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Research Article

Theoretical Investigation on HFIP-Catalyzed Diastereoselective (3+2) Annulation of Indolyl Alcohol and Bicyclobutane to Access Tetracyclic Spiroindolenine

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Abstract

The first theoretical investigation on HFIP-catalyzed (3+2) annulation of indolyl alcohol, bicyclobutane and trace water-promoted C−O bond formation between ketene, alkyl halide was provided by our DFT calculation. At first, the reaction is initiated under HFIP dual activation of two substrates via hydrogen bonding. The indumentum ion is generated from indolyl alcohol after removal of hydroxyl. Then, the converge with additional ester enolate proceeds via two paths. The stepwise sequence contains nucleophilic attack followed by intramolecular Friedel−Crafts alkylation and deprotonation yielding tetracyclic Spiro indolenine. The concerted process is (3+2) annulation to exocyclic double bond. For the second case, alcohol is initially generated from alkyl halide via SN2 path promoted by trace water. Subsequently, α,α-disubstituted ester is formed through nucleophilic attack on ketene in concerted mode. Comparatively, (3+2) annulation is rate-limiting for HFIP-catalyzed diastereoselective reaction. SN2 is rate-limiting for trace water-promoted C−O bond formation.

Keywords: (3+2) annulation; C−O bond formation; HFIP; ketene; Spiro indolenine

1.Introduction

As the most compact hydrocarbon ring, bicycle [1.1.0] butane (BCB) has gained much attention in synthetic chemistry with central C−C bond conferring substantial strain [1]. This strain enables diverse C−C bond cleavage involving ring-opening, insertion, annulation and molecular rearrangement just like the case of cyclopropane as ubiquitous structural motif in cycloaddition [2,3]. Among these, annulation was extensively explored since it provided much valuable bridged framework in organic synthesis. For instance, Boychik obtained fluor-substituted bicycle [1.1.1] pentane (BCP) [4]. Tang reported silver-catalyzed dearomatize [2π+2σ] cycloaddition of indole with bicyclobutane to access induline fused bicycle [2.1.1] hexane [5]. Hu discovered Lewis's acid-catalyzed formal cycloaddition between silyl enol ether and bicycle [1.1.0] butane [6]. Tang gave enantioselective (4 + 3)/thia-(3 + 2) cycloaddition of bicyclobutane and examination via divergent synthesis of bridged sulfur heterocycle [7]. There was formal [2π+2σ] cycloaddition of para-quinone methide with bicycle [1.1.0] butane, 1,3-dipolar cycloaddition of bicyclobutane with isagoge to tetracyclic 2-oxa-3-azabicyclo [3.1.1] heptane and palladium-catalyzed decarboxylative (4 + 3) cycloaddition to 2-oxabicyclo [4.1.1] octane [8-10].

In this field of related structure [11], BCH is well-known for synthetic chemists owing to potential as bio isostere of meta- and para-substituted arene. Mykhailiuk demonstrated where to go next in saturated bio isosteres of benzene [12]. Levertov explored water-soluble non-classical benzene mimetics [13]. Denisenko researched saturated bio isosteres of ortho-substituted benzenes [14]. Then they found 2-oxabicyclo [2.1.1] hexanes as saturated bio-isosteres of the ortho-substituted phenyl ring [15]. This progress improves the pharmacokinetic and physicochemical properties of bioactive molecules. BCH is categorized into all-carbon, spiro-containing, and heteroatom-substituted frameworks structurally. Recently, there emerged enantioselective strategies for all-carbon BCHs such as intermolecular [π2+σ2] photocycloaddition reactions of 2(1H)-quinolones, bicycle [1.1.0] butanes and divergent access to chiral compounds from α, β-unsaturated ketones [16,17]. With various utility, hexafluoro isopropanol (HFIP) is effective in activating BCB with α-cyano chalcone or α-halo hydroxamate to access functionalized Spiro cyclobutene by Shajahan [18-20].

Under this background, many progresses have been made by Biju group. They identified indolyl alcohols effectively trapped by nucleophiles in generating olefins [21]. They presented Spiro indolenine derivatives as key motifs in natural products and pharmaceutical molecules [22]. The chiral phosphoric acid catalysis was employed with N-unsubstituted indolyl alcohols by Studer's group [23]. Notably, the latest breakthrough was HFIP-promoted (3+2) annulation of BCBs with indolyl alcohols [24] and trace water-promoted C−O bond formation between ketene, alkyl halide synthesizing α,α-disubstituted ester [25]. Although spiro-BCH was

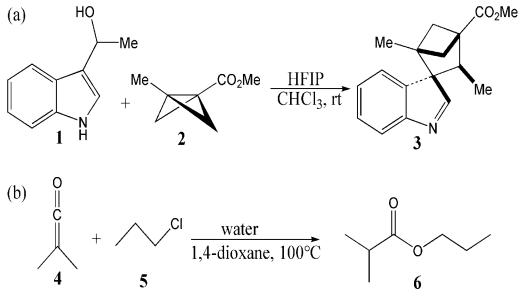
synthesized in highly diastereoselective manner over expected tetracyclic indole, how indumentum ion was generated under activation of HFIP? Why stepwise nucleophilic attack, intramolecular Friedel−Crafts alkylation was competitive with concerted (3+2) annulation? What's the concrete process to afford α,α-disubstituted ester via water-promoted SN2 and nucleophilic attack?

2 Computational details

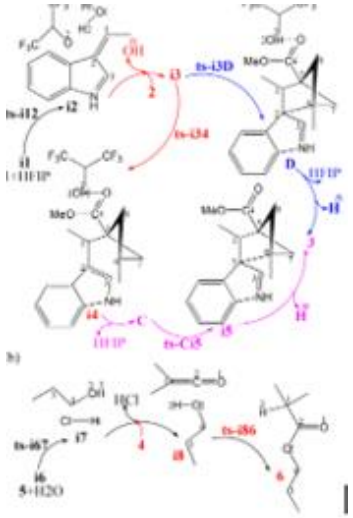
Structures were optimized at M06-2X/6-31G(d) level with GAUSSIAN09 [26]. Among various DFT methods [27], M06-2X functional has smaller deviation between experimental and calculated value than B3LYP hybrid functional [28,29]. With 6-31G(d) basis set, it can provide best compromise between time consumption 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 298, 398 K and 1 atm in acetonitrile, 1,4-dioxane. 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 HFIP-catalyzed (3+2) annulation of indolyl alcohol 1 and bicyclobutane 2 leading to tetracyclic Spiro indolenine 3 as well as trace water-promoted C−O bond formation between ketene 4 and alkyl halide 5 synthesizing α,α-disubstituted ester 6 (Scheme 1). As illustrated by Scheme 2, the reaction is initiated under HFIP activation of 1 and 2 via hydrogen bonding. First, indumentum ion A is generated from 1 after removal of hydroxyl. Then, the additional ester enolate B may converge via two plausible paths. In stepwise sequence, the nucleophilic attack of B on A affords intermediate C, which undergoes intramolecular Friedel−Crafts alkylation followed by deprotonation yielding spiro product 3. The concerted process is (3+2) annulation of B and exocyclic double bond of A. For the second case, initially, alcohol E is generated from alkyl halide 5 via SN2 path promoted by trace water. Subsequently, α,α-disubstituted ester 6 is formed through nucleophilic attack on ketene 4. Figure 1 listed schematic structures of optimized TSs in Scheme 2. Table 1 gave activation energy for all steps.



Scheme 1 (a) HFIP-catalyzed (3+2) annulation of indolyl alcohol 1 and bicyclobutane 2 leading to tetracyclic Spiro indolenine 3, (b) trace water-promoted C−O bond formation between ketene 4 and alkyl halide 5 synthesizing α,α-disubstituted ester 6.



Scheme 2: Proposed reaction mechanism of (a) HFIP-catalyzed (3+2) annulation of **1** and **2** to **3**, (b) trace water-promoted C−O bond formation between **4** and **5** to **6**. TS is named according to the two intermediates it connects.

3.1 Indumentum ion generation, nucleophilic attack, intramolecular F−C alkylation, (3+2) annulation

Two substrates are both activated by HFIP via hydrogen bonding to initiate the reaction. At first, the complex i1 binding 1 and HFIP is formed as starting point of step 1, from which indumentum ion A is generated via ts-i12 with the activation energy of 22.4 kcal mol−1 endothermic by 7.8 kcal mol−1 producing i2 (black dash line of Figure 1a). The transition vector corresponds to providing of proton H2 by HFIP to hydroxyl O1H1 of 1 to assemble water molecule as O2···H2···O1H1 along with breaking of C1···O1 single bond as well as O1H1···F H bonding (1.49, 1.04, 2.29, 2.55 Å) (Figure S1a). Once hydroxyl is removed in form of H2O with the help of HFIP, the positive in polonium ion A is afforded and reactive to converge with bicyclobutane 2.

The activation of 2 by HFIP via hydrogen bonding forms ester enolate B, the reaction of which with A may via two plausible paths. In stepwise sequence, the intermediate i3 binding A and B is taken as new starting point of next two steps. The nucleophilic attack of B on A occurs via ts-i34 with reduced activation energy of 18.8 kcal mol−1 endothermic by 10.3 kcal mol−1 in step 2 leading to intermediate i4 (red dash line of Figure 1a). The transition vector is complicated involving nucleophilic addition of C5 to C1 as C5···C1 single bond, and resultant cleavage of C5···C6 (2.21, 2.08 Å) (Figure S1b). Without HFIP, i4 turns to be complex C ready for the next step.

Subsequently, C undergoes intramolecular Friedel−Crafts alkylation with mediate activation energy of 6.9 kcal mol−1 via ts-Ci5 in step 3 exothermic by -10.1 kcal mol−1 giving i5 (magenta dash line of Figure 1a). It is noticable to see the approaching of C2 to C6 from atomic motion through simple transition vector denoted as C2···C6 to complete ring closure (2.58 Å). Owing to positive electron located on NH, the desired neutral spiro-BCH product 3 is readily to be yielded by deprotonation of i5.

Alternatively, the concerted process is also located via ts-i3D with higher activation energy of 26.2 kcal mol−1 than that of stepwise case via ts-i34 yet more exothermic by -17.4 kcal mol−1 leading to D (blue dash line of Figure 1a). The transition vector confirms this (3+2) annulation of B with exocyclic double bond of A. That not only includes dual bonding of C5···C1, C2···C6 but simulate stretching of C1···C2 from double to single and C5···C6 breaking down. D is a complex involving HFIP and desired spiro-BCH scaffold, from which product 3 is obtained after deprotonation. Given excellent disaster selectivity of 3 in experiment, the concerted manner is more favorable than stepwise case from thermodynamic perspective. Thus (3+2) annulation is determined to be rate-limiting for HFIP-catalyzed diastereoselective reaction of indolyl alcohol and bicyclobutane to tetracyclic spiroindolenin

TS	$\Delta G^{\neq}_{gas}$	$\Delta G^{\neq}_{sol}$
ts-i12	25.5	22.4
ts-i34	22.0	18.8
ts-i3D	28.4	26.2
ts-Ci5	10.1	6.9
ts-i67	28.8	23.4
ts-i86	10.7	12.2

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

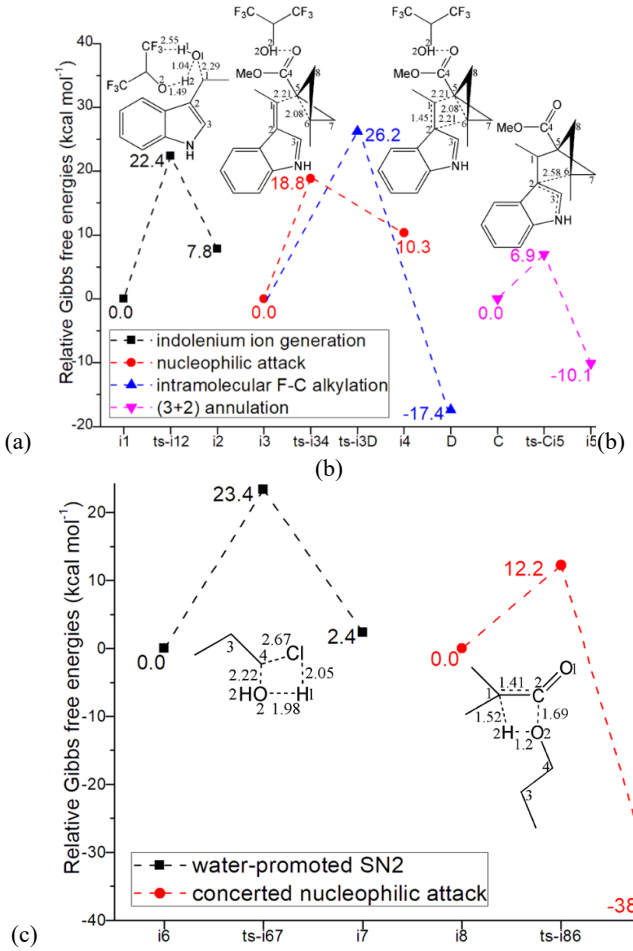


Figure 1: Relative Gibbs free energy profile in solvent phase starting from complex (a) **i1**, **i3**, **C** (b) **i6**, **i8** (Bond lengths of optimized TSs in Å).

3.2 Trace water-promoted SN2 and concerted nucleophilic attack

The metal-free C−O bond formation was also described from reactive ketene 4 and alkyl halide 5 mediated by trace water. Initially, 5 and water

forms intermediate i6, from which typical SN2 path takes place via ts-i67 with activation energy of 23.4 kcal mol−1 endothermic by 2.4 kcal mol−1 affording intermediate i7 in step 1 (black dash line of Figure 1b). From the transition vector, water is functioned as separated hydroxyl and proton. Cl is replaced by hydroxyl via O2···C4···Cl then combines H as HCl molecule via O2···H1···Cl (2.22, 2.67, 1.98, 2.05 Å) (Figure S1c). Once C4-O2 single bond is available, alcohol E is generated from i7 after removal of HCl. Then additional ketene 4 and E assemble intermediate i8 as new starting point of step 2. The nucleophilic attack of E on 4 proceeds via ts-i86 in concerted mode with reduced activation energy of 12.2 kcal mol−1 exothermic huge by -38.1 kcal mol−1 yielding α,α-disubstituted ester 6 (red dash line of Figure 1b). The transition vector contains hydroxyl breaking via O2···H2, elongation of C1=C2 from double to single and concerted linkage of O2···C2, H2···C1 (1.2, 1.41, 1.69, 1.52 Å) (Figure S1d). The C1 turns to be sp3 hybrid together with formal ester bond C2-O2. Comparatively, trace water-promoted SN2 is determined to be rate-limiting for metal-free C−O bond formation of ketene and alkyl halide.

4 Conclusions

In summary, the first theoretical investigation was provided by our DFT calculation on HFIP-catalyzed (3+2) annulation of indolyl alcohol, bicyclobutane and trace water-promoted C−O bond formation between ketene, alkyl halide. For the first case, the reaction is initiated under HFIP dual activation of two substrates via hydrogen bonding. The indumentum ion is generated from indolyl alcohol after removal of hydroxyl. Then, the converge with additional ester enolate proceeds via two plausible paths. The stepwise sequence contains nucleophilic attack followed by intramolecular Friedel−Crafts alkylation and deprotonation yielding product tetracyclic Spiro indolenine. The concerted process is (3+2) annulation to exocyclic double bond. For the second case, initially, alcohol is generated from alkyl halide via SN2 path promoted by trace water. Subsequently, α,α-disubstituted ester is formed through nucleophilic attack on ketene in concerted mode. Given excellent diastereoselective, the concerted manner is more favorable than stepwise case from thermodynamic perspective. Thus (3+2) annulation is determined to be rate-limiting for HFIP-catalyzed diastereoselective reaction. Comparatively, trace water-promoted SN2 is rate-limiting for metal-free C−O bond formation.Electronic Supplementary Material

Supplementary data available: [Computation information and cartesian coordinates of stationary points; Calculated relative energies for the ZPE-corrected Gibbs free energies (Gags), and Gibbs free energies (Gol) for all species in solution phase at 298, 398 K.]

Species	Ga_{gs}	$Go_{l(Chloroform)}$
1+hp	0.00	0.00
i1	-9.10	-1.62
ts-i12	16.44	20.77
i2	-0.15	6.19
1-oh	0.00	0.00
A	4.67	2.46
2+hp	0.00	0.00
B	-13.87	-8.90
1+2+hp-oh	0.00	0.00
i3	8.35	10.56
ts-i34	30.39	29.39
ts-i3D	36.71	36.80
i4	21.33	20.89
D	-8.02	-6.81
1+2-oh	0.00	0.00
C	0.52	3.73
ts-Ci5	10.60	10.66
i5	-9.74	-6.37
1+2-oh-h	0.00	0.00
3	9.19	6.18
	Ga_{gs}	$Go_{l(1,4\text{-dioxane})}$
5+h2o	0.00	0.00
i6	-3.90	-1.84
ts-i67	24.91	21.51
i7	-1.02	0.52
5+h2o-hcl	0.00	0.00
E	6.99	7.61
5+h2o-hcl+4	0.00	0.00
i8	2.80	4.98
ts-i86	13.45	17.20

Table S1: Calculated relative energies (all in kcal mol-1, relative to isolated species) for the ZPE-corrected Gibbs free energies (ΔGgas), Gibbs free energies for all species in solution phase (ΔGsol) at 298, 398 K by M06-2X/6-311++G(d,p)//M06-2X/6-31G(d) method and difference between absolute energy.

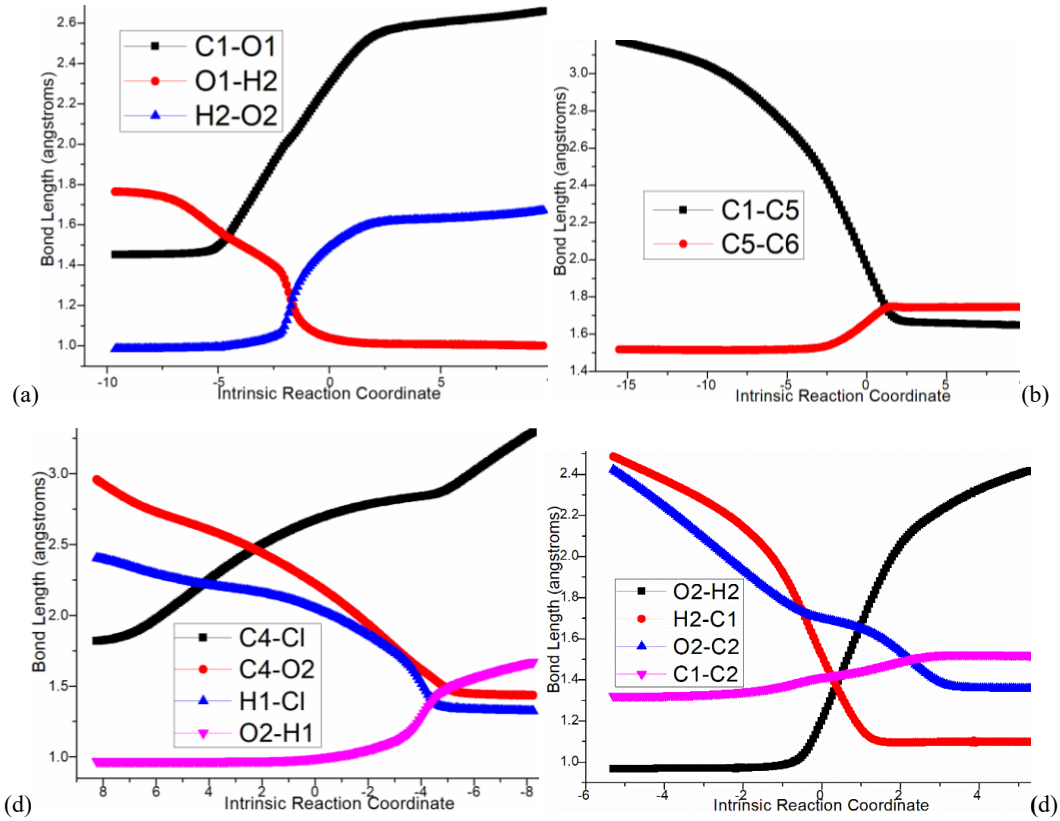


Figure S 1: Evolution of bond lengths along the IRC for (a) **ts-i12** (b) **ts-i34** (c) **ts-i67** (d) **ts-i86** at M06-2X/6-311++G(d,p) level.

TS	$\Delta G^{o}_{ga's}$	Ga^{s}_{ol}
ts-i12 (209i)	25.54	22.39
ts-i34 (333i)	22.04	18.83
ts-i3D (272i)	28.36	26.24
ts-Ci5 (174i)	10.08	6.93
ts-i67 (562i)	28.81	23.35
ts-i86 (1721i)	10.65	12.22

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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