

Paul M Zimmerman

List of Publications by Year in descending order

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122
papers

8,626
citations

66234

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45213

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124
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124
docs citations

124
times ranked

8178
citing authors

#	ARTICLE	IF	CITATIONS
1	Heavy atom oriented orbital angular momentum manipulation in metal-free organic phosphors. <i>Chemical Science</i> , 2022, 13, 789-797.	3.7	18
2	Interplay Between Applied Force and Radical Attack in the Mechanochemical Chain Scission of Poly(acrylic acid). <i>Journal of Physical Chemistry A</i> , 2022, 126, 521-528.	1.1	2
3	Changes in ligand coordination mode induce bimetallic C=C coupling pathways. <i>Dalton Transactions</i> , 2022, 51, 3977-3991.	1.6	2
4	Investigation of Thermally Activated Delayed Fluorescence in Donor-Acceptor Organic Emitters with Time-Resolved Absorption Spectroscopy. <i>Chemistry of Materials</i> , 2022, 34, 2161-2175.	3.2	9
5	The many-body electronic interactions of Fe(II)-porphyrin. <i>Journal of Chemical Physics</i> , 2022, 156, 094110.	1.2	2
6	Glycosyl Exchange of Unactivated Glycosidic Bonds: Suppressing or Embracing Side Reactivity in Catalytic Glycosylations. <i>Journal of Organic Chemistry</i> , 2022, 87, 5817-5826.	1.7	2
7	Predicting reaction conditions from limited data through active transfer learning. <i>Chemical Science</i> , 2022, 13, 6655-6668.	3.7	21
8	Metal-Free Organic Triplet Emitters with On-Off Switchable Excited State Intramolecular Proton Transfer. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	25
9	State-specific solvation for restricted active space spin-flip (RAS-SF) wave functions based on the polarizable continuum formalism. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	1
10	Fully variational incremental CASSCF. <i>Journal of Chemical Physics</i> , 2021, 154, 014105.	1.2	8
11	Toward Full Configuration Interaction for Transition-Metal Complexes. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1598-1609.	1.1	10
12	Combined Theoretical and Experimental Investigation of Lewis Acid-Carbonyl Interactions for Metathesis. <i>ACS Catalysis</i> , 2021, 11, 4381-4394.	5.5	6
13	Experimental and Theoretical Characterization of Ultrafast Water-Soluble Photochromic Photoacids. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4120-4131.	1.2	11
14	Impact of Ring-Fusion on the Excited State Decay Pathways of N-Annulated Perylene Diimides. <i>Journal of Physical Chemistry C</i> , 2021, 125, 10500-10515.	1.5	3
15	An Ion-Pairing Approach to Stereoselective Metal-Free Ring-Opening Metathesis Polymerization. <i>Angewandte Chemie</i> , 2021, 133, 14071-14077.	1.6	5
16	Mechanochemical Release of N-Heterocyclic Carbenes from Flex-Activated Mechanophores. <i>Angewandte Chemie</i> , 2021, 133, 13671-13675.	1.6	8
17	The Role of the Core Attachment Positioning in Triggering Intramolecular Singlet Exciton Fission in Perylene Diimide Tetramers. <i>Journal of Physical Chemistry B</i> , 2021, 125, 5114-5131.	1.2	9
18	An Ion-Pairing Approach to Stereoselective Metal-Free Ring-Opening Metathesis Polymerization. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 13952-13958.	7.2	14

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19	Mechanochemical Release of N -Heterocyclic Carbenes from Flex-Activated Mechanophores. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 13559-13563.	7.2	36
20	Giving superabsorbent polymers a second life as pressure-sensitive adhesives. <i>Nature Communications</i> , 2021, 12, 4524.	5.8	32
21	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
22	Using PP to Identify Ni Bidentate Phosphine Complexes <i>In Situ</i> . <i>Inorganic Chemistry</i> , 2021, 60, 13400-13408.	1.9	1
23	An Open-Shell Coronoid with Hybrid Chichibabin-Schlenk Conjugation. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 22496-22504.	7.2	15
24	An Open-Shell Coronoid with Hybrid Chichibabin-Schlenk Conjugation. <i>Angewandte Chemie</i> , 2021, 133, 22670-22678.	1.6	3
25	Brønsted-Acid-Catalyzed Intramolecular Carbonyl-Olefin Reactions: Interrupted Metathesis vs Carbonyl-Ene Reaction. <i>Journal of Organic Chemistry</i> , 2021, 86, 3008-3016.	1.7	12
26	Using Adhesives to Capture Microplastics from Water. <i>ACS ES&T Engineering</i> , 2021, 1, 1698-1704.	3.7	11
27	Increasing the CO_2 Reduction Activity of Cobalt Phthalocyanine by Modulating the σ -Donor Strength of Axially Coordinating Ligands. <i>ACS Catalysis</i> , 2021, 11, 13203-13216.	5.5	33
28	Studies of Catalyst-Controlled Regioselective Acetalization and Its Application to Single-Pot Synthesis of Differentially Protected Saccharides. <i>Journal of the American Chemical Society</i> , 2021, 143, 18592-18604.	6.6	8
29	A Comparison of Exact and Model Exchange-Correlation Potentials for Molecules. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 12012-12019.	2.1	13
30	Experimental and Computational Studies on Regiodivergent Chiral Phosphoric Acid Catalyzed Cycloisomerization of Mupirocin Methyl Ester. <i>Chemistry - A European Journal</i> , 2020, 26, 4583-4591.	1.7	5
31	The Mechanics of the Bicycle Pedal Photoisomerization in Crystalline <i>cis,cis</i> -1,4-Diphenyl-1,3-butadiene. <i>Journal of Physical Chemistry A</i> , 2020, 124, 8897-8906.	1.1	6
32	Mechanistic Study of Isotactic Poly(propylene oxide) Synthesis using a Tethered Bimetallic Chromium Salen Catalyst. <i>ACS Catalysis</i> , 2020, 10, 8960-8967.	5.5	13
33	Activating intramolecular singlet exciton fission by altering π -bridge flexibility in perylene diimide trimers for organic solar cells. <i>Chemical Science</i> , 2020, 11, 8757-8770.	3.7	22
34	Charge transfer via spin flip configuration interaction: Benchmarks and application to singlet fission. <i>Journal of Chemical Physics</i> , 2020, 153, 064109.	1.2	10
35	Calculation of spin-orbit couplings using RASCI spinless one-particle density matrices: Theory and applications. <i>Journal of Chemical Physics</i> , 2020, 153, 214107.	1.2	18
36	Revealing the Strong Relationships between Ligand Conformers and Activation Barriers: A Case Study of Bisphosphine Reductive Elimination. <i>ACS Catalysis</i> , 2020, 10, 7136-7145.	5.5	25

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37	Fluoride Migration Catalysis Enables Simple, Stereoselective, and Iterative Glycosylation. <i>Journal of the American Chemical Society</i> , 2020, 142, 7235-7242.	6.6	43
38	What Does the Machine Learn? Knowledge Representations of Chemical Reactivity. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1290-1301.	2.5	19
39	Quantum Chemical Investigation of Dimerization in the Schlenk Equilibrium of Thiophene Grignard Reagents. <i>Journal of Physical Chemistry A</i> , 2020, 124, 1480-1488.	1.1	7
40	Nickel-Catalyzed Three-Component Cycloadditions of Enoates, Alkynes, and Aldehydes. <i>Journal of Organic Chemistry</i> , 2020, 85, 2956-2965.	1.7	9
41	Mercury Magnetic Isotope Effect: A Plausible Photochemical Mechanism. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3711-3719.	1.1	9
42	New Direct Approach for Determining the Reverse Intersystem Crossing Rate in Organic Thermally Activated Delayed Fluorescent (TADF) Emitters. <i>Journal of the American Chemical Society</i> , 2020, 142, 8074-8079.	6.6	52
43	Learning To Predict Reaction Conditions: Relationships between Solvent, Molecular Structure, and Catalyst. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3645-3654.	2.5	36
44	Evaluation of full valence correlation energies and gradients. <i>Journal of Chemical Physics</i> , 2019, 150, 244117.	1.2	26
45	Functionalized and Degradable Polyphthalaldehyde Derivatives. <i>Journal of the American Chemical Society</i> , 2019, 141, 14544-14548.	6.6	37
46	Hydroxyl Radical-Coupled Electron-Transfer Mechanism of Flavin-Dependent Hydroxylases. <i>Journal of Physical Chemistry B</i> , 2019, 123, 8065-8073.	1.2	12
47	Exact exchange-correlation potentials from ground-state electron densities. <i>Nature Communications</i> , 2019, 10, 4497.	5.8	54
48	Toward one-pot olefin/thiophene block copolymers using an in situ ligand exchange. <i>Journal of Polymer Science Part A</i> , 2019, 57, 1601-1605.	2.5	2
49	5,10-Dimesityldiindeno[1,2- <i>a</i> ': <i>2</i> ''- <i>1</i> ''- <i>i</i> ']phenanthrene: a stable biradicaloid derived from Chichibabin's hydrocarbon. <i>Chemical Science</i> , 2019, 10, 3413-3420.	3.7	33
50	Using ultra-fast spectroscopy to probe the excited state dynamics of a reported highly efficient thermally activated delayed fluorescence chromophore. <i>Journal of Materials Chemistry C</i> , 2019, 7, 4210-4221.	2.7	16
51	Chemoenzymatic α -Quinone Methide Formation. <i>Journal of the American Chemical Society</i> , 2019, 141, 20269-20277.	6.6	38
52	Catalytic Carbonyl-Olefin Metathesis of Aliphatic Ketones: Iron(III) Homo-Dimers as Lewis Acidic Superelectrophiles. <i>Journal of the American Chemical Society</i> , 2019, 141, 1690-1700.	6.6	63
53	Examining the Ways To Bend and Break Reaction Pathways Using Mechanochemistry. <i>Journal of Physical Chemistry C</i> , 2018, 122, 6996-7004.	1.5	20
54	Excited States of Methylene, Polyenes, and Ozone from Heat-Bath Configuration Interaction. <i>Journal of Physical Chemistry A</i> , 2018, 122, 2714-2722.	1.1	80

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55	Uncovering reaction sequences on surfaces through graphical methods. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7721-7729.	1.3	10
56	Spin-Switching Transmetalation at Ni Diimine Catalysts. <i>ACS Catalysis</i> , 2018, 8, 3655-3666.	5.5	20
57	Trials and tribulations of designing multitasking catalysts for olefin/thiophene block copolymerizations. <i>Journal of Polymer Science Part A</i> , 2018, 56, 132-137.	2.5	10
58	Iterative submatrix diagonalisation for large configuration interaction problems. <i>Molecular Physics</i> , 2018, 116, 107-117.	0.8	3
59	Methods for exploring reaction space in molecular systems. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2018, 8, e1354.	6.2	164
60	Discovery of conical intersection mediated photochemistry with growing string methods. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 27394-27405.	1.3	24
61	Coupled double triplet state in singlet fission. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 30083-30094.	1.3	80
62	Interrupted carbonyl-olefin metathesis via oxygen atom transfer. <i>Science</i> , 2018, 361, 1363-1369.	6.0	47
63	Stepwise basis set selection. <i>Journal of Computational Chemistry</i> , 2018, 39, 2153-2162.	1.5	1
64	Fully Conjugated [4]Chrysaorene. Redox-Coupled Anion Binding in a Tetradicaloid Macrocyclic. <i>Journal of the American Chemical Society</i> , 2018, 140, 14474-14480.	6.6	35
65	Investigating the Optical Properties of Thiophene Additions to <i>s</i> -Indacene Donors with Diketopyrrolopyrrole, Isoindigo, and Thienothiophene Acceptors. <i>Journal of Physical Chemistry C</i> , 2018, 122, 27713-27733.	1.5	11
66	Predicting and Controlling Entangled Two-Photon Absorption in Diatomic Molecules. <i>Journal of Physical Chemistry A</i> , 2018, 122, 8198-8212.	1.1	25
67	Ligand-Induced Reductive Elimination of Ethane from Azopyridine Palladium Dimethyl Complexes. <i>Journal of the American Chemical Society</i> , 2018, 140, 11408-11415.	6.6	15
68	Virtual Screening of Hole Transport, Electron Transport, and Host Layers for Effective OLED Design. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2440-2449.	2.5	22
69	Heteroatom and Side Chain Effects on the Optical and Photophysical Properties: Ultrafast and Nonlinear Spectroscopy of New Naphtho[1,2- <i>b</i> :5,6- <i>b'</i>]difuran Donor Polymers. <i>Journal of Physical Chemistry C</i> , 2018, 122, 17049-17066.	1.5	20
70	Enacting Two-Electron Transfer from a Double-Triplet State of Intramolecular Singlet Fission. <i>Journal of the American Chemical Society</i> , 2018, 140, 7760-7763.	6.6	46
71	Charge Transfer and Aggregation Effects on the Performance of Planar vs Twisted Nonfullerene Acceptor Isomers for Organic Solar Cells. <i>Chemistry of Materials</i> , 2018, 30, 4263-4276.	3.2	49
72	Reliable and efficient reaction path and transition state finding for surface reactions with the growing string method. <i>Journal of Computational Chemistry</i> , 2017, 38, 645-658.	1.5	40

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73	Recovering dynamic correlation in spin flip configuration interaction through a difference dedicated approach. <i>Journal of Chemical Physics</i> , 2017, 146, 014103.	1.2	38
74	Incremental full configuration interaction. <i>Journal of Chemical Physics</i> , 2017, 146, 104102.	1.2	86
75	Evaluating the Effect of Heteroatoms on the Photophysical Properties of Donor–Acceptor Conjugated Polymers Based on 2,6-Di(thiophen-2-yl)benzo[1,2-b:4,5-b']difuran: Two-Photon Cross-Section and Ultrafast Time-Resolved Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2017, 121, 14382-14392.	1.5	27
76	Regiodivergent Glycosylations of 6-Deoxy-erythronolide B and Oleandomycin-Derived Macrolactones Enabled by Chiral Acid Catalysis. <i>Journal of the American Chemical Society</i> , 2017, 139, 8570-8578.	6.6	63
77	Singlet–Triplet Gaps through Incremental Full Configuration Interaction. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4712-4720.	1.1	42
78	Finding reaction mechanisms, intuitive or otherwise. <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 501-504.	1.5	65
79	Entrances, Traps, and Rate-Controlling Factors for Nickel-Catalyzed C–H Functionalization. <i>ACS Catalysis</i> , 2017, 7, 7352-7362.	5.5	48
80	Simulated Mechanism for Palladium-Catalyzed, Directed β -Arylation of Piperidine. <i>ACS Catalysis</i> , 2017, 7, 5466-5477.	5.5	33
81	Mechanistic Investigations of the Iron(III)-Catalyzed Carbonyl-Olefin Metathesis Reaction. <i>Journal of the American Chemical Society</i> , 2017, 139, 10832-10842.	6.6	77
82	Strong correlation in incremental full configuration interaction. <i>Journal of Chemical Physics</i> , 2017, 146, 224104.	1.2	46
83	Mechanistic Insight into Thiophene Catalyst-Transfer Polymerization Mediated by Nickel Diimine Catalysts. <i>Macromolecules</i> , 2017, 50, 9121-9127.	2.2	20
84	Density Functional Physicality in Electronic Coupling Estimation: Benchmarks and Error Analysis. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3242-3248.	2.1	14
85	Isospecific, Chain Shuttling Polymerization of Propylene Oxide Using a Bimetallic Chromium Catalyst: A New Route to Semicrystalline Polyols. <i>Journal of the American Chemical Society</i> , 2017, 139, 11048-11054.	6.6	63
86	Exploring the relationship between vibrational mode locality and coupling using constrained optimization. <i>Journal of Chemical Physics</i> , 2016, 144, 124111.	1.2	29
87	Impact of Preferential π -Binding in Catalyst-Transfer Polycondensation of Thiazole Derivatives. <i>ACS Macro Letters</i> , 2016, 5, 1411-1415.	2.3	33
88	Experimental and Computational Assessment of Reactivity and Mechanism in C(sp ³)–N Bond-Forming Reductive Elimination from Palladium(IV). <i>Journal of the American Chemical Society</i> , 2016, 138, 6049-6060.	6.6	79
89	An Unusual Iron-Dependent Oxidative Deformylation Reaction Providing Insight into Hydrocarbon Biosynthesis in Nature. <i>ACS Catalysis</i> , 2016, 6, 3293-3300.	5.5	13
90	Iron(III)-catalysed carbonyl–olefin metathesis. <i>Nature</i> , 2016, 533, 374-379.	13.7	179

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91	Computational Mechanism for Initiation and Growth of Poly(3-hexylthiophene) Using Palladium $\langle i \rangle N \langle /i \rangle$ -Heterocyclic Carbene Precatalysts. <i>Macromolecules</i> , 2016, 49, 7632-7641.	2.2	21
92	Estimating the Derivative Coupling Vector Using Gradients. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 5074-5079.	2.1	10
93	Achieving Accurate Reduction Potential Predictions for Anthraquinones in Water and Aprotic Solvents: Effects of Inter- and Intramolecular H-Bonding and Ion Pairing. <i>Journal of Physical Chemistry C</i> , 2016, 120, 22235-22247.	1.5	41
94	The Mechanism of Acceptorless Amine Double Dehydrogenation by $\langle i \rangle N, N \langle /i \rangle$ -Amide Ruthenium(II) Hydrides: A Combined Experimental and Computational Study. <i>ACS Catalysis</i> , 2016, 6, 4799-4813.	5.5	56
95	Studies of the Mechanism and Origins of Enantioselectivity for the Chiral Phosphoric Acid-Catalyzed Stereoselective Spiroketalization Reactions. <i>Journal of the American Chemical Society</i> , 2016, 138, 444-456.	6.6	89
96	Mechanism for Forming B,C,N,O Rings from NH_3 and BH_3 and CO_2 via Reaction Discovery Computations. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1135-1144.	1.1	15
97	Optimizing Vibrational Coordinates To Modulate Intermode Coupling. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 1883-1891.	2.3	29
98	Structure and Dynamics of the $\langle \sup \rangle 1 \langle /sup \rangle$ (TT) State in a Quinoidal Bithiophene: Characterizing a Promising Intramolecular Singlet Fission Candidate. <i>Journal of Physical Chemistry C</i> , 2015, 119, 28258-28268.	1.5	56
99	Orbitals with intermediate localization and low coupling: Spanning the gap between canonical and localized orbitals. <i>Journal of Chemical Physics</i> , 2015, 143, 014106.	1.2	8
100	Highly Active Nickel Catalysts for C-H Functionalization Identified through Analysis of Off-Cycle Intermediates. <i>Journal of the American Chemical Society</i> , 2015, 137, 7636-7639.	6.6	71
101	Hexane Cracking on ZSM-5 and Faujasite Zeolites: a QM/MM/QCT Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 28836-28853.	1.5	31
102	Single-ended transition state finding with the growing string method. <i>Journal of Computational Chemistry</i> , 2015, 36, 601-611.	1.5	160
103	Navigating molecular space for reaction mechanisms: an efficient, automated procedure. <i>Molecular Simulation</i> , 2015, 41, 43-54.	0.9	82
104	Unraveling the Crucial Role of Metal-Free Catalysis in Borazine and Polyborazylene Formation in Transition-Metal-Catalyzed Ammonia-Borane Dehydrogenation. <i>ACS Catalysis</i> , 2015, 5, 3478-3493.	5.5	47
105	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
106	Enantioselective Synthesis of Piperidines through the Formation of Chiral Mixed Phosphoric Acid Acetals: Experimental and Theoretical Studies. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 11194-11198.	7.2	59
107	Restricted active space spin-flip (RAS-SF) with arbitrary number of spin-flips. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 358-366.	1.3	64
108	A Correlated Electron View of Singlet Fission. <i>Accounts of Chemical Research</i> , 2013, 46, 1339-1347.	7.6	150

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109	Automated discovery of chemically reasonable elementary reaction steps. <i>Journal of Computational Chemistry</i> , 2013, 34, 1385-1392.	1.5	179
110	Reliable Transition State Searches Integrated with the Growing String Method. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3043-3050.	2.3	177
111	Growing string method with interpolation and optimization in internal coordinates: Method and examples. <i>Journal of Chemical Physics</i> , 2013, 138, 184102.	1.2	145
112	Restricted active space spin-flip configuration interaction: Theory and examples for multiple spin flips with odd numbers of electrons. <i>Journal of Chemical Physics</i> , 2012, 137, 164110.	1.2	69
113	Efficient exploration of reaction paths via a freezing string method. <i>Journal of Chemical Physics</i> , 2011, 135, 224108.	1.2	154
114	Selection and Validation of Charge and Lennard-Jones Parameters for QM/MM Simulations of Hydrocarbon Interactions with Zeolites. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1695-1703.	2.3	67
115	Mechanism for Singlet Fission in Pentacene and Tetracene: From Single Exciton to Two Triplets. <i>Journal of the American Chemical Society</i> , 2011, 133, 19944-19952.	6.6	397
116	On the nature of electron correlation in C60. <i>Journal of Chemical Physics</i> , 2011, 135, 194306.	1.2	26
117	Singlet fission in pentacene through multi-exciton quantum states. <i>Nature Chemistry</i> , 2010, 2, 648-652.	6.6	356
118	Simultaneous Two-Hydrogen Transfer as a Mechanism for Efficient CO ₂ Reduction. <i>Inorganic Chemistry</i> , 2010, 49, 8724-8728.	1.9	70
119	Excited states of methylene from quantum Monte Carlo. <i>Journal of Chemical Physics</i> , 2009, 131, 124103.	1.2	70
120	The Role of Free N-heterocyclic Carbene (NHC) in the Catalytic Dehydrogenation of Ammonia-Borane in the Nickel NHC System. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 2201-2205.	7.2	115
121	Oligomerization and Autocatalysis of NH ₂ BH ₂ with Ammonia-Borane. <i>Inorganic Chemistry</i> , 2009, 48, 1069-1081.	1.9	108
122	Catalytic Dehydrogenation of Ammonia Borane at Ni Monocarbene and Dicarbene Catalysts. <i>Inorganic Chemistry</i> , 2009, 48, 5418-5433.	1.9	72