202100885.	2.1	3
2	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
3	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
4	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
5	A theoretical study on the hydrogenation of CO₂to methanol catalyzed by ruthenium pincer complexes. Dalton Transactions, 2022, 51, 10020-10028.	3.3	10
6	Low-cost synthesis of small molecule acceptors makes polymer solar cells commercially viable. Nature Communications, 2022, 13, .	12.8	38
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	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
9	Methanol oxidation over rutile Au1@TiO2 catalyst: Importance of facets and oxygen vacancy. Applied Surface Science, 2021, 542, 148541.	6.1	14
10	Poly(Amino Acid) Coordination Nanoparticle as a Potent Sonosensitizer for Cancer Therapy. ACS Applied Bio Materials, 2021, 4, 881-889.	4.6	2
11	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
12	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
13	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
14	Theoretical investigation of Prolylâ€Histidineâ€catalyzed intermolecular aldol reaction. Journal of Physical Organic Chemistry, 2021, 34, e4203.	1.9	0
15	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
16	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
17	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
18	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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19	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
20	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
21	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
22	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
23	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
24	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
25	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
26	The reaction paths of CH₂O decomposition on CuO(111) surface: A DFT study. Journal of Physical Organic Chemistry, 2020, 33, e4017.	1.9	4
27	Rutile TiO2 supported single atom Au catalyst: A facile approach to enhance methanol dehydrogenation. Molecular Catalysis, 2020, 482, 110670.	2.0	8
28	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
29	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
30	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
31	RÃ¼cktitelbild: Asymmetric Guerbet Reaction to Access Chiral Alcohols (Angew. Chem. 28/2020). Angewandte Chemie, 2020, 132, 11768-11768.	2.0	0
32	Palladium-Catalyzed Highly Regioselective Hydrocarboxylation of Alkynes with Carbon Dioxide. ACS Catalysis, 2020, 10, 7968-7978.	11.2	36
33	Transition-metal-free polycyclic indoline formation via a free radical pathway: a computational mechanistic study. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	3
34	Asymmetric Guerbet Reaction to Access Chiral Alcohols. Angewandte Chemie, 2020, 132, 11505-11512.	2.0	20
35	Asymmetric Guerbet Reaction to Access Chiral Alcohols. Angewandte Chemie - International Edition, 2020, 59, 11408-11415.	13.8	60
36	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

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37	Theoretical Study on Nitrogenous Heterocyclic Assisted Aldimine Condensation. Acta Chimica Sinica, 2020, 78, 437.	1.4	7
38	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
39	Ruthenium-catalyzed deoxygenative hydroboration of carboxylic acids: a DFT mechanistic study. New Journal of Chemistry, 2019, 43, 11493-11496.	2.8	5
40	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
41	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
42	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
43	Transitionâ€Metalâ€Free Hydrogen Autotransfer: Diastereoselective Nâ€Alkylation of Amines with Racemic Alcohols. Angewandte Chemie, 2019, 131, 10638-10646.	2.0	12
44	Transitionâ€Metalâ€Free Hydrogen Autotransfer: Diastereoselective Nâ€Alkylation of Amines with Racemic Alcohols. Angewandte Chemie - International Edition, 2019, 58, 10528-10536.	13.8	65
45	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
46	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
47	Rapid screening of the hydrogen bonding strength of radicals by electrochemiluminescent probes. Chemical Communications, 2019, 55, 5563-5566.	4.1	5
48	Mechanisms of Ketone/Imine Hydrogenation Catalyzed by Transitionâ€Metal Complexes. Energy and Environmental Materials, 2019, 2, 292-312.	12.8	34
49	3D-QSAR studies of D3R antagonists and 5-HT1AR agonists. Journal of Molecular Graphics and Modelling, 2019, 86, 132-141.	2.4	6
50	A Hydride-Shuttle Mechanism for the Catalytic Hydroboration of CO₂. Inorganic Chemistry, 2018, 57, 3054-3060.	4.0	30
51	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
52	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
53	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
54	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

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55	Structure Simulation and Hostâ€“Guest Interaction of Histidine-Intercalated Hydrotalciteâ€“Montmorillonite Complex. Minerals (Basel, Switzerland), 2018, 8, 198.	2.0	4
56	Metalâ€“Substrate Cooperation Mechanism for Dehydrogenative Amidation Catalyzed by a PNN-Ru Catalyst. Inorganic Chemistry, 2018, 57, 8778-8787.	4.0	24
57	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
58	Investigation on terpolymer of ethylene/propylene/Ï‰-bromo-Î±-olefins catalyzed by titanium complexes. Journal of Materials Science, 2017, 52, 5981-5991.	3.7	6
59	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
60	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
61	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
62	DFT Mechanistic Study on Alkene Hydrogenation Catalysis of Iron Metallaboratrane: Characteristic Features of Iron Species. Organometallics, 2017, 36, 3530-3538.	2.3	18
63	Borneol Is a TRPM8 Agonist that Increases Ocular Surface Wetness. PLoS ONE, 2016, 11, e0158868.	2.5	19
64	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
65	Dimerization of SLX4 contributes to functioning of the SLX4-nuclease complex. Nucleic Acids Research, 2016, 44, 4871-4880.	14.5	14
66	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
67	Quinolylâ€Amidinates Chelating Bimetallic Magnesium and Mononuclear Aluminum Complexes for Ïµâ€Caprolactone Polymerization. ChemistrySelect, 2016, 1, 5660-5665.	1.5	9
68	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
69	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
70	Theoretical Study on N-N Activation by Thiolate-bridged Dinuclear Dinitrogen Transition-metal Complexes. Acta Chimica Sinica, 2016, 74, 340.	1.4	4
71	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
72	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

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73	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
74	Homolytic or Heterolytic Dihydrogen Splitting with Ditantalum/Dizirconium Dinitrogen Complexes? A Computational Study. Organometallics, 2015, 34, 1255-1263.	2.3	8
75	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
76	Bent and planar structures of Î¼â€“Î·2:Î·2-N2dinuclear early transition metal complexes. Dalton Transactions, 2014, 43, 11658.	3.3	6
77	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
78	Guest-modulation of the mechanical properties of flexible porous metalâ€“organic frameworks. Journal of Materials Chemistry A, 2014, 2, 9691-9698.	10.3	18
79	Targeting MLL1 H3K4 Methyltransferase Activity in Mixed-Lineage Leukemia. Molecular Cell, 2014, 53, 247-261.	9.7	252
80	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
81	Structural basis for protein-RNA recognition in telomerase. Nature Structural and Molecular Biology, 2014, 21, 507-512.	8.2	71
82	A theoretical study on the alkene insertion step in Rh-Yanphos catalyzed hydroformylation. Chinese Chemical Letters, 2013, 24, 1083-1086.	9.0	7
83	CO assisted N₂functionalization activated by a dinuclear hafnium complex: a DFT mechanistic exploration. Physical Chemistry Chemical Physics, 2013, 15, 901-910.	2.8	13
84	3D-QSAR and docking studies on 2-arylbenzoxazole and linker-Y transthyretin amyloidogenesis inhibitors. Science China Chemistry, 2013, 56, 1550-1563.	8.2	7
85	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
86	Mechanistic Studies on the Carboxylation of Hafnocene and ansa-Zirconocene Dinitrogen Complexes with CO2. Organometallics, 2013, 32, 7077-7082.	2.3	13
87	WHICH IS THE PROTON-SHUTTLE IN ISOXANTHOPTERIN DEAMINASE? QM/MM MD UNDERSTANDING. Journal of Theoretical and Computational Chemistry, 2013, 12, 1341002.	1.8	1
88	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
89	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
90	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

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91	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
92	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
93	Rational Design and Study on Recognition Property of Paracetamol-Imprinted Polymer. Applied Biochemistry and Biotechnology, 2010, 160, 328-342.	2.9	16
94	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
95	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
96	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
97	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
98	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
99	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
100	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
101	A novel algorithm for a rotation invariant template matching. Optoelectronics Letters, 2008, 4, 379-383.	0.8	3
102	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
103	Dynamics and cooperativity of Trp-cage folding. Archives of Biochemistry and Biophysics, 2008, 475, 140-147.	3.0	29
104	Nature of Asynchronous Hydrogen Transfer in Ketone Hydrogenation Catalyzed by Ru Complex. Journal of Physical Chemistry C, 2008, 112, 13524-13527.	3.1	28
105	A DFT Study on Formation of Bisaryl Oxime Ether from Benzaldehyde and Phenoxyamine. Chemistry Letters, 2008, 37, 656-657.	1.3	3
106	Models for binding cooperativities of inhibitors with transthyretin. Archives of Biochemistry and Biophysics, 2007, 466, 85-97.	3.0	14
107	Study of the properties of molecularly imprinted polymers by computational and conformational analysis. Analytica Chimica Acta, 2007, 581, 137-146.	5.4	64
108	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

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109	Initial Conformational Changes of Human Transthyretin under Partially Denaturing Conditions. Biophysical Journal, 2005, 89, 433-443.	0.5	26
110	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
111	Toughening of polyethylene terephthalate/amorphous copolyester blends with a maleated thermoplastic elastomer. Journal of Applied Polymer Science, 2003, 89, 797-805.	2.6	16
112	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
113	Ab initio study on the mechanism of reaction HNCO+NH2. Science in China Series B: Chemistry, 2002, 45, 365-372.	0.8	3
114	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
115	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
116	Ab initio MO study of reaction mechanism for carbonyl migration of Co complex. Science Bulletin, 2000, 45, 1176-1178.	1.7	5
117	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
118	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
119	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
120	Theoretical Study on the Mechanism of the Benzaldehydes Deoxyfluorination by Sulfuryl Fluoride and Tetramethylammonium Fluoride. Journal of Physical Organic Chemistry, 0, , .	1.9	1