

Yi Ren

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	COMPASS Force Field for 14 Inorganic Molecules, He, Ne, Ar, Kr, Xe, H ₂ , O ₂ , N ₂ , NO, CO, CO ₂ , NO ₂ , CS ₂ , and SO ₂ , in Liquid Phases. <i>Journal of Physical Chemistry B</i> , 2000, 104, 4951-4957.	2.6	181
2	The $\hat{\pm}$ -Effect in Gas-Phase SN ₂ Reactions: Existence and the Origin of the Effect. <i>Journal of Organic Chemistry</i> , 2007, 72, 5660-5667.	3.2	90
3	G2(+) Investigation on the $\hat{\pm}$ -Effect in the SN ₂ Reactions at Saturated Carbon. <i>Chemistry - A European Journal</i> , 2007, 13, 677-682.	3.3	55
4	The $\hat{\pm}$ -Effect in Gas-Phase SN ₂ Reactions Revisited. <i>Organic Letters</i> , 2006, 8, 119-121.	4.6	49
5	Highly efficient extraction of actinides with pillar[5]arene-derived diglycolamides in ionic liquids via a unique mechanism involving competitive host-guest interactions. <i>Dalton Transactions</i> , 2016, 45, 19299-19310.	3.3	49
6	Exploring the Reactivity Trends in the E ₂ and S _N 2 Reactions of X ⁺ + CH ₃ CH ₂ Cl (X = F, Cl, Br, HO, HS, HSe, NH ₂ , PH ₂), <i>Tj ETQqO O 0,rgBT /Overlock 10 T</i> <i>Theory and Computation</i> , 2009, 5, 1597-1606.	5.8	44
7	Nonaggregational Shape-Persistent Cyclo[6]aramide and Its Macrocyclic Effect toward Binding Secondary Ammonium Salts in Moderately Polar Media. <i>Organic Letters</i> , 2013, 15, 4670-4673.	4.6	35
8	Macrocyclic shape-persistence of cyclo[6]aramide results in enhanced multipoint recognition for the highly efficient template-directed synthesis of rotaxanes. <i>Chemical Science</i> , 2017, 8, 2091-2100.	7.4	32
9	Cyclo[6]aramide-Tropylium Charge Transfer Complex as a Colorimetric Chemosensor for Differentiation of Intimate and Loose Ion Pairs. <i>Organic Letters</i> , 2015, 17, 5950-5953.	4.6	29
10	Does $\hat{\pm}$ -effect exist in E ₂ reactions? A G2(+) investigation. <i>Journal of Computational Chemistry</i> , 2009, 30, 358-365.	3.3	28
11	A G2(+) level investigation of the gas-phase non-identity SN ₂ reactions of halides with halodimethylamine. <i>Journal of the American Society for Mass Spectrometry</i> , 2004, 15, 673-680.	2.8	26
12	The $\hat{\pm}$ -effect exhibited in gas-phase S _N 2@N and S _N 2@C reactions. <i>Journal of Computational Chemistry</i> , 2013, 34, 1997-2005.	3.3	25
13	Theoretical study of the N ₁₀ clusters without double bonds. <i>International Journal of Quantum Chemistry</i> , 2001, 82, 34-43.	2.0	22
14	Modified Gaussian-2 level investigation of the identity ion-pair SN ₂ reactions of lithium halide and methyl halide with inversion and retention mechanisms. <i>Journal of Computational Chemistry</i> , 2004, 25, 461-471.	3.3	19
15	Halogen versus halide electronic structure. <i>Science China Chemistry</i> , 2010, 53, 210-215.	8.2	19
16	Reversibly Tunable Lower Critical Solution Temperature Behavior Induced by H-Bonded Aromatic Amide Macrocyclic and Imidazolium Host-Guest Complexation. <i>Organic Letters</i> , 2017, 19, 18-21.	4.6	19
17	Unexpected Selectivity in Sodium Borohydride Reductions of $\hat{\pm}$ -Substituted Esters: Experimental and Theoretical Studies. <i>European Journal of Organic Chemistry</i> , 2006, 2006, 1981-1990.	2.4	18
18	RECENT DEVELOPMENT IN THE STUDY OF SN ₂ REACTIONS AT HETEROATOMS AND ION PAIR SYSTEMS. <i>Journal of Theoretical and Computational Chemistry</i> , 2006, 05, 121-140.	1.8	18

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19	A rare case for binding a diquat salt by two cyclo[6]aramides. <i>Supramolecular Chemistry</i> , 2015, 27, 436-443.	1.2	18
20	Density functional theory study of tautomerization of 2-aminothiazole in the gas phase and in solution. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 247-258.	2.0	15
21	Theoretical study on the role of cooperative solvent molecules in the neutral hydrolysis of ketene. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 493-506.	1.4	14
22	Theoretical Study on the Identity Ion Pair SN ₂ Reactions of LiX with CH ₃ SX (X = Cl, Br, and I): ^Å Structure, Mechanism, and Potential Energy Surface. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6615-6621.	2.5	12
23	Ab initio computational modeling on the tautomerism of monochalcogenocarboxylic acids CH ₃ C(=O)XH (X = S, Se, and Te) in the polar and aprotic solution. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 921-929.	2.0	11
24	Comprehensive Theoretical Studies on the Gas Phase S _N ² Reactions of Anionic Nucleophiles toward Chloroamine and <i>N</i> -Chlorodimethylamine with Inversion and Retention Mechanisms. <i>Journal of Physical Chemistry A</i> , 2011, 115, 13965-13974.	2.5	10
25	Origin of Enhanced Reactivity of a Microsolvated Nucleophile in Ion Pair S _N ² Reactions: The Cases of Sodium <i>p</i> -Nitrophenoxide with Halomethanes in Acetone. <i>Journal of Physical Chemistry A</i> , 2015, 119, 3878-3886.	2.5	10
26	Pyridine-incorporated cyclo[6]aramide for recognition of urea and its derivatives with two different binding modes. <i>Supramolecular Chemistry</i> , 2017, 29, 730-740.	1.2	10
27	Counter-ion effect in the nucleophilic substitution reactions at silicon: a G2M(+) level theoretical investigation. <i>Theoretical Chemistry Accounts</i> , 2008, 119, 407-411.	1.4	7
28	Theoretical investigation of ion pair SN ₂ reactions of alkali isothiocyanates with alkyl halides. Part 1. Reaction of lithium isothiocyanate and methyl fluoride with inversion mechanism. <i>International Journal of Quantum Chemistry</i> , 2005, 101, 104-112.	2.0	6
29	Theoretical study of the gas-phase ion pairs SN ₂ reactions of LiX with CH ₃ SY (X, Y = F, Cl, Br, I). <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1487-1494.	2.0	4
30	AB INITIO COMPUTATIONAL INVESTIGATIONS ON THE GAS-PHASE HOMODIMERIZATION AND KETO-ENOL TAUTOMERISM OF THE MONOCHALCOGENOCARBOXYLIC ACIDS CH ₃ C(=O)XH (X = S, Se, Te). <i>Journal of Theoretical and Computational Chemistry</i> , 2011, 10, 41-51.	1.8	4
31	Tautomerism of monochalcogenosilanoic acids CH ₃ Si(=O)XH (X = S, Se, Te) in the gas phase and in the polar and aprotic solution: An ab initio computational investigation. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 142-150.	2.0	3
32	Comprehensive mechanistic study of ion pair SN ₂ reactions of lithium isocyanate and methyl halides. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 1653-1663.	2.0	2
33	EXPLORING THE POTENTIAL ENERGY SURFACE OF THE CATALYZED ISOMERIZATION OF NITROSOMETHANE TO FORMALDOXIME. <i>Journal of Theoretical and Computational Chemistry</i> , 2007, 06, 187-195.	1.8	2
34	Theoretical study of the gas-phase SN ₂ reactions of X ⁻ with CH ₃ OY (X, Y = Cl, Br, I). <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1142-1149.	2.0	1
35	Density functional theory study on the reactions of X ⁻ with CH ₃ SY (X, Y = F, Cl, Br, I). <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1373-1381.	2.0	1
36	A Mechanism Study of a Novel Acid-Activatable Michael-Type Fluorescent Probe for Thiols. <i>Chinese Journal of Chemical Physics</i> , 2015, 28, 277-287.	1.3	0