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Research Article

Theoretical Investigation on TCT-DMSO-Catalyzed Thioalkylation and Regioselective Intramolecular Cyclization Cascade of 2-Alkylnylaniline to build 3-Methylthiolated Indole

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Abstract

The first theoretical investigation on TCT-DMSO-catalyzed dialkylations and regioselective intramolecular cyclization cascade of 2-alkylnylaniline was provided by our DFT calculation. Upon treatment of DMSO with TCT, the dimethyl alkoxysulfonium salt was afforded after removal of one chloride ion. Then, with additional two DMSO, this species was converted to DMSO-stabilized methyl sulfenium electrophile equivalent, methoxy sulfonium salt and TCT derivative. Next, a proton trapping occurred between the latter two followed by dissociation of methoxy sulfonium salt into dimethyl sulfide and formaldehyde. Finally, the electrophilic addition of DMSO-stabilized methylsulfenium to triple bond of 2-alkynylaniline took place accompanied by nucleophilic attack of amine group leading to product 3 methy lthiolated indole together with recovered DMSO and a released proton. The first DMSO attack dimethyl alkoxysulfonium is determined to be rate-limiting.

Keywords: regioselective cyclization; dialkylation; DMSO; indole; alkylamine

1.Introduction

As a crucial class of building blocks, sulfone, sulfoxide and substituted methyl sulfide have been widely used in pharmaceutical industry [1-3]. It's desirable to introduce such motif especially S-methyl d3 analogues. In this field, DMSO/DMSO-d6 was usually applied as methylthiolating "SMe/SCD_3" sources in organic transformation. Dai developed lewis acid-catalyzed, copper(II)-mediated synthesis of heteroaryl thioethers under base-free condition [4]. Sharma discovered copper acetate−DMSO promoted methylthiolation of arene and heteroarene [5]. Mamedov gave bromine-promoted one-pot furo[b]annulation and α-C(sp2)-thiomethylation cascade of (E)-3-Styrylquinoxalin-2(1H)-ones with dimethyl sulfoxide [6]. Li reported application of DMSO as a methylthiolating reagent in organic synthesis [7]. However, an electrophilic activator is needed to activate DMSO/DMSO-d6 including acetic anhydride, oxalyl chloride, methanesulfonic anhydride, tosyl chloride and thionyl chloride. Due to above limits, many activators are not suitable for substrates sensitive to acidic condition such as DMSO/SOC_{l2}-mediated synthesis of thiomethylnaphthalene from propargyl alcohol, oxysulfenylation of alkene with dimethyl sulfoxide/oxalyl chloride, and 3-Methylthioindole via intramolecular cyclization of 2-alkynylaniline mediated by DMSO/DMSO-d6 and SOCl2.

Trichloro triazine (TCT) is well-known reagent in activation of DMSO due to environmental friend, mild nature, and commercial availability [11-13]. Ma achieved Beckmann rearrangement of ketoxime promoted by cyanuric chloride and dimethyl sulfoxide [14]. Kochanowska-Karamian obtained marine indole alkaloids as potential drug leads for control of depression and anxiety [15]. Sugahara researched palladium-catalyzed amination of aryl sulfides with anilines [16]. In addition, considering synthetic utilization of sulfenyl [17], Zhang discussed divergent synthesis of 2-methylthioindole and 2-unsubstituted indole derivatives mediated by SOCl2 and dimethyl/diethyl sulfoxides [18]. As powerful and straightforward strategy leading to 3-sulfenylindoles, there were also Mersin's synthesis of N-alkyl-3-sulfonylindoles and N-alkyl-3-sulfanylindoles by cascade annulation of 2-alkynyl-N, N-dialkylamines and Zhang's formation of Rascal in an interrupted pamperer reaction mediated by hypervalent iodine(III) reagent [19,20]. Thereby sulfonium salts were proved to be versatile intermediates generated from activation of DMSO by TCT.

Under this background, many progresses have been reported in recent years. There is construction of 4-(methylation) isochromosomes skeleton through regioselective intramolecular cyclization of 2-alkynylbenzoate by an [21], halogen and chalcogen cation pools stabilized by DMSO of Adhikari [22], intramolecular tetracyclization/fluorom ethylthiolation of alkynes by Li and synthesis of 3-methylthio-benzo[b]furans/thiophenes via intramolecular cyclization of 2-alkynylanisoles/sulphones of Zhang

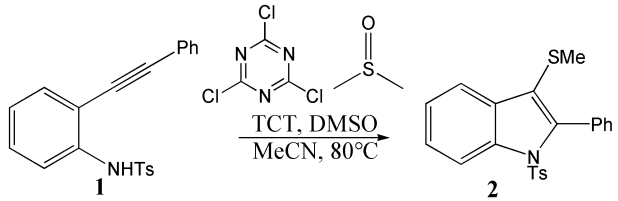
[23,24]. The latest breakthrough was Xing's dialkylation and regioselective intramolecular cyclization cascade of 2-alkylnylaniline mediated by TCT-DMSO [25]. Although 3-methylthiolated indole was synthesized, how dimethyl alkoxysulfonium salt was afforded via treatment of DMSO with TCT? What's the concrete process to generate methyl sulfonium electrophile equivalent stabilized by DMSO? How electrophilic addition to triple bond of 2-alkynylaniline occurred, accompanied by nucleophilic attack of amine group in concerted pathway through deprotonation and DMSO release delivering final product?

2 Computational details

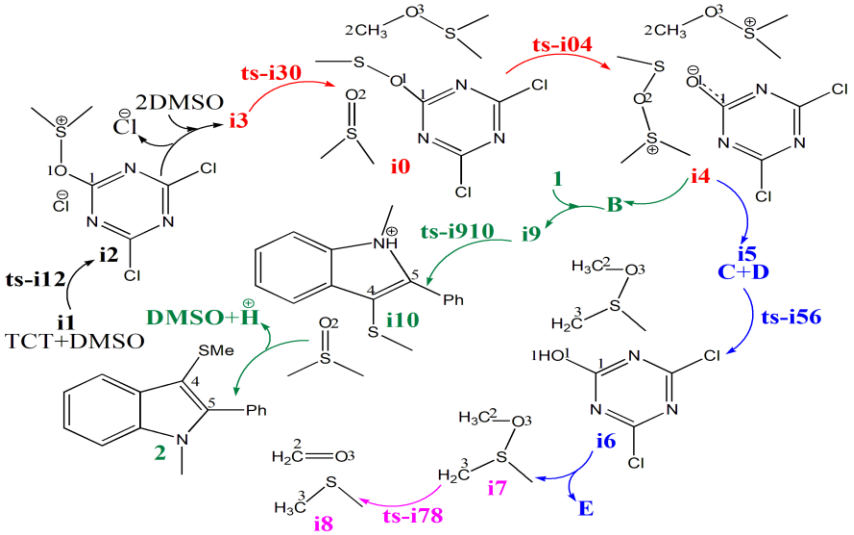
Structures were optimized at M06-2X/6-31G(d) level with GAUSSIAN09 [26]. Among various DFT methods [27], M06-2X functional has smaller deviation between experimental and calculated value than B3LYP hybrid functional [28,29]. With 6-31G(d) basis set, it can provide best compromise between time consumption and energy accuracy. It was also found to give accurate results for stepwise (2 + 2) cycloaddition, enantioselective (4 + 3) and Diels−Alder reaction [30,31]. Together with good performance on noncovalent interaction, it is suitable for this system [32-34]. To obtain zero-point vibrational energy (ZPVE), harmonic frequency calculations were carried out at M06-2X/6-31G(d) level gaining thermodynamic corrections at 353 K and 1 atm in acetonitrile (CH3CN). At M06-2X/6-311++G(d,p) level, the solvation-corrected free energies were obtained using integral equation formalism polarizable continuum model (IEFPCM) [35-39] on M06-2X/6-31G(d)-optimized geometries. NBO procedure was performed with Natural bond orbital (NBO3.1) obtaining lone pair and bond to characterize bonding orbital interaction and electronic properties [40-42]. Using Multiwfn_3.7_dev package [43].

3 Results and Discussion

The mechanism was explored for TCT-DMSO-catalyzed dialkylation and regioselective intramolecular cyclization cascade of 2-alkylnylaniline 1 to access 3-methylthiolated indole 2 (Scheme 1). As illustrated by Scheme 2, first, a dimethyl alkoxysulfonium salt was afforded upon treatment of DMSO with TCT after removal of one chloride ion. Then, with further addition of two DMSO, this species was converted to complex binding DMSO-stabilized methyl sulfonium electrophile equivalent along with methoxy sulfonium salt and TCT derivative. Next, a proton trapping occurred between the latter two followed by dissociation of methoxy sulfonium salt into dimethyl sulfide DMS and formaldehyde. Finally, via concerted path, the electrophilic addition of DMSO-stabilized methyl sulfonium to triple bond of 2-alkynylaniline 1 took place accompanied by nucleophilic attack of amine group leading to final product 3 methyl thiolated indole 2 together with recovered DMSO and a proton release. Figure 1 listed schematic structures of optimized TSs in Scheme 2. Table 1 gave activation energy for all steps.



Scheme 1: TCT-DMSO-catalyzed dialkylation and regioselective intramolecular cyclization cascade of 2-alkylnylaniline 1 to build 3-methylthiolated indole 2.



Scheme 2: Proposed reaction mechanism of TCT-DMSO-catalysed dialkylation and regioselective intramolecular cyclization cascade of **1** to **2**. TS is named according to the two intermediates it connects.

3.1 Dimethyl alkoxysulfonium and 2DMSO addition

The first complex i1 binding DMSO and TCT is formed as starting point of step 1, from which the activation energy is 15.0 kcal mol−1 via ts-i12 exothermic by -0.8 kcal mol−1 producing i2 (black dash line of Figure 1). Upon treatment of DMSO with TCT, a dimethyl alkoxysulfonium salt A was afforded after removal of one chloride ion. The transition vector corresponds to closure of O1 of DMSO to C1 of TCT as O1···C1 and cleavage of C1-Cl single bond as well as stretching of S-O1 from double to single (1.56, 1.9, 1.58 Å). Once O1-C1 is bonded in A, the positive charge is located on S ready for next step.

Then, the intermediate i3 binding additional two DMSO and A is taken as new starting point of next two steps (red dash line of Figure 1). The first DMSO attack occurs via ts-i30 with increased activation energy of 28.4 kcal mol−1 in step 2. The transition vector is complicated involving breaking of S1···C2, linkage of C_2···O_3 and resultant elongation of S2···O3 from double to single (2.28, 1.98, 1.55 Å) (Figure S1a). The

methoxy sulfonium salt C is generated in resultant intermediate i0 with typical S_2-O_3 single bond.

Subsequently, the second DMSO attack takes place from i0 via ts-i04 in step 3 with mediate activation energy of 10.4 kcal mol−1 exothermic by -2.2 kcal mol−1. It is noticeable to see the transfer of SMe from O1 to O_2 from detailed atomic motion of transition vector denoted as O1···S1···O2 along with S_3···O_2 weakened from double to single (1.94, 2.27, 1.54 Å). Once S1-O2 single bond is formed, the positive charge is transferred to S3 of DMSO-stabilized methylsulfenium electrophile equivalent B and negative charge on O1 of TCT derivative D.

TS	$\Delta G^{\neq}_{gas}$	$\Delta G^{\neq}_{sol}$
ts-i12	22.1	15.0
ts-i30	28.5	28.4
ts-i04	9.7	10.4
ts-i56	11.2	20.5
ts-i78	11.9	9.3
ts-i910	9.8	10.0

Table 1: The activation energy (in kcal mol^{-1}) of all reactions in gas and solvent

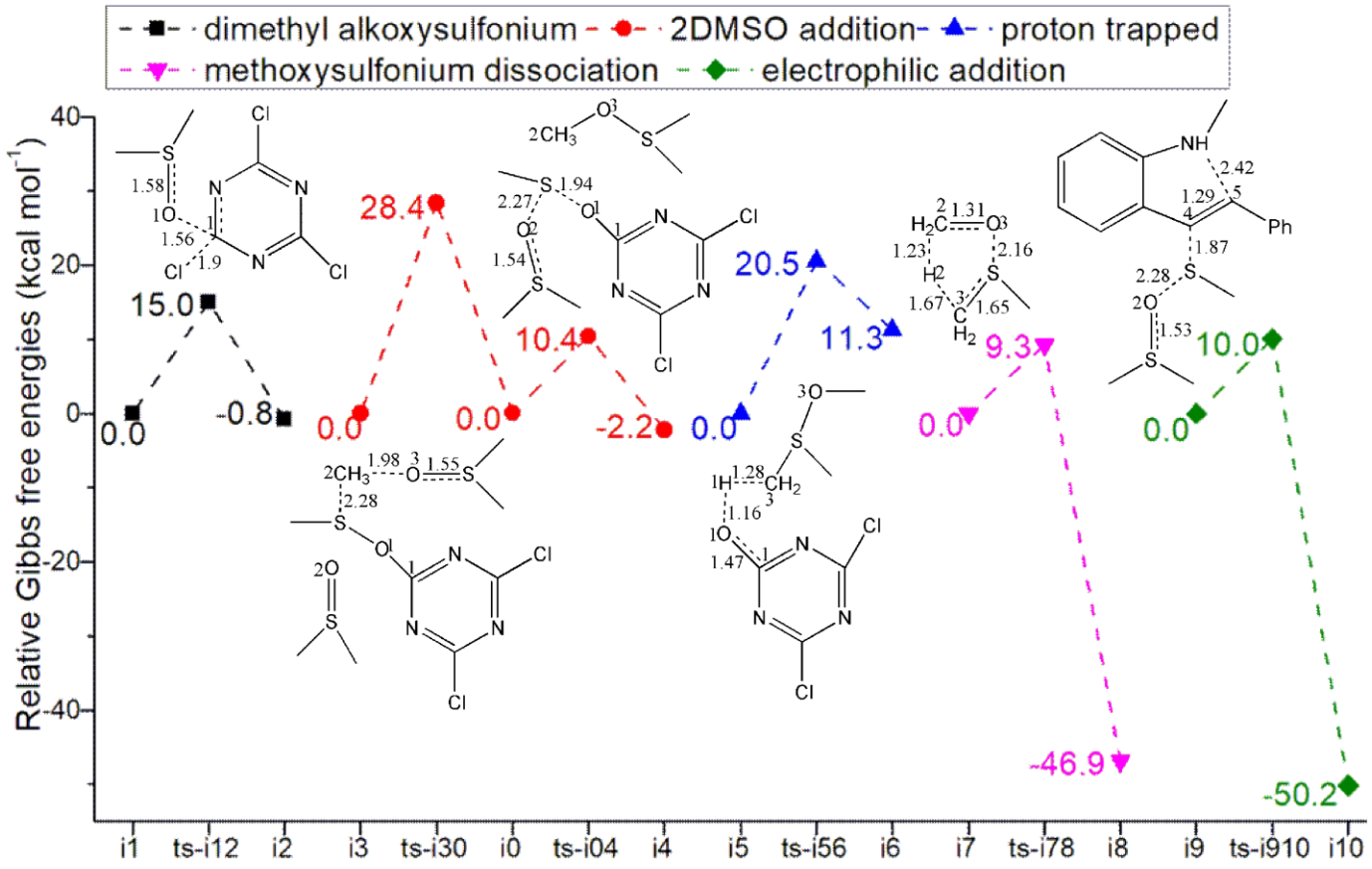


Figure 1: Relative Gibbs free energy profile in solvent phase starting from complex i1, i3, i5, i7, i9 (Bond lengths of optimized TSs in Å).

3.2 Proton trapption, methoxysulfonium dissociation, electrophilic addition of 2-alkynylaniline

Next, involving positive S2 of methoxysulfonium salt C and negative O1 of TCT derivative D, a neutral intermediate i5 is given as new starting point of step 4. A proton trapption proceeds between C and D via ts-i56 with activation energy of 20.5 kcal mol−1 endothermic by 11.3 kcal mol−1 giving intermediate i6 (blue dash line of Figure 1). The transition vector suggests facile proton H1 transfer from methyl C_3 to O1 affording methylene and hydroxyl of TCT derivative E. After release E, i6 converts to i7 for the following frocess. (1.28, 1.16 Å) (Figure S1b).

From i7, the dissociation of methoxysulfonium salt undergoes via ts-i78 with decreased activation energy of 9.3 kcal mol−1 exothermic huge by -46.9 kcal mol−1 in step 5 (magenta dash line of Figure 1). The transition vector is multiple not only including proton shift via C_2···H_2···C_3 but breaking down of S2···O_3, contraction of C2-O3 from single to double (1.23, 1.67, 2.16, 1.31 Å) (Figure S1c). Therefore, the stable intermediate i8 is obtained binding dimethyl sulfide DMS and formaldehyde CH_2O.

Finally, the 2-alkynylaniline 1 and DMSO-stabilized methylsulfenium B forms i9 as new starting point of step 6. The electrophilic addition of B to triple bond of 1 takes place via ts-i910 with reduced activation energy of 10.0 kcal mol−1 exothermic by -50.2 kcal mol−1 accompanied by nucleophilic attack of amine group in concerted mode yielding i10 (olive dash line of Figure 1). The transition vector contains bonding of S to alkyne C_4, breaking of S···O_2 and concerted nucleophilic addition of N to alkyne C_5, stretching of C_4-C_5 from triple to double (2.28, 1.87, 2.42, 1.29

Å) (Figure S1d). The 5-membered aza-ring closure is achieved in last i10 with typical C_5-N single, C_4=C_5 double bond. The product 3 methylthiolated indole 2 is yielded together with a released proton and recovered DMSO. Comparatively, the first DMSO attack dimethyl alkoxysulfonium salt in step 2 is determined to be rate-limiting for TCT-DMSO-catalyzed thioalkylation and intramolecular cyclization cascade producing3-methylthiolated indole.

4 Conclusions

In summary, the first theoretical investigation was provided by our DFT calculation on TCT-DMSO-catalyzed thioalkylation and regioselective intramolecular cyclization cascade of 2-alkylnylaniline. The dimethyl alkoxysulfonium salt was afforded upon treatment of DMSO with TCT after removal of one chloride ion. Then, with additional two DMSO, this species was converted to DMSO-stabilized methylsulfenium electrophile equivalent, methoxysulfonium salt and TCT derivative via two steps. Next, a proton trapption occurred between the latter two followed by dissociation of methoxysulfonium salt into dimethyl sulfide DMS and formaldehyde CH_2O. Finally, the electrophilic addition of DMSO-stabilized methylsulfenium to triple bond of 2-alkynylaniline took place accompanied by nucleophilic attack of amine group leading to product 3 methylthiolated indole together with recovered DMSO and a released proton in concerted mode. The first DMSO attack dimethyl alkoxysulfonium salt in step 2 is determined to be rate-limiting. Electronic Supplementary Material

Supplementary data available: [Computation information and cartesian coordinates of stationary points; Calculated relative energies for the ZPE-corrected Gibbs free energies (ΔG_{gas}), and Gibbs free energies (ΔG_{sol}) for all species in solution phase at 353 K.

Species	ΔG_{gas}	$\Delta G_{sol(CH3CN)}$
tct+dmso	0.00	0.00
i1	-12.49	-7.07
ts-i12	9.59	7.89
i2	-0.25	-7.88
tct+dmso-cl	0.00	0.00
A	106.40	-5.64
tct+3dmso-cl	0.00	0.00
i3	51.86	-33.60
ts-i30	80.31	-5.21
i0	59.74	-33.55
ts-i04	69.48	-23.19
i4(B+C+D)	49.96	-35.81
C+D	0.00	0.00
i5	-89.22	-6.38
ts-i56	-77.98	14.16
i6	-79.96	4.89
C+D-E	0.00	0.00
i7	-72.24	13.47
ts-i78	-60.37	22.72
i8(dms+hcho)	-116.71	-33.38
B+1	0.00	0.00
i9	-18.89	-6.92
ts-i910	-9.13	3.13
i10	-61.25	-57.11
B+1-dmso-h	0.00	0.00
2	-145.83	-95.12

Table S1: Calculated relative energies (all in kcal mol^{-1}, relative to isolated species) for the ZPE-corrected Gibbs free energies (ΔG_{gas}), Gibbs free energies for all species in solution phase (ΔG_{sol}) at 353 K by M06-2X/6-311++G(d,p)//M06-2X/6-31G(d) method and difference between absolute energy.

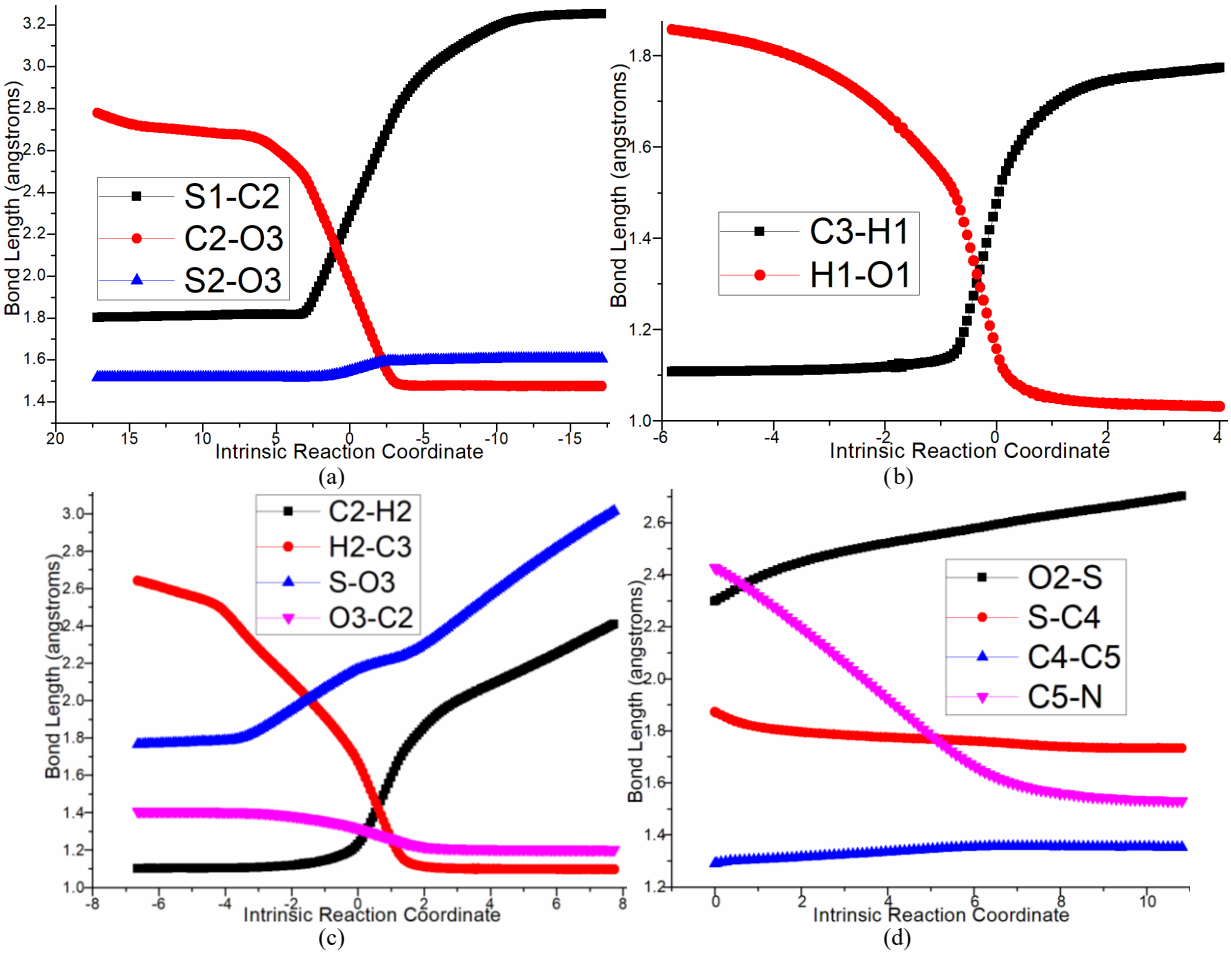


Figure S1: Evolution of bond lengths along the IRC for (a) ts-i30 (b) ts-i56 (c) ts-i78 (d) ts-i910 at M06-2X/6-311++G(d,p) level.

TS	$\Delta G^{\neq}_{gas}$	$\Delta G^{\neq}_{sol}$
ts-i12 (70i)	22.1	15.0
ts-i30 (511i)	28.5	28.4
ts-i04 (152i)	9.7	10.4
ts-i56 (738i)	11.2	20.5
ts-i78 (688i)	11.9	9.3
ts-i910 (187i)	9.8	10.0

Table S2: The activation energy (local barrier) (in kcal mol−1) of all reactions in the gas, solution phase calculated with M06-2X/6-311++G(d,p)//M06-2X/6-31G(d) method.

Author contributions: Conceptualization, Nan Lu; Methodology, Nan Lu; Software, Nan Lu; Validation, Nan Lu; Formal Analysis, Nan Lu; Investigation, Nan Lu; Resources, Nan Lu; Data Curation, Nan Lu; Writing-Original Draft Preparation, Nan Lu; Writing-Review & Editing, Nan Lu; Visualization, Nan Lu; Supervision, Nan Lu; Project Administration, Nan Lu. All authors have read and agreed to the published version of the manuscript.

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Conflict of interest: The authors declare no conflict of interest.

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