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Theoretical Investigation on DABCO-Mediated aza-Michael Reaction of Sulfonyli-Minoindoline and α,β-Unsaturated Aldehyde to Construct 3-Sulfonyl α-Carboline

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Abstract

The first theoretical investigation on DABCO-mediated aza-Michael reaction of sulfonyli-minoindoline and α,β-unsaturated aldehyde was provided by our DFT calculation. First, 2-aminotosyl indole is given in equilibrium with 2-sulfonamidoindoline via deprotonation with the help of DABCO. Then, it undergoes aza-Michael reaction with α,β-unsaturated aldehyde to form transient carbanion. The ring closure occurs leading to four-membered transient 1,2-thiazetidine, from which the sulfonyl moiety is recovered along with ring opening to release tension. Next, the intramolecular aldol-type reaction proceeds through nucleophilic attack of indole moiety onto aldehyde group followed by proton transfer giving carboannulated product and new hydroxyl group. At last, the final product 3-sulfonyl α-carboline is furnished through dehydration and oxidation. Comparatively, the dehydration is determined to be rate-limiting.

Keywords: DABCO; aza-Michael; Sulfonyl Migration; Intramolecular Aldol; 3-Sulfonyl α-Carboline

Introduction

Among heterocyclic compounds, α-Carbolines display numerous biological activities and various applications in natural product synthesis [1, 2]. Hung reported synthesis of α-and δ-carbolines by sequential Pd-catalyzed site-selective C–C and twofold C–N coupling reaction [3]. The neocryptolepine is especially used in treatment of infectious diseases and malaria [4]. In addition, sulfonyl moiety is crucial to improve physicochemical properties in pharmacophores [5]. Therefore, many progresses have been achieved in synthesis of α-carbolines and sulfonyl derivatives. For instance, Chatterjee explored perspectives on metal-catalysed syntheses of carbolines (α/β/γ/δ) [6]. Li obtained synthesis of carboline derivatives using domino annulation strategies [7]. Zhang discovered synthesis strategies for *A*-, *B*-, *Γ*- and δ-carbolines [8]. There were also lew-is-base dependent (3+3) annulations of acetoxy allenoates with iminoindolines of Debnath and divergent reactivity of δ- and B′-acetoxy allenoates with 2-sulfonamidoindoles *via* phosphine catalysis to enter dihydro-α-carboline, and spiro-cyclopentene motifs [9, 10]. Although several methods are available for accessing α-carbolines, reports on synthesis of sulfonyl carbolines are relatively rare.

In this field, Zhang exploited visible-light-induced oxidative cyclization of N-propargylanilines with sulfinic acids to 3-sulfonated quinoline derivatives [11]. Yuan researched synthesis of 3-sulfonylquinolines by visible-light promoted metal-free cascade cycloaddition involving N-prop-argylanilines and sodium sulfinates [12]. Recently, tosyl migration reactions emerged as efficient and alternative strategy in construction of sulfonated heterocycles. Gharpure summarized harnessing Gold(I)-catalyzed hydroamination/1,3-sulfonyl migration cascade for divergent synthesis of isoxazolidine and isoxazoline from O-alkynyl hydroxylamine and TMSOTf-mediated aminocyclization of N-homopropargyl hydroxylamines for stereoselective synthesis of 3-sulfonyl cyclic nitrones [13, 14]. Joseph gave recent advances in catalytic synthesis of arylsulfonyl compounds. Sundaravelu found metal-catalyzed C–S bond formation using sulfur surrogates [15, 16]. The interest is continued in recent years such as Palladium-catalyzed benzannulations of 1-(Indol-2-Yl)but-3-Yn-1-Ols as easy access to functionalized carbazoles, Gold(I)-catalyzed, iodonium monochloride-mediated carboannulations of indole/benzofuran-based acetylenic substrates and Palladium(0)-catalyzed heteroannulations of allenamides to δ-carbolines, benzofuro[3,2- b]Pyridines [17-20].

In view of bis-α-carbolines important in bioactive alkaloids [21], another breakthrough of Das

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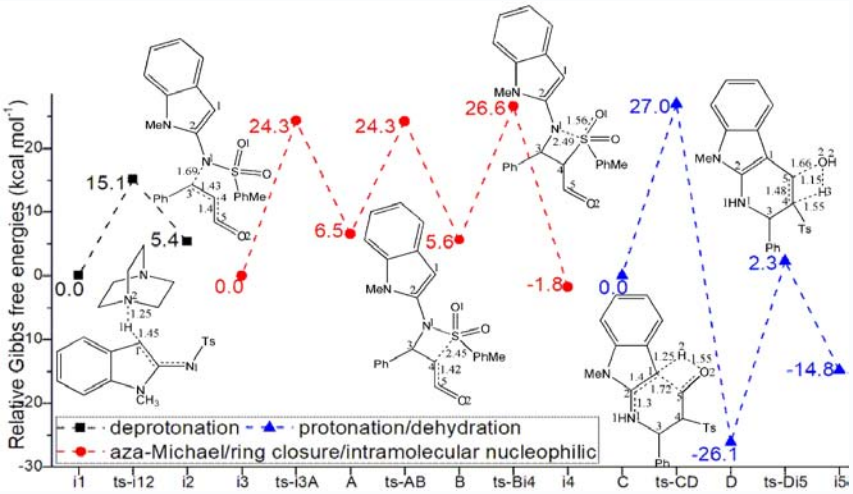


Figure 1: Relative Gibbs free energy profile in solvent phase starting from complex i1, i3, C (Bond lengths of optimized TSs in Å).

group was DABCO-mediated aza-Michael reaction of sulfonyli-minoindoline and *α,β*-unsaturated aldehyde in aprotic solvent (DMF) at 150°C [22]. Although 3-sulfonyl-*α*-carboline was constructed as major product, how DABCO triggered N to C migration of the tosyl group? Why 2-aminotosyl indole was in equilibrium with 2-sulfonamidoindoline assisted by base [23]? How intramolecular nucleophilic attack on the sulfonyl moiety may form an adduct via transient 1,2-thiazetidine intermediate [24]? What's the concrete process of intra-molecular aldol-type reaction through nucleophilic attack by C3 of indole moiety onto the aldehyde group [25]? This approach avoids toxic metal catalyst/reagents and uses simple/low-cost substrates. Why carboline is yielded exclusively if the reaction was carried out in MeOH at 110°C?

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 423 K and 1 atm in n,n-dimethylformamide (DMF). 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].

Results and Discussion

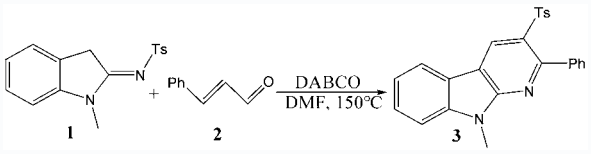
The mechanism was explored for DABCO-mediated aza-Michael reaction of sulfonyli-minoindoline 1 and *α,β*-unsaturated aldehyde 2 leading to 3-sulfonyl *α*-carboline 3 (Scheme 1). As illustrated by Scheme 2, initially, 2-aminotosyl indole is given in equilibrium with 2-sulfonamidoindoline 1 *via* deprotonation with the help of DABCO. Then it undergoes aza-Michael reaction with *α,β*-unsaturated aldehyde 2 to form transient carbanion. The ring closure occurs leading to four-membered transient 1,2-thiazetidine, from which the sulfonyl moiety is recovered along with ring opening to release tension. Next, the intramolecular aldol-type reaction proceeds through nucleophilic attack of indole moiety onto the aldehyde group followed by proton transfer leading to carboannulated product and new hydroxyl group. At last, the final product 3-sulfonyl α-carboline 3 is furnished through dehydration and oxidation. Figure 1 listed schematic structures of optimized TSs in Scheme 2. Table 1 gave activation energy for all steps.

Deprotonation/aza-Michael/intramolecular nucleophilic attack/ring opening

Initially, the first complex i1 is formed as starting point of step 1 binding DABCO and 2-sulfonamidoindoline 1 (black dash line of Figure 1). With the help of DABCO, 1 was deprotonated *via* ts-i12 with the activation energy of 15.1 kcal mol^{-1} endothermic by 5.4 kcal mol^{-1} resulting in i2. The transition vector corresponds to leaving of H1 from C1 to N2 as C1···H1···N2 (1.45, 1.25 Å) (Figure S1a). Once proton H1 is captured by N of DABCO denoted as BH+, the 2-aminotosyl indole 1' is given in equilibrium with 1 participated in next step, where the double bond is shifted on C1-C2 and negative charge is located on N1.

After removal of pronated DABCO, the assemble of *α,β*-unsaturated aldehyde 2 and 1' makes i3 as new starting point of following process (red dash line of Figure 1). Then aza-Michael reaction takes place via ts-i3A with increased activation energy of 24.3 kcal mol^{-1} in step 2 endothermic slightly by 6.5 kcal mol^{-1} to form transient carbanion A. The transition vector suggests nucleophilic addition of negative N1 to possitive C3 and the resultant stretching of C3···C4, shortening of C4···C5 (1.69, 1.43, 1.4 Å). When the typical single bond is formed on N1-C3, the negative charge is transferred on C4 in A.

Subsequently from A, the ring closure occurs via intramolecular nucleophilic attack of negative C4 to S, which not only generates four-membered transient 1,2-thiazetidine B but also makes *π* electron on double bond S=O1 positioned on O1. *via* ts-AB in step 3, the activation energy is decreased to 17.7 kcal mol^{-1} endothermic by 5.6 kcal mol^{-1}. The transition vector contains closing of C4 to S



Scheme 1: DABCO-mediated aza-Michael reaction of sulfonyli-minoindoline 1 and *α,β*-unsaturated aldehyde 2 leading to 3-sulfonyl α-carboline 3.

and elongation of sulfonyl moiety S=O1. Therefore, B is obtained with typical single bond C4-S and S-O1 after completion of this step. Obviously, B is also reactive with strained tetracyclic ring to initiate next step.

Next, the sulfonyl moiety of B is recovered as S=O1 via ts-Bi4 with activation energy of 21.0 kcal mol^{-1} exothermic by -1.8 kcal mol^{-1} affording adduct intermediate i4. Seen from the transition vector, the atomic motion is about contraction of S···O1 from single to double and breaking down of S···N1 (1.56, 2.49 Å). The release of tension makes i4 stable owing to ring-opening on S-N1. The negative charge is also shifted on N1, which is therefore readily to accept proton returned from pronated DABCO. The neutral complex C is obtained ready for the following process.

Intramolecular aldol-proton transfer/dehydration

C is taken as new starting point of next two steps (blue dash line of Figure 1). The intramolecular aldol-type reaction proceeds *via* ts-CD with increased activation energy of 27.0 kcal mol^{-1} in step 5 exothermic by -26.1 kcal mol^{-1} leading to carboannulated product D. The transition vector reveals a complicated concert process (Figure S1b). In addition to nucleophilic attack by C1 of indole moiety onto C5 of aldehyde group as C1···C5, the second proton H2 is transferred from C1 to O2 as C1···H2···O2 (1.72, 1.25, 1.55 Å). The complex D is stable six-membered ring involving typical C1-C5 single bond, novel O2H2 hydroxyl group and double bond C1=C2 remain unchanged.

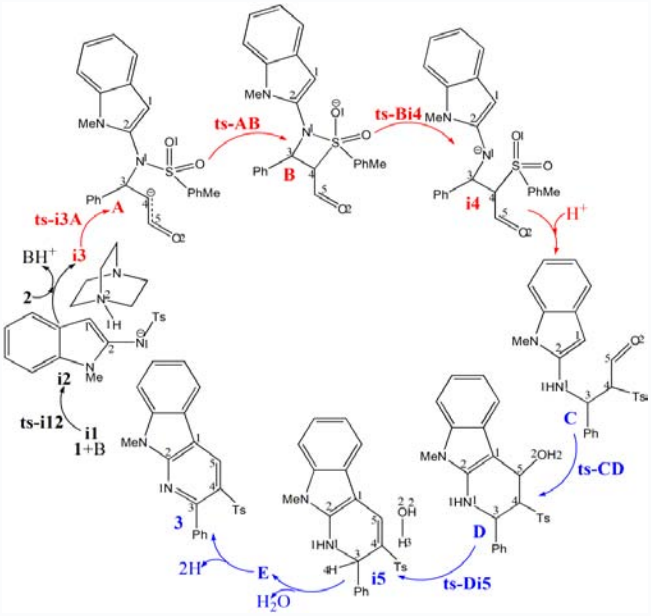
At last, the dehydration takes place via ts-Di5 in step 6 with activation energy of 28.4 kcal mol^{-1} exothermic by -14.8 kcal mol^{-1} giving i5. The transition vector is about cleavage of C4···H3, C5···O2, linkage of H2O2···H3 and shortening of C4···C5 (1.55, 1.66, 1.15, 1.48 Å) (Figure S1c). *Via* this step, not only a new water molucule is assembled and departured, but double bond is formed on C4=C5 in i5, from which the final product 3-sulfonyl *α*-carboline 3 is furnished through dehydrogenation oxidation on C3, N1. Comparatively, the dehydration of step 6 is determined to be rate-limiting for DABCO-mediated aza-Michael reaction of sulfonyli-minoindoline and *α,β*-unsaturated aldehyde to 3-sulfonyl *α*-carboline.

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

TS	$\Delta G^{\neq}_{gas}$	$\Delta G^{\neq}_{sol}$
ts-i12	13.31	15.14
ts-i3A	28.70	24.34
ts-AB	19.91	17.71
ts-Bi4	22.90	21.00
ts-CD	30.25	26.95
ts-Di5	33.17	28.42

Conclusions

In summary, the first theoretical investigation was provided by our DFT calculation on DABCO-mediated aza-Michael reaction of sulfonyli-minoindoline and *α,β*-unsaturated aldehyde. First, 2-aminotosyl indole is given in equilibrium with 2-sulfonamidoindoline via deprotonation with the help of DABCO. Then, it undergoes aza-Michael reaction with *α,β*-unsaturated aldehyde to form transient carbanion. The ring closure occurs leading to four-membered transient 1,2-thiazetidine, from which the sulfonyl moiety is recovered along with ring opening to release tension. Next, the intramolecular aldol-type reaction proceeds through nucleophilic attack of indole moiety onto aldehyde group followed by proton transfer giving carboannulated product and new hydroxyl group. At last, the final product 3-sulfonyl *α*-carboline is furnished through dehydration and oxidation. Comparatively, the dehydration of step 6 is determined to be rate-limiting.



Scheme 2: Proposed reaction mechanism of DABCO-mediated aza-Michael reaction of 1 and 2 leading to 3. TS is named according to the two intermediates it connects.

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 423 K.]

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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