A DFT Mechanistic Study on the Aza-Aldol Reaction of Boron Aza-Enolates: Relative Stability of Six-Membered Transition State and its Relevance to the Coordination Mode of the Leaving Group

Sho Miyakawa[1], Ray Miyazaki[1], Tomoya Miura[2,4], and Jun-ya Hasegawa[1,3,*]

[1] Institute for Catalysis, Hokkaido University, N21W10, Kita-ku, Sapporo 001-0021, Japan

[2] Department of Synthetic Chemistry and Biological Chemistry, Kyoto University, Katsura, Kyoto 615-8510, Japan

[3] Interdisciplinary Research Center for Catalytic Chemistry, National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8565, Japan

[4] Present address: Division of Applied Chemistry, Okayama University, Tsushimanaka 3-1-1, Okayama 700-8530, Japan

E-mail: hasegawa@cat.hokudai.ac.jp

Abstract

The mechanism of the aza-aldol reaction between boron aza-enolate and benzaldehyde is investigated using density functional theory calculations. The result shows that the *syn-E* isomer is preferentially formed, consistent with experimental observations. The six-membered ring transition state (TS) with the boat form leads to the *E* isomer, while more unstable chair TS does to the *Z* isomer. The preference of the *syn* isomer is determined by the interactions between the substituents of the aza-enolate and benzaldehyde. Structural distortion and intrinsic reaction coordinate analyses of simplified model systems provide insights into the origin of the relative stability of the rate-determining TS with boat and chair forms. The boat TS is an early TS; thus, minimal structural distortions of the reactant are required to reach this TS. The Lewis pair interactions between the boron and imine group during B-N elimination also influenced the relative stability of the TSs. This interaction involves the nitrogen lone-pair in the boat TS, while the π(N=C) orbital is involved in the chair TS. The Lewis pair with the lone-pair stabilizes the TS more than

that with the π orbital. The boron aza-enolate with 9-BBN generates an ate complex and forms C-C bonds sequentially, whereas that with Bpin does not generate an ate complex and exhibits the concerted formation of B-O and C-C bonds. Thus, the higher electrophilicity of boron such as 9-BBN enhances the reactivity by facilitating the formation of the ate complex. A reaction design is proposed to reverse the *syn*/*anti* selectivity. Proof-of-concept DFT calculations suggested that the modification of the imine group would change relative stability of the boat/chair TSs and give *anti*-product.

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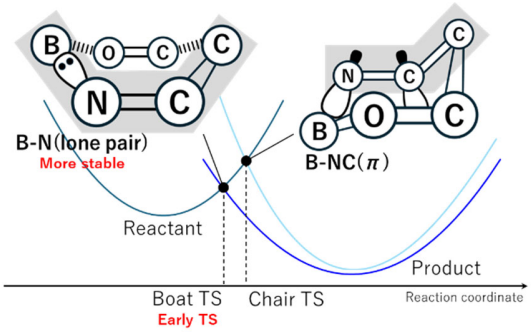

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A DFT study on aza-aldol reaction of boron aza-enolates. Relative stability of boat vs chair transition state, which determines diastereoselectivity, is relevant to the coordination mode of the leaving imine group.

1. Introduction

The aldol reaction with boron enolates enables the formation of carbon-carbon bonds in a highly diastereoselective manner and has been extensively studied.[1] One mechanistic study proposed a six-membered ring transition state (TS) in the chair conformation,[2] and a reaction that proceeds through a chair-type TS was designed using calculations based on the classical force field.[3] Conversely, ab initio MO calculations showed that the boat-type TS was the most stable, whereas the chair-type TS was slightly unstable.[4] A force field development was conducted based on this result.[5] Density functional theory (DFT) calculations subsequently showed that the boat-type TS is energetically favorable, however, the chair-type TS is similar in energy.[6] The TS structure is determined by the interactions in the stereoisomers of the enolate.[2, 7] Because diastereoselectivity depends on the TS, theoretical analysis of the TSs has been an essential tool in mechanistic analysis.

Signifiant progress in the aza-aldol reactions of boron aza-enolates with aldehydes was reported in the earliest studies.[8] Boron aza-enolates are nitrogen analogs of boron enolates. A computational study was conducted for the TS structure in the reaction of N-ethenylboronamine (CH_2=CH-NH-BH_2) with formaldehyde at the MP2/6-31G* level based on the RHF/3-21G optimized structures.[8d] According to this study, an ate complex was initially generated by the interaction of the boron atom in the aza-enolate and the carbonyl oxygen of the aldehyde. The subsequent carbon-carbon bond-forming reaction can proceed by one of three six-membered ring TSs: a chair structure (Chair), a boat structure with a boron atom in the body of the boat (Boat-A), and a boat structure with a boron atom occupying the bow (Boat-B) (Figure 1). The Boat-A TS resulted in the lowest activation energy of the three TSs; however, fundamental mechanistic analysis for the boat/chair preference is still necessary. In addition, the origin of the diastereoselectivity should be discussed in terms of the interactions between the substituents at the pseudo-equatorial and pseudo-axial positions.

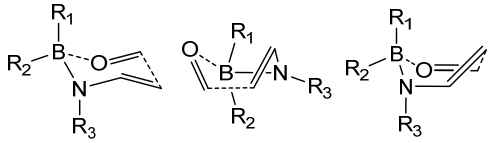
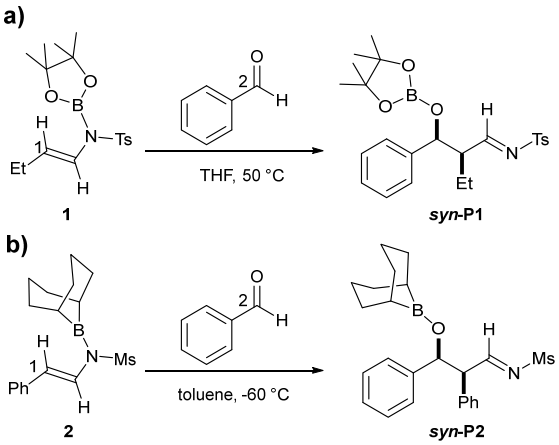


Figure 1. Three types of TS structures.

We recently reported a highly diastereoselective reaction of *N*-sulfonyl-1,2,3-triazoles with 9-borabicyclo[3.3.1]nonane (9-BBN–H) or 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (HBpin) in the presence of transition metal catalysts and aldehydes that proceeds via the generation of aza-enolates

(Scheme 1 and Scheme S1).[9] Based on a previous theoretical study[8d] and the stereoselectivity of these reactions, we considered that the reaction mechanism proceeds via a Boat-A type six-membered ring TS. However, a characteristic feature of our reaction is the presence of bulky substituents on the aldehyde and aza-enolate, which induce high stereoselectivity. Therefore, a realistic model with an asymmetric aza-enolate or aldehyde is required to investigate the reaction pathway. In addition, boron exhibits different reactivities in the 9-BBN–H and HBpin, used in our experiments. We sought to clarify the reasons for this difference with computational models (**1** and **2**) which have the same substituents as in our experiment.



Scheme 1. Aza-aldol reactions of a) HBpin-derived boron aza-enolate[9] and b) 9-BBN–H-derived boron aza-enolate.[10]

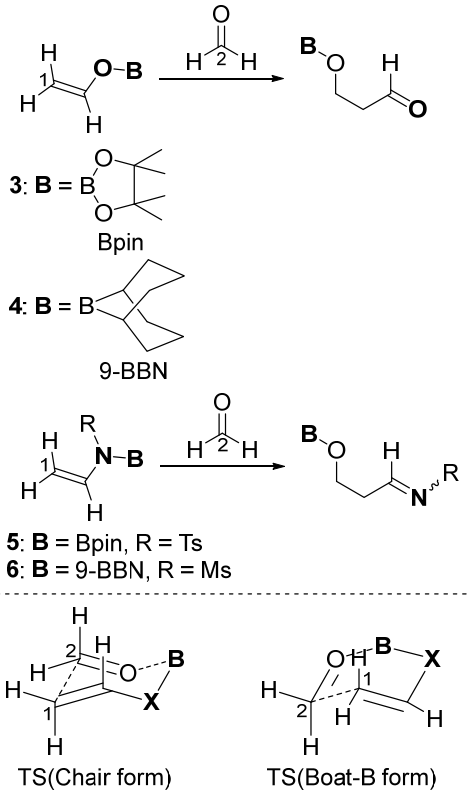
In this study, we elucidate the origin of the high diastereoselectivity of the aza-aldol reaction[9-10] with aza-enolates, **1** and **2**, with benzaldehyde (**PhCHO**) using DFT calculations. Simplified boron enolates and aza-enolates possessing Bpin or 9-BBN (**3** - **6**) was also adopted to investigate the role of substituents on boron and the boat/chair preference in the aldol and aza-aldol reactions, which is a fundamental issue commonly observed in ring-type TSs. In addition, aza-aldol reactions with more bulky substituents, *t*-Bu group, at the C1 position of **1** were investigated, and the selectivity in the opposite cases was examined. Finally, a designing principle to reverse *syn*/*anti* selectivity was proposed and verified by an *in-silico* proof-of-concept reaction.

2. Results and Discussion

2.1 Relative stability of the boat and chair type TSs in the aldol and aza-aldol reactions

To understand the effect of the substituents on boron in Bpin and 9-BBN simplified model systems

shown in Scheme 2 were investigated using DFT calculations. Enolates **3** and **4** and aza-enolates **5** and **6** are analogs of **1** and **2**, respectively. The Ph substituents on boron enolate, boron aza-enolate, and formaldehyde were replaced by hydrogen atoms, while the Bpin and Ts substituents on **5** along with the 9-BBN and Ms substituents on **6** were retained. The boat and chair configurations of the TS of these simple systems were obtained. The Boat-A conformation of the TS in the reaction of the aza-enolate with 9-BBN was more unstable than the Boat-B configuration by 11.3 kcal mol^{-1}. The Boat-A form was excluded from the discussion owing to its high energy. Both Chair and Boat-B type TSs were obtained in the other systems. The TS energies are relative to the sum of the energies of the reactants in the isolated system.



Scheme 2. Aldol-type reaction of boron enolates and boron aza-enolates.

Table 1 presents Gibbs activation energy of the reactions. In the aldol reaction of boron enolates with the alkoxy boron substrate **3**, the boat TS was 1.8 kcal mol^{-1} more stable than the chair TS. In the reaction of substrate **4**, in which the boron atom bears an alkyl group (9-BBN), the chair TS was slightly more stable than the boat TS by only 0.4 kcal mol^{-1}, indicating that the chair configuration is accessible. The relative stabilities of the boat and chair forms are affected by the interaction of the substituents on the

substrate. This result is qualitatively consistent with previous ab initio MO calculations.[4-5] The boat TS of the aza-enolate is advantageous for both **5** and **6**, with an energy difference of 5.5 kcal mol^{-1}, particularly when the boron bears an alkoxy substituent. In the case of 9-BBN, the energy difference between the boat and chair TSs decreased to 2.1 kcal mol^{-1}. 9-BBN stabilizes chair TS more than the boat TS in the reaction with enolates and aza-enolates.

Table 1. Relative Gibbs energy of TSs of aldol-type reaction of simple enolates and aza-enolates with formaldehyde. Isolated molecules in the reactant state are taken as reference energy. Structural optimization and Gibbs energy calculations (298.15 K) were performed at the ωB97XD/6-311+G** level. Structural deformation energy was evaluated with potential energy at the same level of calculation. Units are in kcal mol^{-1}.

B = Bpin	Enolate (**3**)			Aza-enolate (**5**)		
	Chair	Boat-B	$\Delta_{\mathrm{boat-chair}}$	Chair	Boat-B	$\Delta_{\mathrm{boat-chair}}$
$\Delta G^{\ddagger}$	26.3	24.6	−1.8	27.5	22.0	−5.5
$\Delta E_K^{\mathrm{struct}}$	48.2	40.2	−7.9	50.8	34.3	−16.5
B = 9-BBN	Enolate (**4**)			Aza-enolate (**6**)		
	Chair	Boat-B	$\Delta_{\mathrm{boat-chair}}$	Chair	Boat-B	$\Delta_{\mathrm{boat-chair}}$
$\Delta G^{\ddagger}$	17.6	18.0	0.4	22.0	19.9	−2.1
$\Delta E_K^{\mathrm{struct}}$	37.3	30.4	−6.9	52.2	28.6	−23.5

To form the TS structure, each molecular component is distorted from the reactant structure. This distortion energy is related to the relative energies of the TSs. The total distortion energy $\Delta E_K^{\mathrm{struct}}$ is defined as the sum of that of the enolates/aza-enolates, and aldehydes in the TS structures, as in Equation (1):

$$\Delta E_K^{\mathrm{struct}} = \sum_i \{E_i(X_{K,\mathrm{TS}}) - E_i(X_{\mathrm{R}})\} \quad (1)$$

where i runs over the molecular components (enolate/aza-enolate, formaldehyde), and K is Chair or Boat-B. X_{R} and $X_{K,\mathrm{TS}}$ are the molecular structures of the reactant state and TS, respectively. The contribution of these components to the energy difference between the chair and boat TSs is shown as $\Delta_{\mathrm{boat-chair}}$ in Table 1.

The distortion effect $\Delta E^{\mathrm{struct}}$ was larger in the chair TS than in the boat TS regardless of the substrate, indicating that the structural changes required to form the chair TS are accompanied by significant strain.

The difference between the chair and boat TSs ($\Delta_{boat-chair}$) in the aza-aldol reaction of **5** (B=Bpin) and **6** (B=9-BBN) was 16.5 kcal mol^{-1} and 23.5 kcal mol^{-1}, respectively. The difference in the enolate reaction of **3** and **4** was 7.9 kcal mol^{-1} and 6.9 kcal mol^{-1}, respectively.

Figure 2 shows the TSs of the aldol-type reaction with aza-enolate-containing Bpin (**5**). Those of the other three reactions are presented in Section S2. The structures of the Boat-B-type TSs are more similar to those of the reactant than those of the chair-type TSs. The C1-C2 bond in the Boat-B TS measures 2.35 Å, 0.14 Å longer than the Chair type TS (2.21 Å). The B-N distance in the Boat-B type TS (1.56 Å) is shorter than that in the Chair type (1.61 Å), while the B-O distance in the Boat-B type TS (1.64 Å) is longer than that in the Chair type (1.57 Å). The angle of ∠B (defined in Figure 2 and described in detail in section S3) in Boat-B is 341.7°, which is larger than that in the Chair type TS (337.2°), indicating that the Boat-B TS has a flat structure (∠B=360°) similar to that of the reactant. This trend was similar to that observed in the other three systems; therefore, the Boat-B type TS was characterized as an early transition state, whereas the chair type TS was characterized as a relatively late transition state.

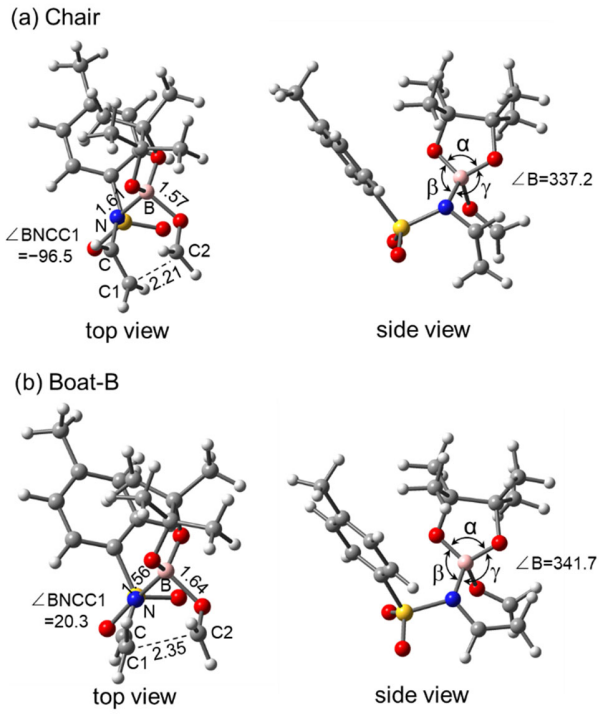


Figure 2. Optimized transition state structure of the aldol reaction between aza-enolate **5** and formaldehyde. "∠B" is defined as ∠B = α + β + γ (section S3). The other transition state structures are also discussed in section S3.

The distortion energy contribution associated with the structural change in the reactant to form the transition state ($\Delta^{\mathrm{struct}}_{\mathrm{boat-chair}} = \Delta E^{\mathrm{struct}}_{\mathrm{Boat-B}} - \Delta E^{\mathrm{struct}}_{\mathrm{Chair}}$) is further decomposed into the contribution from the molecular components (enolate/aza-enolate and formaldehyde). The contributions of both enolate/aza-enolate and formaldehyde were negative in all cases (Table 2), indicating that the formation of the chair-type TS involves a higher degree of structural distortion than the boat-type TS in both enolate/aza-enolate and formaldehyde. The distortion energy of the enolate/aza-enolate was greater than that of formaldehyde. For example, in the case of enolate with Bpin, the enolate exhibited a distortion energy of -5.8 kcal mol^{-1} while that of formaldehyde was -2.1 kcal mol^{-1}.

Further decomposition analysis was conducted and revealed that the planar-to-tetrahedral distortion of the boron moiety in the enolate/aza-enolate contributes to the $\Delta^{\mathrm{struct}}_{\mathrm{boat-chair}}$ value. In this analysis, structural optimization was performed with some structural parameters fixed to those of the TS. The $\Delta^{\mathrm{struct}}_{\mathrm{boat-chair}}$ value was evaluated with the energy of the partial optimization. Three structural parameters were chosen; (1) dihedral angle B-X-C-C, (2) the ∠B angle, and (3) the ∠B angle plus B-X bond length. As shown in Table 2, 56 % to 99 % of $\Delta^{\mathrm{struct}}_{\mathrm{boat-chair}}$ was recovered when ∠B plus B-X were fixed to the TS structure. The B-X-C-C angle was clearly not a significant factor. A greater degree of distortion is naturally necessary to reach the late TS structures, such as Chair TS, than the early TS structures, such as Boat-B TS.

Table 2. The distortion energy difference between the chair and boat transition states, $\Delta^{\mathrm{struct}}_{\mathrm{boat-chair}} = \Delta E^{\mathrm{struct}}_{\mathrm{boat}} - \Delta E^{\mathrm{struct}}_{\mathrm{chair}}$, is decomposed into several components. X = O and N for enolate and aza-enolate, respectively.

fragment	component[a]	Enolate		Aza-enolate	
		Bpin	9-BBN	Bpin	9-BBN
total		−7.9	−6.9	−16.5	−23.5
formaldehyde		−2.1	−3.0	−3.2	−9.0
enolate/aza-enolate		−5.8	−3.9	−13.2	−14.5
	BXCC fixed	−1.0	0.1	−2.7	4.4
	∠B fixed	−2.0	−2.0	−6.8	−7.4
	∠B+BX fixed	−4.2	−3.9	−8.7	−8.1

[a] "BXCC" denotes dihedral angle B-X-C1-C2. "∠B" denotes a summation of three angles made of three adjacent atoms centered on the

B atom. See section S3 in SI. “BX” denotes the B-X bond distance.

The intrinsic reaction coordinate (IRC) was obtained to understand the structural changes upon conversion of the TS to the product. As shown in Figure 3, the boat TS has a longer C1-C2 bond and shorter B-X (X = O or N) bond than the chair TS, which provides further evidence that the boat TS is an early TS and the chair TS is a late TS. The chair TS is on the IRC plot obtained from the boat TS; however, the B-X bond of the chair TS dissociates earlier than that of the boat TS as the reaction coordinate proceeds to the product. The reason is that, in the case of the boat TS, the lone pair of the leaving carbonyl (X = O) or imine group (X = N) interacts with the boron during the B-X bond dissociation. In contrast, in the case of the chair TS, the C-X π orbital undergoes this interaction. The Kohn-Sham (KS) orbitals with B-X bonding character are summarized in Figure S10, showing the interactions of the lone-pair and π-orbital in the Boat-B and Chair TSs, respectively. In Section S4, the B-X bond energy is evaluated. In the boat TS, the B-X bond energy is 6-13 kcal/mol higher compared to the chair TS. This result shows that a lone pair is a better Lewis base than a π orbital. Figure 2 shows the dihedral angle B-N-C-C1, which indicates the position of boron relative to the molecular plane of the enolate. The dihedral angles B-N-C-C1 in the chair and boat TSs were -96.5° and 20.3°, which indicates that the boron in the chair TS is located perpendicular to the molecular plane, while that in the boat TS is located essentially in the molecular plane. A similar trend was observed in all other cases involving 9-BBN and the aza-enolate (Section S2). Accordingly, this B-N-C-C1 angle is helpful in distinguishing between the boron-lone pair interaction and the boron-π interaction. We hereafter use this dihedral angle to identify the interaction between boron and aza-enolates.

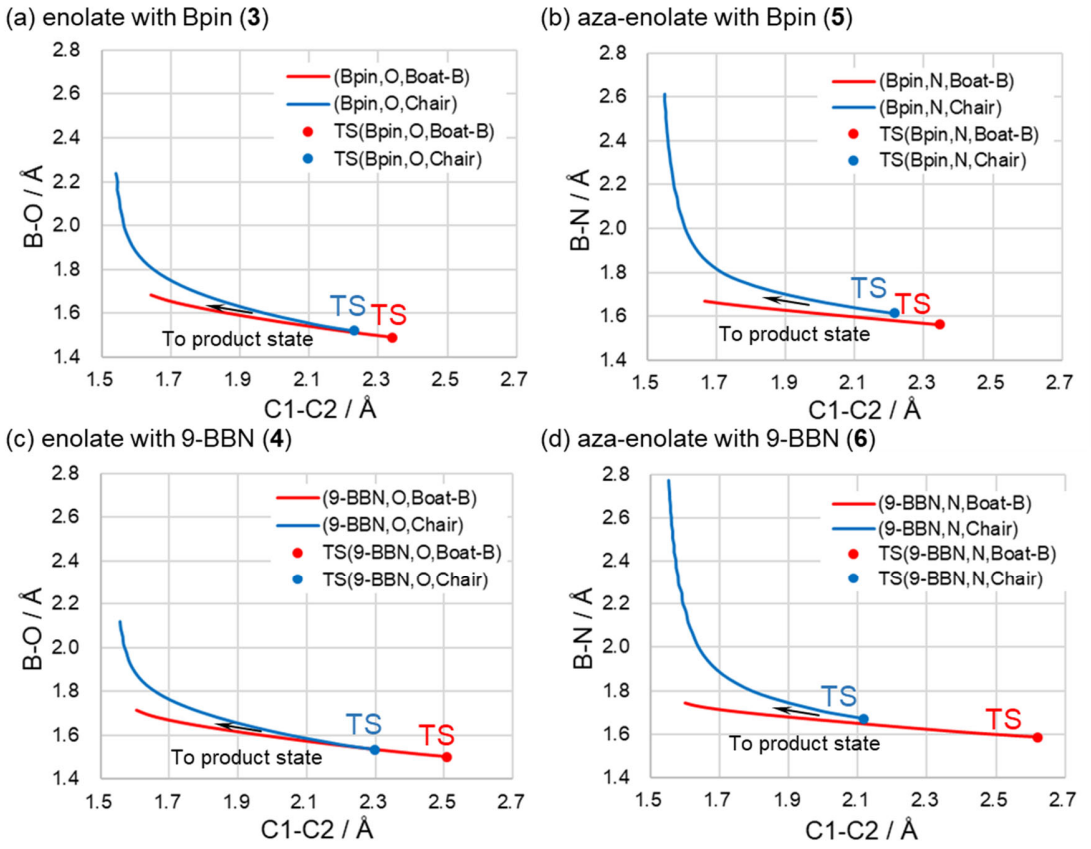


Figure 3. IRC from TS to product side. (a) enolate with Bpin (**3**), (b) aza-enolate with Bpin (**5**), (c) enolate with 9-BBN (**4**), and (d) aza-enolate with 9-BBN (**6**). TS is represented by filled circle. The IRC was obtained until the termination of the calculation due to the instability in the IRC calculation.

The barrier height depends on the substituent (Bpin or 9-BBN). The Gibbs energies of the Bpin and 9-BBN cases are listed in Table 1. The activation energies of both the enolate and aza-enolate with 9-BBN were lower than that of those with Bpin. In both the enolate and aza-enolate, the structural distortion energy ΔE^{struct} of the 9-BBN TS is lower than that of the Bpin TS by 9.8 kcal mol^{-1} and 5.7 kcal mol^{-1}, respectively. This implies that the TS with 9-BBN is an earlier TS than that with Bpin, which is consistent with the IRC analysis (Figure 3). The reactants with 9-BBN undergo less distortion to form the TS, resulting in a lower activation barrier. Due to the stronger Lewis acidity of the boron atom in 9-BBN compared to Bpin, the stabilization is attributed to the formation of Lewis pairs between boron and nitrogen.

2.2 Aza-aldol reaction of aza-enolate with Bpin

The energy profile of the aza-aldol reactions of **1** (Scheme 1a) is shown in Figure 4. In this profile, the energy is quoted relative to that of the **1···PhCHO** state, which is the most stable aggregate of **1** and **PhCHO**. A boat-shaped TS (Boat-B), in which boron was located at the bow end, and a chair-shaped TS were obtained. We also attempted to determine the TS corresponding to Boat-A; however, the steric repulsion between the Ts group and Bpin destabilized the Boat-A TS, and the calculations converged to a chair-type TS. Four TS structures were obtained: two Boat-B structures in which the Ph group of benzaldehyde occupied the pseudo-axial (**TS1-1a**) or pseudo-equatorial (**TS1-1b**) positions, and two chair-type structures in which the Ph group occupied the axial (**TS1-1c**) or equatorial (**TS1-1d**) positions (Figure 4). The three-dimensional structures of these TSs are shown in Figure S6.

The rate-determining step was the formation of the transition state TS1, in which C-C bond formation and B-N bond cleavage proceeded concertedly. The reaction pathway with the lowest activation barrier, with an activation Gibbs energy of 21.2 kcal mol^{-1}, proceeded via a boat-shaped six-membered ring TS, **TS1-1a**, to produce the most stable product, ***syn-E*-P1**. Conversely, the pathway to reach the *anti*-product proceeds via the **TS1-1b** and **TS1-1d** transition states with activation barriers of 24.0 kcal mol^{-1} and 26.1 kcal mol^{-1}, respectively, to produce ***anti-E*-P1** and ***anti-Z*-P1**, respectively. The ***anti-Z*-P1** intermediate is converted to the ***anti-E*-P1** product via the isomerization with energy barrier of 16.7 kcal mol^{-1}, and the reaction pathway via **TS1-1b** would dominantly leads the ***anti-E*-**P1 product. The *syn*/*anti* diastereoselectivity is determined by TS1. The *syn*/*anti* ratio of the product estimated from the activation barrier of this transition state was 99/1, which is qualitatively consistent with the experimental results (*syn*/*anti* > 95/5).

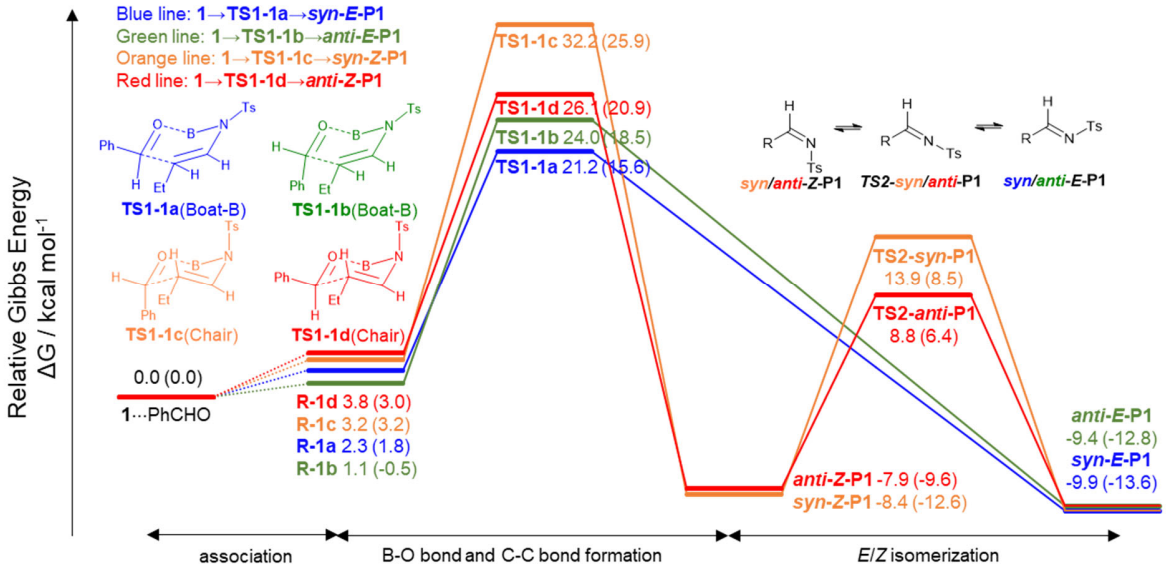


Figure 4. Gibbs energy diagram of the aza-aldol reaction of **1** at the ωB97XD/6-311G(2d,p) level with tetrahydrofuran solvation effect. Frequency calculations adopted a temperature of 323 K. The numbers in parentheses are the relative potential energy. All energy values are relative to the **1···PhCHO** state.

TS1-1a was the most stable of the four transition states. The boat type **TS1-1a** and **TS1-1b** are more stable than the chair-type **TS1-1c** and **TS1-1d** transition states, consistent with the simplified model system. Table 3 summarizes the energy and structural properties of **TS1-1a** to**TS-1d**. Bond distances of newly formed bonds such as B-O and C1-C2 are longer in the boat TS than in the chair TS, while the dissociating B-N bond is shorter. In addition, the ∠B and ∠N values show that the boron and nitrogen moieties are more planar in the boat TS, indicating that the boat TS is an earlier TS than the chair TS. The dihedral angle B-N-C=C in the boat TSs ranges from 12.3° to 21.2°, indicating that the orientation of the boron during the dissociation of the B-N bond is preferable for interaction with the lone pair of the imino moiety. In contrast, the B-N-C=C angle in the chair TSs ranges from -96.6 to -96.0°, and the π orbital of the imino group, rather than the lone pair, participates in the interaction. The KS orbitals with B-N bonding character (Figure S10e) show that the nitrogen lone-pair in the imino group bonds to the boron atom in the boat TS, while the π orbital forms this bonding interaction in the chair TS.

Table 3. DFT calculation of transition states **TS1-1a**, **TS1-1b**, **TS1-1c**, and **TS1-1d**. ∠B is the sum of the bond angles that a boron forms with two adjacent oxygen and nitrogen atoms. ∠N is the sum of the bond angles that a nitrogen forms with adjacent boron, carbon and sulfur atoms. B-N-C=C is the dihedral angle between the boron-nitrogen bond and carbon-carbon double bond.

Transition State	$\Delta G^{\ddagger}$ [kcal mol^{-1}][a]	B-O [Å]	B-N [Å]	C1-C2 [Å][b]	∠B [deg.]	∠N [deg.]	B-N-C=C [deg.]
TS1-1a (Boat-B)	21.2	1.55	1.60	2.24	337.2	351.2	21.2
TS1-1b (Boat-B)	24.0	1.58	1.58	2.22	337.4	353.4	12.3
TS1-1c (Chair)	32.2	1.52	1.66	2.05	332.4	339.9	-96.0
TS1-1d (Chair)	26.1	1.49	1.69	2.03	332.1	339.0	-90.6

[a]Relative Gibbs energy. [b]For the definition of C1 and C2, see Scheme 1a.

Among boat TSs, **TS1-1a** is more stable than **TS1-1b** by 2.8 kcal mol^{-1}. The orientation of PhCHO in these transition states differed; the Ph group in **TS1-1a** and **TS1-1b** are located in a pseudo-axial and pseudo-equatorial position, respectively. We compared the structures of these TSs to understand the origin of the relative stabilities (Figure 5). The Ph group in the pseudo-axial position and the Et group in the bowsprit position in **TS1-1a** were farther to avoid steric repulsion, whereas the Ph and Et groups were closer in **TS1-1b**, resulting in greater steric repulsion. The Ph and Et groups are located close to each other in the pseudo-equatorial and bowsprit positions, respectively. Two hydrogen atoms **TS1-1a** are close to the oxygen atom of Bpin (2.70 Å and 2.15 Å), which facilitates attractive hydrogen bonding interactions; however, the Ph group in **TS1-1b** avoids steric repulsion, which inhibits hydrogen bonding with the oxygen atom of Bpin. The corresponding B-H distances are 3.38 Å and 2.24 Å.

In section 2.1, the essential relative stability of Chair and Boat-B TSs was analyzed using simplified model (**3-6**) by eliminating steric effects of substituents. On the other hand, the relative stability was also examined by replacing Et group at the C1 position of **1** with *t*-Bu group to examine how this relative stability would change in the presence of more steric hindrance. The results were similar to those for **1**; calculated activation Gibbs energy for **TS1-7a** and **TS1-7b** was 23.4 kcal mol^{-1} and 25.8 kcal mol^{-1} respectively. See section S10 in SI for more details. Since the *syn* product is generated by avoiding steric repulsion, it is understandable that the introduction of a bulkier group results in the *syn* preference as in **1**. Those for the Chair TS, **TS1-7d** and **TS1-7d**, which produce *anti*- and *syn*-products, were 30.6 kcal mol^{-1} and 37.0 kcal mol^{-1}, respectively.

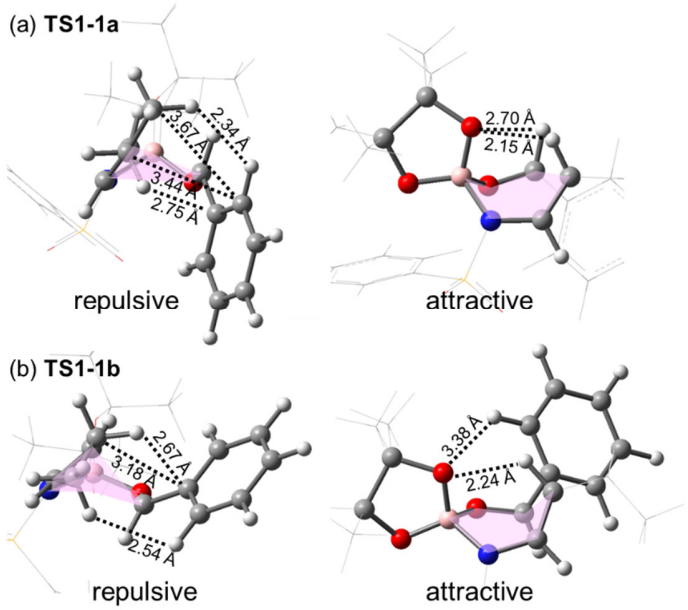


Figure 5. Repulsive and attractive interactions in (a)**TS1-1a** and (b)**TS1-1b**. The six-membered ring in the transition state is colored with pink planes.

The intermediates **R-1a**, **R-1b**, **R-1c**, and **R-1d** led to the formation of TS1. These states correspond to the ends of the IRC on the reactant side of TS1: The distances between the O atom in PhCHO and the B atom in the aza-enolate moiety are 3.34 Å, 3.83 Å, 2.99 Å, and 3.12 Å in **R-1a**, **R-1b**, **R-1c**, and **R-1d**, respectively. No B-O bonds are formed in these structures; thus, no ate complex was formed between the boron aza-enolate and Bpin. This is a characteristic of the aza-aldol reaction with Bpin. A previous study[8d] employing calculations at the HF/3-31G level reported that an ate complex was obtained as an intermediate using a BH_2 group; however, the B-O bond length was 2.5-2.7 Å, which does not indicate the formation of the ate complex. This contrast to the reaction with 9-BBN, in which the ate complex is present as a metastable intermediate (Section 2.3).

The ***syn*-Z-P1** and ***anti*-Z-P1** products are produced via reaction pathways involving **TS1-1c** and **TS1-1d**, respectively. Each product contained an *E*-isomer with respect to its imine moiety. As shown in Figure 4, ***syn*-E-P1** and ***anti*-E-P1** were more stable than ***syn*-Z-P1** and ***anti*-Z-P1** by 1.5 kcal mol^{-1}, respectively. The formation of TSs toward the *syn* form (**TS2-*syn*-P1**) and *anti* form (**TS2-*anti*-P1**) in the isomerization of the imine moiety had activation barriers of 22.3 kcal mol^{-1} and 16.7 kcal mol^{-1}, respectively. The activation energies of these isomerizations are lower than those of the six-membered ring transition state; therefore, they are not the rate-determining steps. Experimental studies have reported that the *E-Z*

isomerization of imines proceeds readily at room temperature.[11] Using C-N bond rotation as the reaction coordinate in locating the TS produced a TS structure with an almost linear Ts-N-C bond (Table S5).

2.3 Aza-aldol reaction of aza-enolate with 9-BBN

The five different reaction pathways of the aza-aldol reaction of **2** (Scheme 1b) were obtained, and the energy profile was shown in Figure 6. Two Boat-B TSs, **TS2-2a** and **TS2-2b**, and were obtained, in which the benzaldehyde's Ph group occupies the pseudo-axial positions and the pseudo-equatorial positions, respectively. Similarly, two Chair TSs, **TS2-2c** and **TS2-2d**, were obtained, with the Ph groups occupying the axial and equatorial positions, respectively. In the case of the Boat-A TS in which boron is located in the body of the boat skeleton, only **TS2-2e**, in which the Ph group occupied a pseudo-equatorial position, was obtained. The pathways involving **TS2-2a** and **TS2-2b** directly lead to ***syn-E*-P2** and ***anti-E*-P2**, respectively, the most stable *E*-products. In the pathway involving **TS2-2c**, **TS2-2d**, and **TS2-2e**, the direct formation of the *Z* isomer is followed by the *E/Z* isomerization to generate the most stable *E*-isomer. The rate-determining step is C–C bond formation. In the pathway via **TS2-2d**, the activation barrier for **TS3-*anti*-P2** (21.7 kcal mol^{-1}), in which the *Z*-product (***anti-Z*-P2**) isomerizes to the more stable *E*-product, is higher than that for **TS2-2d** (19.0 kcal mol^{-1}) and is the rate-determining step. The pathway with the lowest activation barrier is proceeded via **TS2-2a**, with an apparent activation barrier of 13.2 kcal mol^{-1}. Assuming these five reaction pathways, the *syn*/*anti* ratio obtained using Eyring's equation is 87/13, qualitatively reproducing the experimentally observed diastereo-ratio (*syn*/*anti* ≥ 95/5).

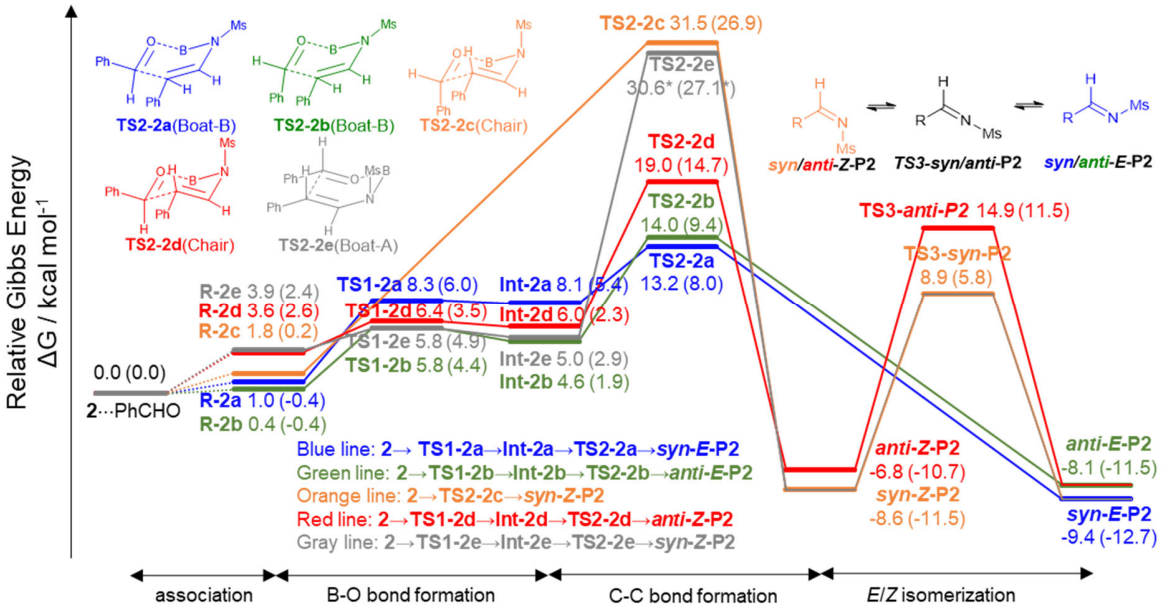


Figure 6. Relative Gibbs energy diagram of the aza-aldol reaction of **2** at ωB97XD/6-311G(2d,p) level. The numbers in parentheses are relative potential energy. For the **TS2-2e** state, single-point calculation at the 6-31G* optimized structure was adopted.

The characteristics of the TS of the reactant **2** were consistent with those of the simplified model system and the aza-aldol reaction of reactant **1**. Boat-B TSs **TS2-2a** and **TS2-2b** were more stable than chair TSs **TS2-2c** and **TS2-2d**. The instability of Boat-A TS **TS2-2e**, in which boron is located in the body of the boat skeleton, was also consistent with the simplified model. The structural parameters of TSs are listed in Table 4. The TSs of Boat-B configurations (**TS2-2a**, **TS2-2b**) have shorter B-N bonds and longer B-O and C1-C2 bonds than those of the chair configurations (**TS2-2c**, **TS2-2d**). Angles B and N were closer to 360 °, indicating greater planarity around the B and N atoms in the Boat-B type TS. These results indicate that the boat and chair TS are early and late TSs, respectively. The dihedral angle B–N–C=C also indicated that the interaction between the imino moiety and boron was similar to that of the model described in section 2.2.

Table 4. The transition state of the C-C formation step between **2** and PhCHO.

	$\Delta G^{‡}$ [kcal mol^{-1}][a]	B–O [Å]	B–N [Å]	C1–C2 [Å][b]	∠B [deg.]	∠N [deg.]	B-N-C=C [deg.]
TS2-2a (Boat-B)	13.2	1.54	1.65	2.22	338.4	356.4	22.9
TS2-2b (Boat-B)	14.0	1.55	1.62	2.12	337.4	357.9	3.8
TS2-2c (Chair)	31.5	1.52	1.71	2.04	334.5	339.6	-91.8
TS2-2d (Chair)	19.0	1.48	1.82	1.94	331.0	334.6	-85.1
TS2-2e (Boat-A)	30.6	1.47	2.00	2.02	329.4	335.0	-95.0

[a]Gibbs energy relative to **2**···PhCHO. For **TS2-2e**, structure optimization failed with the 6-311G(2d,p) basis sets. The result of a single-point calculation at the 6-31G* optimized geometry was used. [b]For the definition of C1 and C2, see Scheme 1b.

The **TS2-2a** is the lowest TS with the activation energy of 13.2 kcal mol^{-1}, which is 8.0 kcal mol^{-1} lower than that of the corresponding pathway in the reaction of reactant **1**. This result indicates that the Lewis acidity of 9-BBN in reactant **2** stabilizes the tetra-coordinated boron more than Bpin. The energy barrier in the formation of **TS2-2b** is 14.0 kcal mol^{-1}, which differs from that of **TS2-2a** by only 0.8 kcal mol^{-1}. This difference is insufficient to precisely discuss the origin of the relative stability of the TS; however, we postulate that the explanation of the instability of **1** is applicable here. In **TS2-2b**, the Ph group of PhCHO occupies the pseudo-equatorial position, whereas that in **TS2-2a** occupies the pseudo-axial position. The steric repulsion of the aza-enolate Ph group in the bowsprit position was slightly greater than in **TS2-2b**, which explains the observed *syn*/*anti* ratio.

The reaction of aza-enolate **2** was characterized by the formation of a B-O bond with PhCHO and subsequent C-C bond formation, yielding a tetracoordinated boron ate complex. Calculations suggest that all pathways leading to the TSs involve tetra-coordinated boron intermediates, except for the pathway leading to **TS2-2c**. **Int-2a**, **Int-2b**, **Int-2d**, and **Int-2e** are tetracoordinated ate complexes. No structural parameters were found to characterize the relative stability of these intermediates (Table S7). The B-O distance and ∠B are approximately 1.6-1.7 Å and 340°, respectively, indicating an sp^3-like structure in which the boron atom is no longer planar. This demonstrates that B-O bond is initially formed followed by C-C bond formation and B-N bond cleavage in the aza-aldol reaction of **2**. The formation of the ate complex is in contrast to that of aza-enolate **1**, in which the bond-forming and cleavage steps proceed concertedly. The formation of the ate complex could enlarge the reaction rate because more frequent access to TS2 is anticipated. In the reaction of **2**, the formation of the tetracoordinate ate complex is due to the

Lewis acidity of the boron in 9-BBN (**2**), which is much more electrophilic than that in Bpin (**1**). Natural bond orbital (NBO) analysis[12] revealed that the energy contribution by the donation of the alkoxy group to the unoccupied boron 2p orbital (LP*) in **1** is 227.2 kcal mol^{-1} (Table S8), whereas that in **2** is only 89.5 kcal mol^{-1} (Table S9). The NBO analysis indicates that the stability of the Lewis pair formed by **2** and the aldehyde contributes to the stability of the ate complex and the TS.

2.4 Reversing *syn*/*anti* selectivity: a proof-of-concept examination

Regarding the *syn*/*anti* selectivity, the aza-enolate **1** and **2** are *syn* selective in the reaction with **PhCHO** as observed in the experiment and DFT calculation. Here, we consider how we obtain *anti* selective aza aldol reaction. We note that the reaction pathway via Chair TS shows *anti* selectivity in **1** and **2** (see discussion in sections 2.1 and S11 in SI) Thus, an approach to destabilize the pathway via Boat-B is discussed. As described in section 2.1, the Boat-B TS is stabilized by the coordination of the N lone-pair to the B atom. Therefore, another group could be attached to the lone-pair not to form the N(lone-pair)-B Lewis pair. As a proof-of-concept (POC) study, we adopted aza-enolate **8** (see Figure 7) in which the N-Ms group in **2** has been replaced by a NH_2 group.

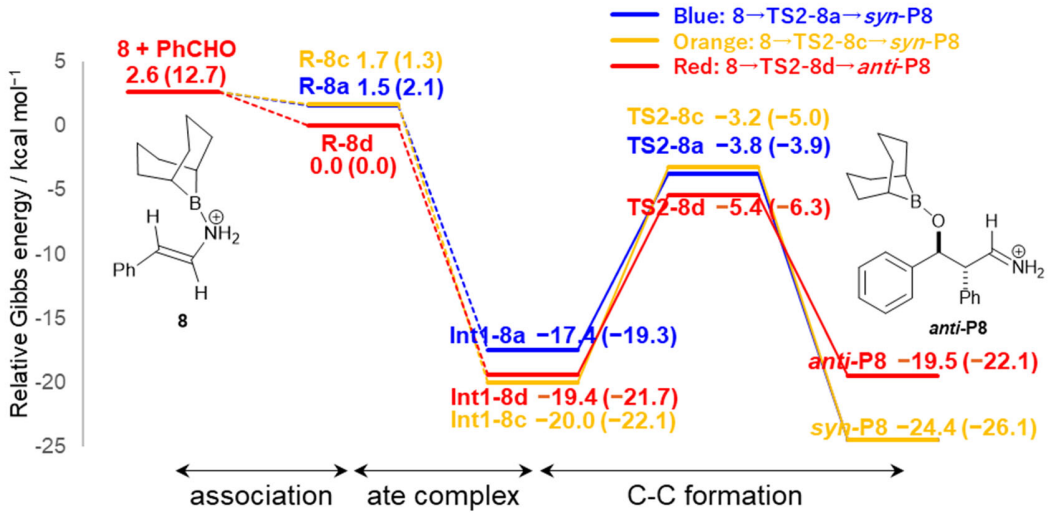


Figure 7. Energy profile of aza-aldol reaction with aza-enolate **8**.

The energy profile of the aza-aldol reaction with **8** and **PhCHO** is shown in Figure 7. Three types of association conformations were examined: **R-8a** leading to Boat-B type TS, **R-8c** and **R-8d** to Chair TS. The association states should be in equilibrium with the reactant state, **8**+**PhCHO**, at early stage of the reaction due to the similar energy levels before and after the association. Among the association states, **R-**

8d was the most stable. Ate-complex formation follows, and **Int1-8c** and **Int1-8d**, which lead to Chair TS, was about 2 kcal mol^{-1} more stable than **Int1-8a** which gives Boat TS. Among the TSs that generate C-C bond, **TS2-8d** that forms *anti* product, ***anti*-P8**, via Chair TS was the most stable. The Boat-B TS, **TS2-8a**, was located at 1.6 kcal mol^{-1} higher in energy. Thus, the result of the present POC study showed that, compared to the **1** and **2** cases, the relative energies of the Boat-B and Chair TSs can be reversed. In the case of **8**, no nitrogen lone pair but N=C π orbital is available for the coordination to boron at the N=C leaving stage of the reaction.

We also compared the apparent activation energy of the reaction pathways. From the equilibrium state of the association, the ate complex is formed. Since the complex formation energy is significantly large, the back reaction would be suppressed. The rate-limiting step is the C-C formation step. Considering these facts, the reaction rate might be proportional to the product of the association equilibrium constant K^{assoc} and the rate constant of the C-C formation k^{C-C}.

$$r \propto K^{assoc} k^{C-C} = \frac{k_B T}{h} e^{-\frac{\Delta G^{assoc} + \Delta G^{\ddagger, C-C}}{RT}} \quad (2)$$

Apparent activation energy of the pathway is given as follows.

$$\Delta G^{\ddagger, app} = \Delta G^{assoc} + \Delta G^{\ddagger, C-C} \quad (3)$$

With this formula, the apparent activation Gibbs energy via **TS2-8d** to form the *anti*-product, **anti-P8**, is 11.4 kcal mol^{-1}, which is the smallest among the pathways. That of the pathway via **TS2-8a** to lead *syn*-product formation was 12.6 kcal mol^{-1}. The result indicates that the anti-selectivity could be obtained by controlling the relative energies of Boat-B and Chair TS.

3. Conclusions

A DFT mechanistic study was conducted for the aza-aldol reaction of aza-enolates and PhCHO. Two types of aza-enolates, **1** and **2**, derived respectively from HBpin and 9-BBN–H were adopted. The result shows that the *syn-E* isomer is preferentially formed, consistent with experimental observations. Most stable six-membered ring Boat-B TS leads to the *E* isomer. The preference of the *syn* isomer is determined by the substituents' interactions between aza-enolate and **PhCHO**.

Aldol and aza-aldol reactions were also studied with simplified model systems to understand the fundamental features of the mechanism. The model system showed that the energies of the six-membered ring TSs of the Boat-B type configurations are lower than those of the Chair type configurations in the aza-aldol reaction, which is in good agreement with the qualitative ab initio calculations of a previous study.[8d] The Boat-B form was found to be an early TS, and the Chair form is a late TS. The Boat-B type

TS structure is similar to that of the reactant and is relatively stable, whereas the Chair type TS is higher in energy because the structure requires a greater degree of distortion. Analysis of the IRC from the TS to the product system shows that in the pathway via the Boat-B TS, the unoccupied boron 2p orbital interacts with the lone pair of the nitrogen on the imine leaving group. Conversely, this boron 2p orbital interacts with the C-N π orbital in the Chair TS. The B-N(lone pair) Lewis pair is more stable than the boron-π Lewis pair; thus, this interaction stabilized the Boat-B TS.

The *E*/*Z*-selectivity originates from the Boat-B/Chair TS. The *syn*/*anti*-selectivity is a consequence of the repulsive interactions arising from the steric hindrance of the substituent Ph group and attractive interactions with the oxygen atom of Bpin. The ate complex was not formed in the reaction of **1**, but was present as a metastable intermediate in the reaction of **2**. NBO analysis revealed a clear difference in the nature of the boron moiety of **1** and **2**, suggesting that the substituent has a significant effect on the electrophilicity of boron, which affects both the transition-state energies and the stability of the ate complex.

The explanation of relative stabilities of the six-membered ring transition states provided by this study will advance our understanding of reaction mechanisms with similar six-membered ring TSs. In particular, the *syn*/*anti* selectivity is also able to be controlled by the energy levels of the Boat-B/Chair TS. A POC study by DFT calculations showed that the elimination of the N lone-pair stabilization effect by the substitution of the N-Ms group by the NH_2 group would reverse the relative energy order of the Boat-B and Chair TS.

4. Computational Details

DFT calculations were performed using the ωB97XD exchange-correlation functional[13] with the Gaussian 16 software.[14] The simplified enolates (**3**, **4**) and aza-enolate (**5**, **6**) were introduced to examine the role of the boron reagent in selecting either Chair or Boat-B forms. To understand the electronic origin of the Chair/Boat-B preference, substitutent groups at C1 of enolate/aza-enolate and C2 of aldehyde were substituted by H atoms to exclude the steric effect on the TS structure. The solvent effect was also excluded in the same reason. Structural optimization and normal mode analysis of the simplified model system were performed at the ωB97XD/6-311+G** level. The Gibbs energy calculation was performed, assuming a temperature of 298.15 K. For the aza-aldol reactions of **1** and **2**, solvent effects were modeled by the self-consistent reaction field (SCRF) method with the polarized continuum model (PCM),[15] and the parameter sets for tetrahydrofuran (THF) and toluene, respectively. Structural optimization and single-point calculations were performed using 6-311G(2d,p) basis functions.[16] The **TS2-2e** TS in the aza-aldol

reaction of **2** could not be obtained using the 6-311G(2d,p) basis set. Instead, single-point calculations based on the 6-31G*-optimized structure were performed using the 6-311G(2d,p) basis set. Normal mode analysis of **1** and **2** was conducted using the temperature used under experimental conditions (323 K and 213 K, respectively). The optimized energy minimum and TS were subjected to normal mode analysis and verified by the number of imaginary frequency. The connectivity between the energy minimum and TS was confirmed by calculating the IRC.[17] For the NBO analysis, the computational routines included in Gaussian 16 (NBO version 3)[12] were used.

Data Availability Statement

The data underlying this study are available in the published article and its Supporting Information.

Supporting Information

Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/****. The information includes the reaction scheme of aza-aldol reactions, structural parameters (section S1), TS structures (section S2), more detailed definition of ∠B and ∠N (section S3), B−X (X = O and N) binding energies (section S4), structures of reactant states, transition states and product states in the aza-aldol reaction (section S5), Structural parameters of transition states of E/Z isomerization (section S6) and the reactant, **TS1-x**, **Int-x** (x=**2a, 2b**, **2d**, **2e**), and products (section S7), NBO analysis (section S8), interaction between boron and carbonyl/imino group (section S9), aza-aldol reaction with a bulkier substituent (section S10), and atomic coordinate of the optimized structures (S11).

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Supporting Information

A DFT Mechanistic Study on the Aza-Aldol Reaction of Boron Aza-Enolates: Relative Stability of Six-Membered Transition State and its Relevance to the Coordination Mode of the Leaving Group

Sho Miyakawa[1], Ray Miyazaki[1], Tomoya Miura[2,4], and Jun-ya Hasegawa[1,3,*]

[1] Institute for Catalysis, Hokkaido University, N21W10, Kita-ku, Sapporo 001-0021, Japan

[2] Department of Synthetic Chemistry and Biological Chemistry, Kyoto University, Katsura, Kyoto 615-8510, Japan

[3] Interdisciplinary Research Center for Catalytic Chemistry, National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8565, Japan

[4] Present address: Division of Applied Chemistry, Graduate School of Natural Science and Technology, Okayama University, Tsushima-naka 3-1-1, Okayama 700-8530, Japan

E-mail: hasegawa@cat.hokudai.ac.jp

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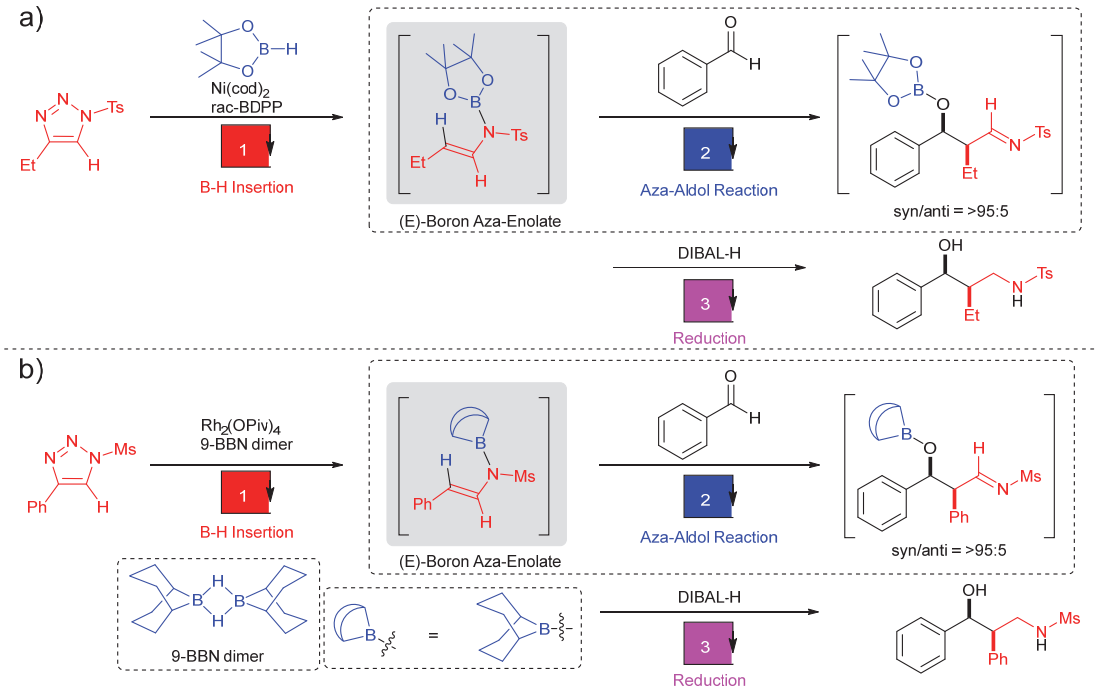
S1. Aza-aldol reaction of HBpin and 9-BBN derived boron aza-enolate



Scheme S1. a) Aza-aldol reaction of HBpin-derived boron aza-enolate[1]. b) Aza-aldol reaction of 9-BBN-derived boron aza-enolate[2].

S2. Transition state structures for the simplified substrates

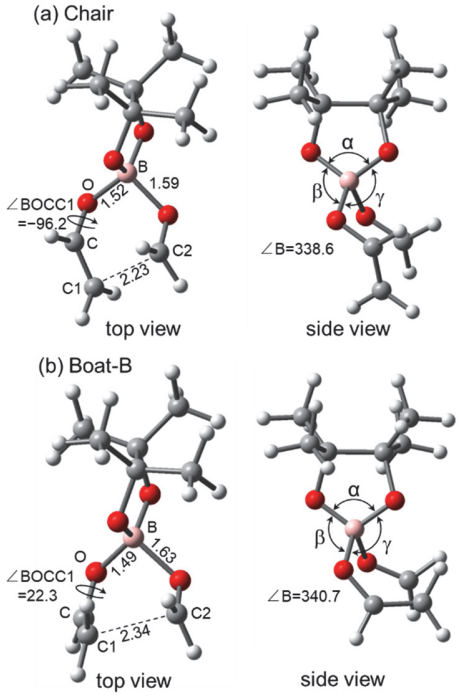


Figure S1. Transition state structures for the O-enolate with Bpin

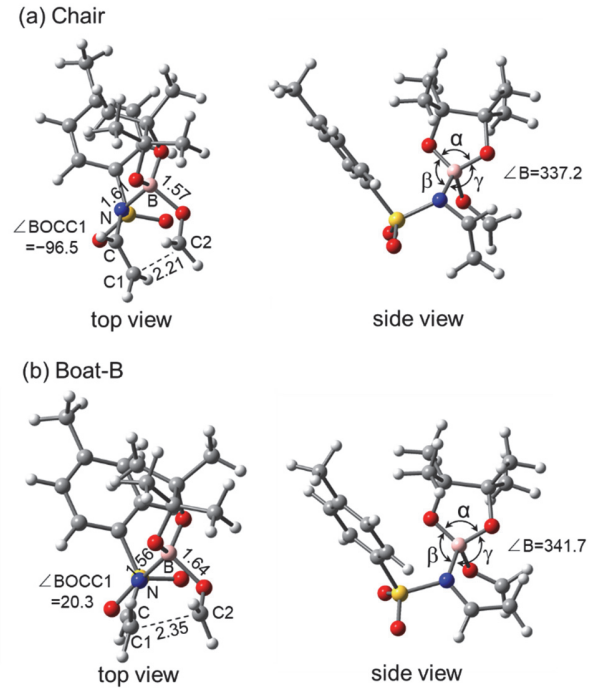


Figure S2. Transition state structures for the N-enolate with Bpin

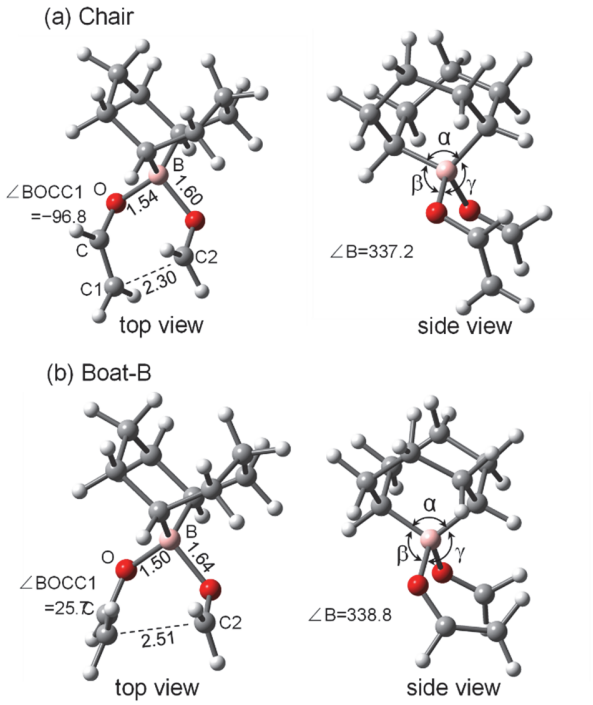


Figure S3. Transition state structures for the O-enolate with 9-BBN

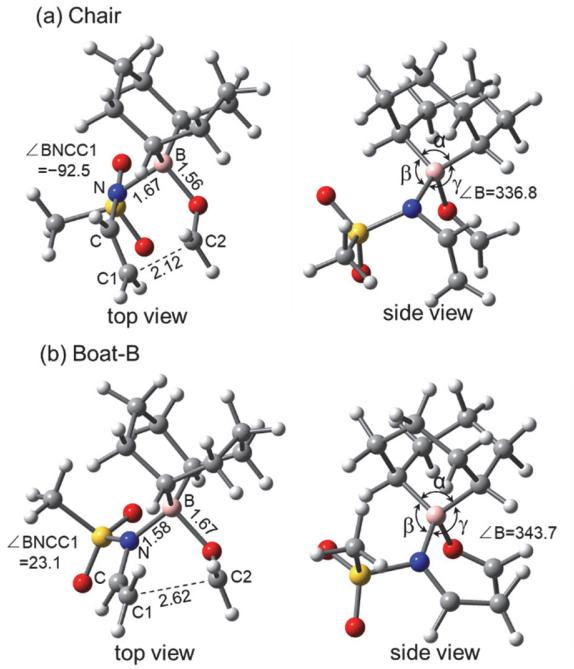


Figure S4. Transition state structures for the N-enolate with 9-BBN

S3. Definition of ∠B and ∠N in Tables 1, 2, 4, and 5

A sum of three angles around boron and nitrogen atoms is defined as ∠B are ∠N, respectively, for comparison of planarity. The ∠B and ∠N values become maximum at 360 degrees, where the boron and nitrogen moiety is planer. The three angles that determines ∠B and ∠N are given in Figure S5. Tables S1 and S2 show the ∠B and ∠N angles and their components.

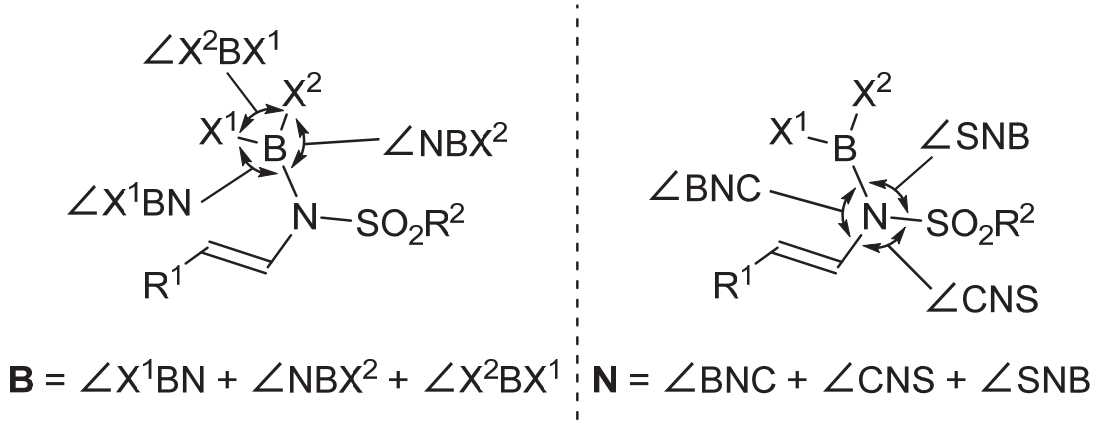


Figure S5. Definition of the three angles that determine ∠B and ∠N.

Table S1. The ∠B and ∠N values and related angles in **1**, **1**···PhCHO and transition states.

	X^1BN	NBX^2	X^2BX^1	∠B	BNC	CNS	SNB	∠N
1	121.9	123.9	114.2	360.0	121.3	115.3	120.8	357.4
1···PhCHO	123.6	122.2	114.2	360.0	121.6	115.7	120.5	357.8
TS-1a	112.5	115.2	109.5	337.2	117.8	114.8	118.6	351.2
TS-1b	110.3	117.7	109.4	337.4	117.2	114.6	121.6	353.4
TS-1c	107.9	115.0	109.5	332.4	105.5	116.1	118.3	339.9
TS-1d	107.1	114.5	110.6	332.2	103.5	117.0	118.5	339.0

Table S2. The ∠B and ∠N values and related angles in **2**, **2**···PhCHO and the transition states.

	X^1BN	NBX^2	X^2BX^1	∠B	BNC	CNS	SNB	∠N
2	122.3	126.3	111.5	360.1	124.0	113.7	122.3	360.0
2···PhCHO	122.3	126.3	111.5	360.1	124.1	113.6	122.2	359.9
TS-2a	112.7	119.3	106.4	338.4	119.4	112.3	124.7	356.4
TS-2b	110.2	120.8	106.5	337.4	119.1	112.9	125.8	357.8
TS-2c	111.2	115.5	107.9	334.5	104.7	117.1	117.7	339.5
TS-2d	109.5	112.5	109.0	331.0	100.3	118.2	116.1	334.6
TS-2e	110.6	107.9	110.9	329.4	96.6	117.4	121.0	335.0

S4. B−X (X = O and N) binding energy

One way to evaluate binding energy, we might calculate energy by simply stretching the target bond. However, we have to evaluate the B−X binding energy in a cyclic transition state. Therefore, we defined the B−X binding energy $E_{\mathrm{bind}}^{\mathrm{B-X}}$ as shown in Scheme S2.

First, the energy of the structure obtained by elongating the B-X bond up to 100 Å from the transition state structure was calculated. The resultant energy was subtracted from the energy of the transition state, yielding the term $E_{\mathrm{bind}}^{(1)}$. In this calculation, no bond was assumed for the C1−C2 interaction, and only the B−X bond was elongated. The $E_{\mathrm{bind}}^{(1)}$ term includes not only the B-X bond energy but also the interaction energy between the enolate and formaldehyde moieties, $E_{\mathrm{bind}}^{(2)}$. Then, the structure was modified by removing Bpin or 9−BBN from the transition state, and the energy of the structure obtained by extending the C1−C2 distance up to 100 Å was subtracted, resulting in $E_{\mathrm{bind}}^{(2)}$. $E_{\mathrm{bind}}^{\mathrm{B-X}}$ was defined by subtracting $E_{\mathrm{bind}}^{(2)}$ from $E_{\mathrm{bind}}^{(1)}$.

$$E_{\mathrm{bind}}^{(1)} = E\left[\ \right] - E\left[\ \right]$$

$$E_{\mathrm{bind}}^{(2)} = E\left[\ \right] - E\left[\ \right]$$

$$E_{\mathrm{bind}}^{\mathrm{B-X}} = E_{\mathrm{bind}}^{(1)} - E_{\mathrm{bind}}^{(2)}$$

Scheme S2 Definition of B−X (X = O and N) binding energy, $E_{\mathrm{bind}}^{\mathrm{B-X}}$, in the transition state. A case of O-enolate with 9-BBN substituents.

The results are shown in Tables S3 and S4. In all cases, the $\Delta E_{\mathrm{bind}}^{\mathrm{boat-chair}}$ values are negative, indicating that the boat conformation has a more negative $E_{\mathrm{bind}}^{\square}$ compared to the chair conformation. It is evident that the B−X bond is more stable in the boat TS conformation than in the chair TS conformation. The bonding between X's lone pair and B in the boat conformation is more stable than the bonding involving the π orbitals of the chair conformation. Therefore, the type of the B−X bonding during dissociation contributes to the relative stability of the transition state.

Table S3 Result of $E_{\mathrm{bind}}^{\square}$, $E_{\mathrm{bind}}^{(1)}$ and $E_{\mathrm{bind}}^{(2)}$. See definition in Scheme S2. Units are in kcal/mol.

	Bpin				9-BBN			
	O-enolate		N-enolate		O-enolate		N-enolate	
	boat	chair	boat	chair	boat	chair	boat	chair
$E_{\mathrm{bind}}^{(1)}$	-167.4	-161.0	-169.7	-159.8	-160.3	-156.8	-157.8	-151.7
$E_{\mathrm{bind}}^{(2)}$	-0.7	-1.6	2.7	1.1	0.8	-1.3	5.7	-1.1
$E_{\mathrm{bind}}^{\square}$	-166.7	-159.4	-172.4	-160.9	-161.1	-155.5	-163.5	-150.5

Table S4 $\Delta E_{\mathrm{bind}}^{\mathrm{boat-chair}}$. $E_{\mathrm{bind}}^{\square}$ of the boat TS structure relative to that of the chair one.

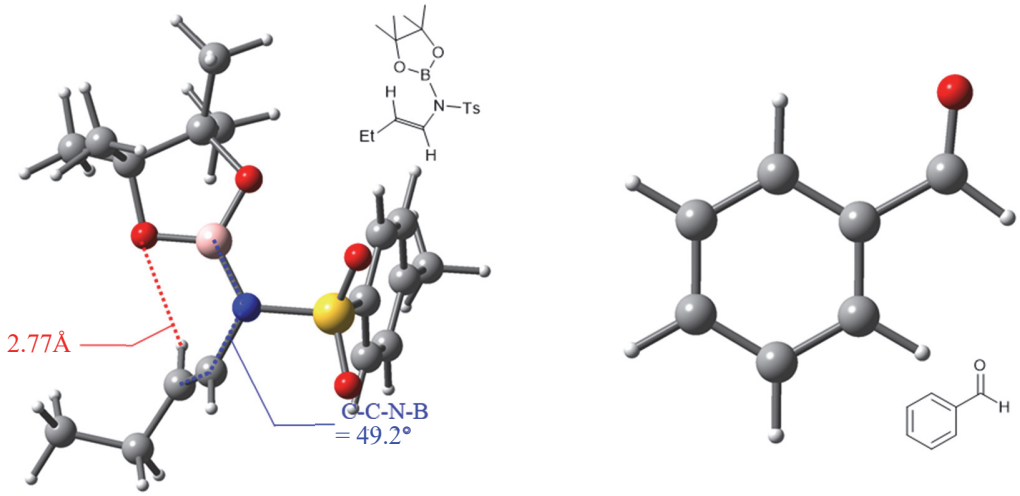
	Bpin		9-BBN	
	O-enolate	N-enolate	O-enolate	N-enolate
$\Delta E_{\mathrm{bind}}^{(1),\mathrm{boat-chair}}$	-6.4	-9.8	-3.5	-6.1
$\Delta E_{\mathrm{bind}}^{(2),\mathrm{boat-chair}}$	0.9	1.6	2.1	6.8
$\Delta E_{\mathrm{bind}}^{\mathrm{boat-chair}}$	-7.3	-11.5	-5.6	-12.9

S5. Structures of reactant states, transition states and product states in the aza-aldol reaction

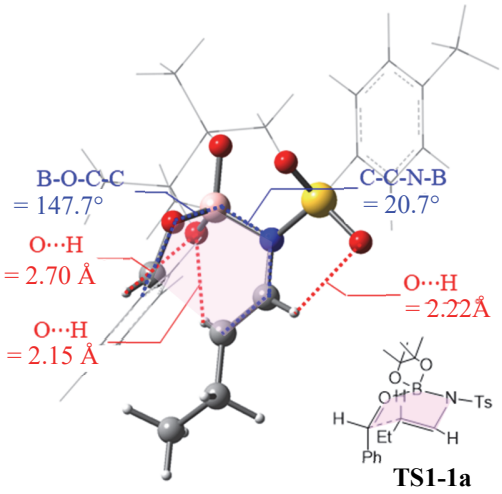
The aza-aldol reaction of **1** has four pathways. Each transition state has obviously different steric hindrances. The structures and their key steric repulsion of reactants, transition states, and products are shown below.

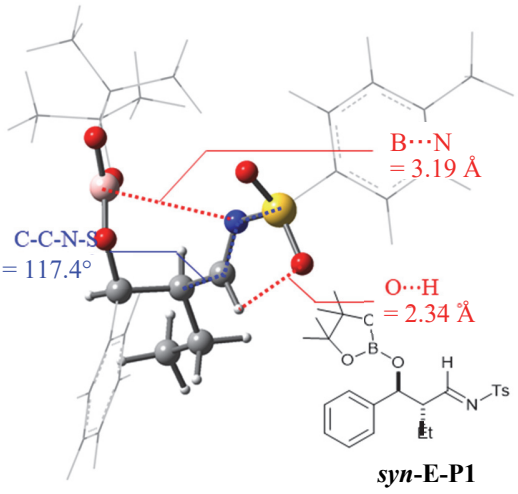
In the transition state of a six-membered ring, we adopt the conventional nomenclature used in cyclohexane to describe the positions of substituents such as axial and equatorial positions. In the context of a boat form, the substituents attached to the four atoms constituting the hull of the boat are referred to as being in *pseudo-axial* position if they project in the direction perpendicular to the approximate plane of the ring. Conversely, substituents projecting within the plane are considered to be in a *pseudo-equatorial* position. Additionally, among the substituents attached to the carbon corresponding to the bow of the boat, those projecting inside the ring are termed in *flagpole* position, while those projecting outside the ring are in *bowsprit* position.

(a) 1 and PhCHO

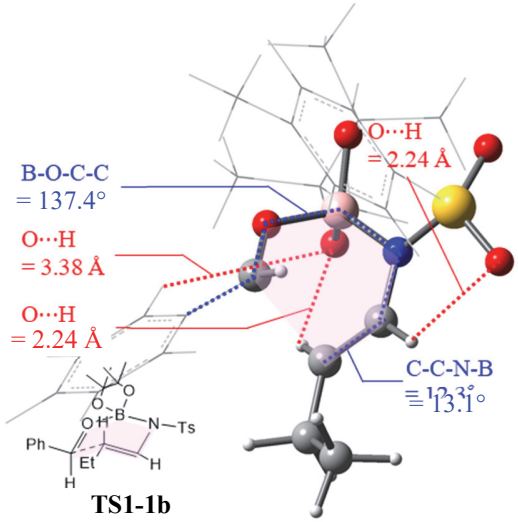


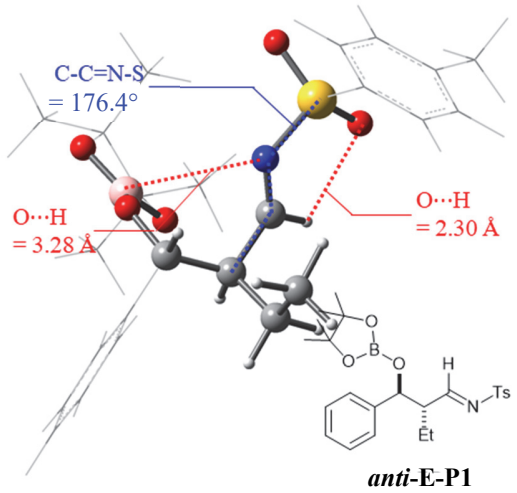
(b) TS1-1a → *syn-E*-P1



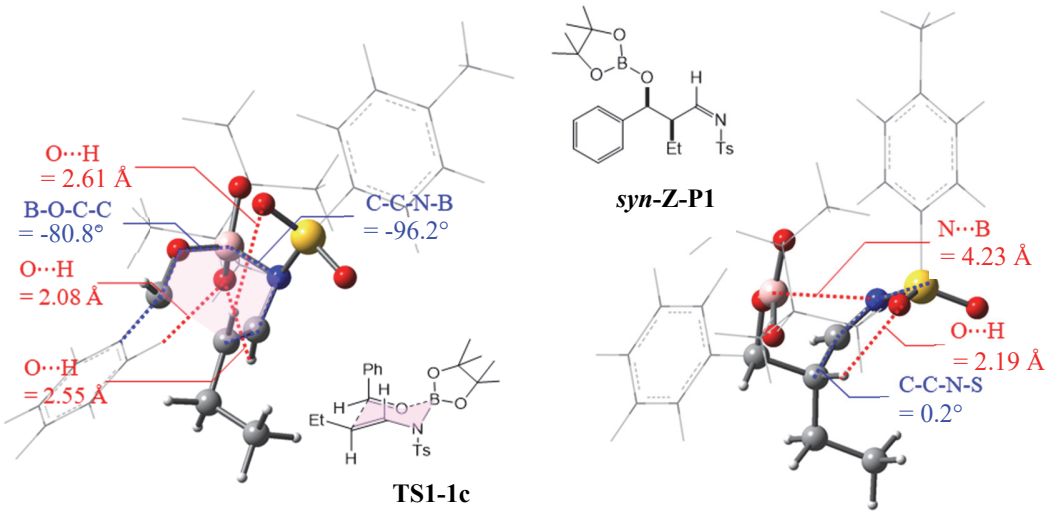


(c) TS1-1b → *anti-E*-P1





(d) TS1-1c → *syn-Z*-P1



(e) TS1-1d → *anti-Z*-P1

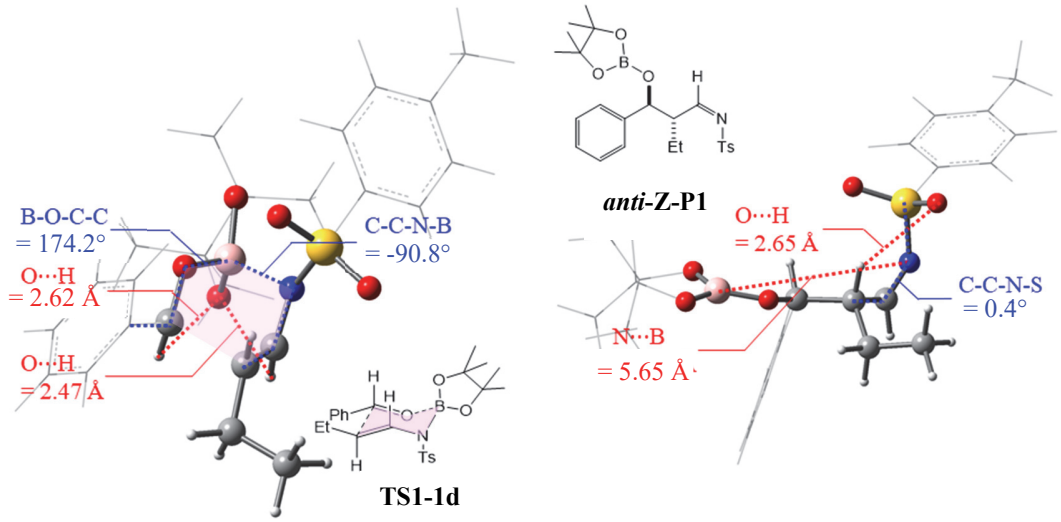
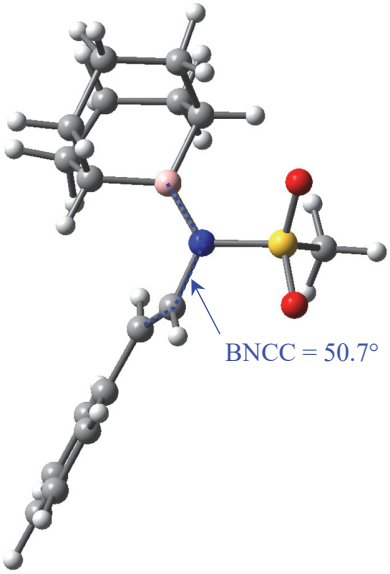


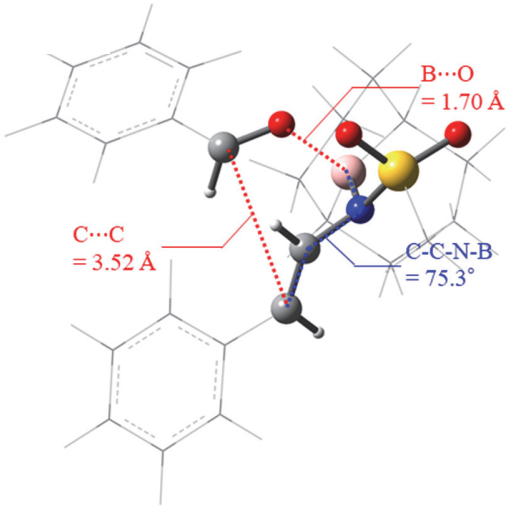
Figure S6. Structures of reactant state, transition states, product states and intermediate states in aza-aldol reaction of **1**.

The aza-aldol reaction of **2** has five pathways. Each transition state has obviously different steric hindrances. The structures and their key steric repulsion of reactants, transition states, and products are shown below.

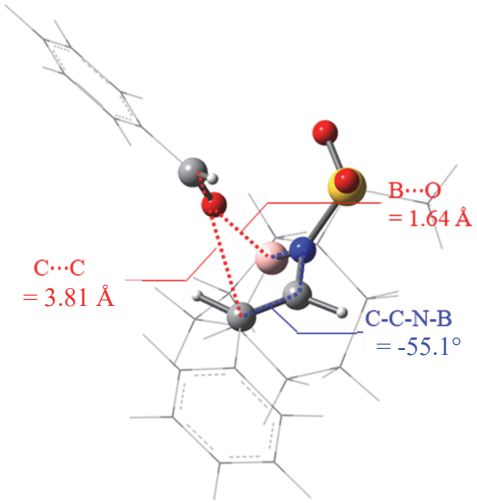
(a) 2



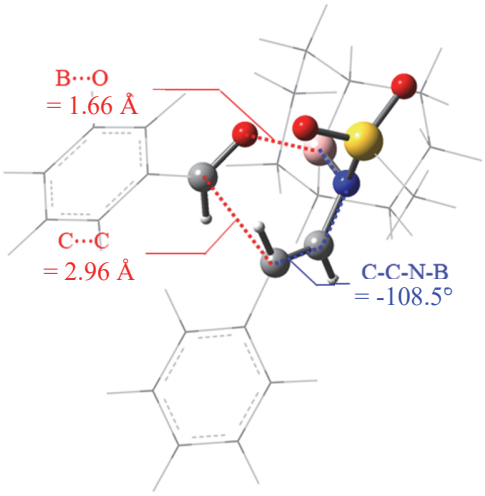
(b) Int-2a



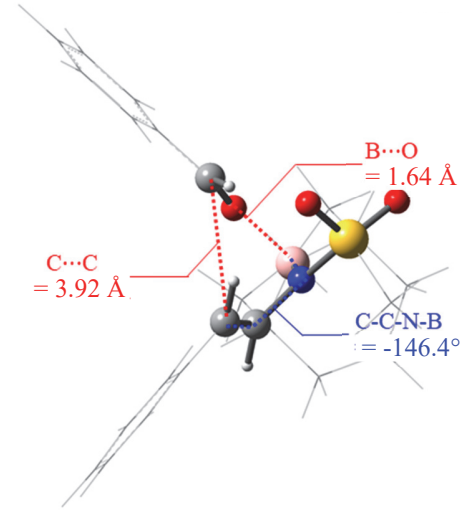
(c)Int-2b



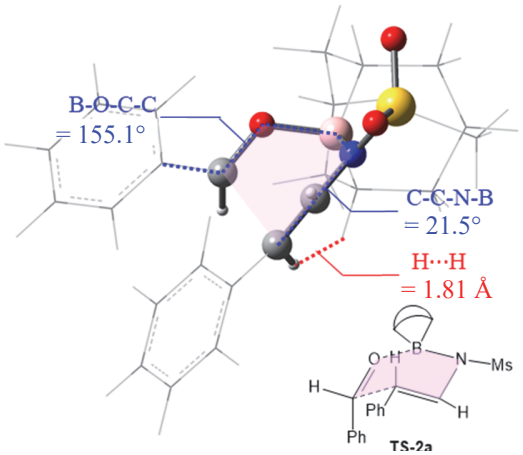
(d)Int-2d



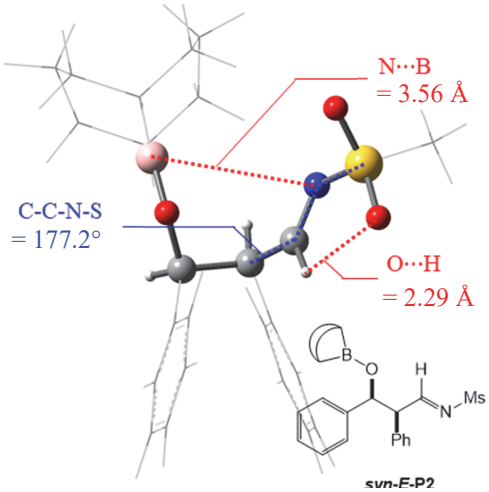
(e)Int-2e



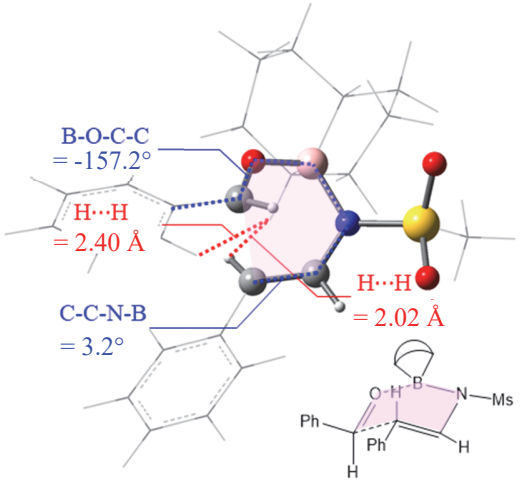
(f) TS2-2a



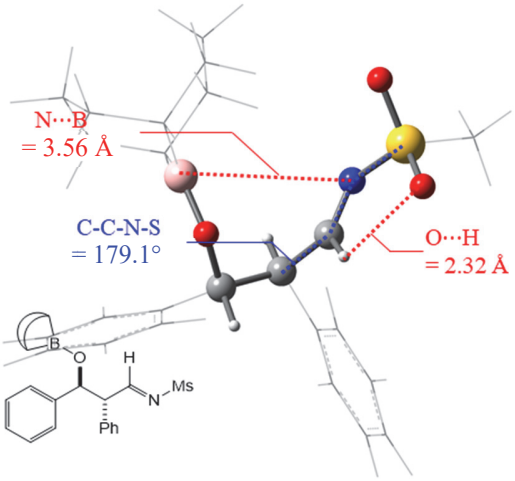
***syn-E*-P2**



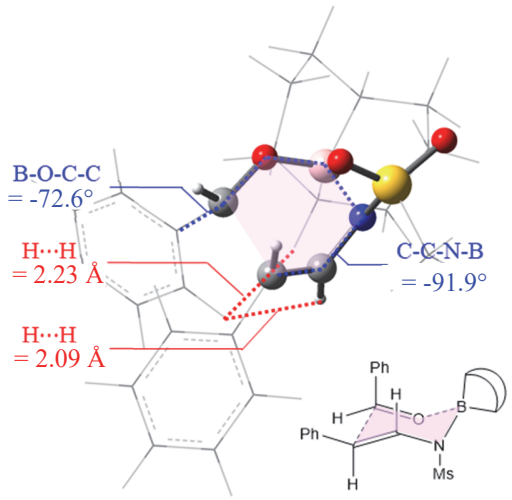
(g) TS2-2b



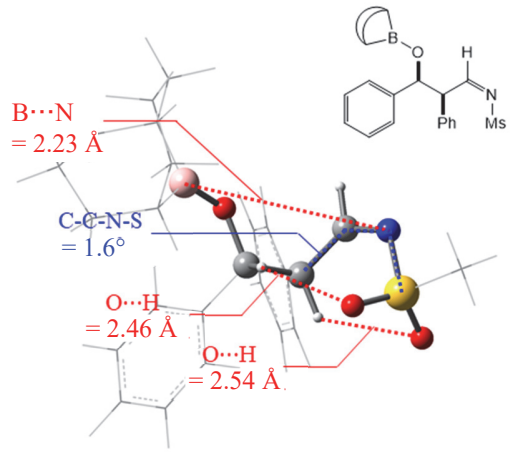
***anti-E*-P2**



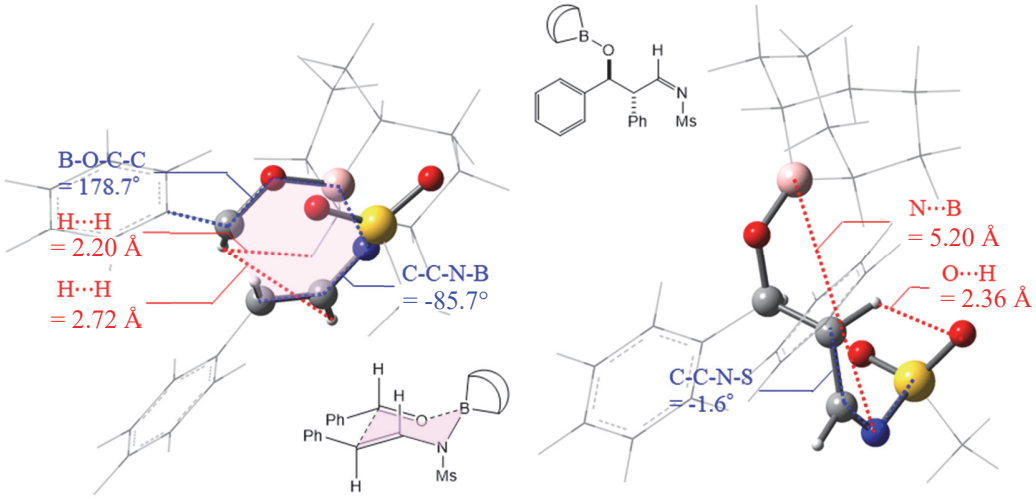
(h) TS2-2c



***syn-Z*-P2**



(i) TS2-2d ***anti-Z*-P2**



(j) TS2-2e ***anyi-Z*-P2**

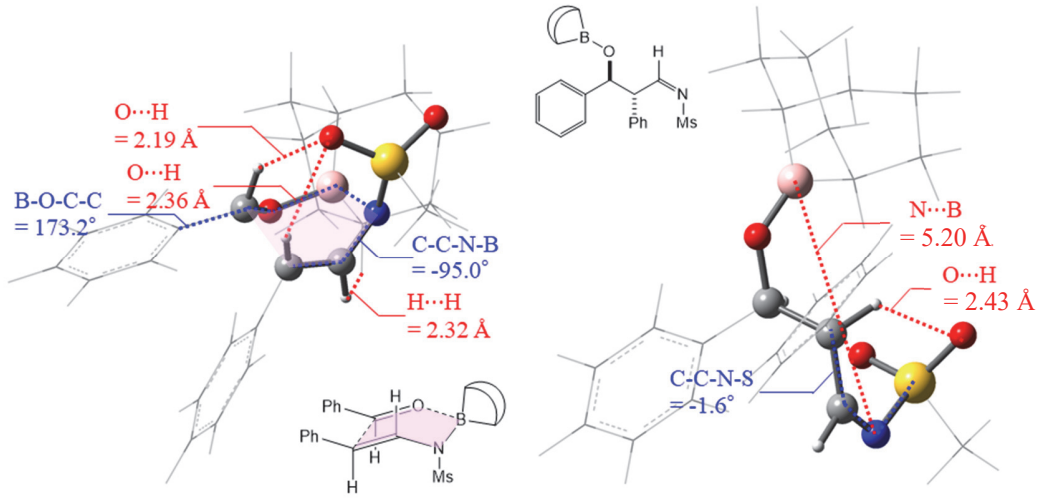


Figure S7. Structures of reactant state, transition states, product states and intermediate states of aza-aldol reaction of **2**.

S6. Structural parameters of the transition state of *E*/*Z* isomerization

Table S5. DFT Calculation of the *E*/*Z* isomerization of **P1**.

	ΔG‡ [kcal/mol][a]	C-N [Å]	S-N [Å]	C-N-S [°]
***syn*-*E*-P1**	-1.5	1.28	1.70	116.2
TS2-*syn*-P1	22.3	1.25	1.59	175.0
***syn*-*Z*-P1**	0.0	1.28	1.69	123.8
***anti*-*E*-P1**	-1.5	1.28	1.70	115.6
TS2-*anti*-P1	16.7	1.26	1.59	171.44
***anti*-*Z*-P1**	0.0	1.28	1.70	118.65

[a]Relative Gibbs energy.

S7. Structural parameters of the reactant states, intermediate states, and transition states, and product states

Table S6. Result of DFT calculation of the substrates and products of **1** and **2**

	ΔG [kcal/mol][a]	B-O [Å]	B-N [Å]	C1-C2 [Å][b]	∠B [deg.]	∠N [deg.]
Reactant state (isolated)						
1+**PhCHO**	1.1		1.45		360.0	357.4
2+**PhCHO**	0.6		1.44		360.0	360.0
Reactant state						
1···**PhCHO**	0.0		1.45		360.0	357.7
2···**PhCHO**	0.0		1.44		360.0	359.9
Product state						
syn-E-Product (***syn-E*-P1**)	-7.9	1.36	3.24	1.56		
anti-E-Product (***anti-E*-P1**)	-7.2	1.35	3.28	1.54		
syn-Z-Product (***syn-Z*-P1**)	-6.9	1.36	4.22	1.55		
anti-Z-Product (***anti-Z*-P1**)	-6.4	1.36	5.70	1.55		
syn-E-Product (***syn-E*-P2**)	-10.8	1.36	3.57	1.57		
anti-E-Product (***anti-E*-P2**)	-9.3	1.37	3.62	1.54		
syn-Z-Product (***syn-Z*-P2**)	-9.9	1.37	4.82	1.56		
anti-Z-Product (***anti-Z*-P2**)	-8.1	1.36	5.23	1.57		

[a]Relative Gibbs energy. [b]For the definition of C1 and C2, see Scheme 1.

Table S7. Results of DFT calculations for the transition states, **TS1-x** and intermediate states, **Int-x (x=2a, 2b, 2d, 2e)**, of **2**.

	$\Delta G^{\ddagger}$, ΔG [kcal/mol][a]	B–O [Å]	B–N [Å]	C1–C2 [Å][b]	∠B [deg.]	∠N [deg.]
Transition state (B–O formation)						
Boat-B (ax) (**TS1-2a**)	7.5	2.01	1.51	3.64	350.4	352.3
Boat-B (eq) (**TS1-2b**)	5.8	2.28	1.48	3.59	353.6	359.9
Chair (eq) (**TS1-2d**)	5.9	2.14	1.49	3.10	352.6	356.8
Boat-A (eq) (**TS1-2e**)	6.3	2.44	1.47	3.42	355.5	360.0
Intermediate state						
Boat-B (ax) (**Int-2a**)	7.5	1.70	1.57	3.52	342.3	346.6
Boat-B (eq) (**Int-2b**)	3.6	1.64	1.55	3.80	339.7	360.0
Chair (eq) (**Int-2d**)	4.9	1.67	1.57	2.94	340.8	349.7
Boat-A (eq) (**Int-2e**)	4.1	1.65	1.56	3.78	340.2	358.8

[a]Gibbs energy relative to **2**···**PhCHO**. $\Delta G^{\ddagger}$ for TS, ΔG for intermediate state. [b]For the definition of C1 and C2, see Scheme 1b.

S8. Natural bond orbital (NBO) analysis for 1 and 2

The interaction energies of three bonds around B atom in **1** and **2** are summarized in Tables S8 and S9, respectively. Spatial distribution of the related NBOs for **1** and **2** is shown in Figures S8 and S9, respectively. The donor-acceptor interaction between the LP orbital of nitrogen and the LP* orbital of boron in **2** was 72.2 kcal mol^{-1}, which is greater than the value of 53.1 kcal mol^{-1} in **1**. On the other hand, the interaction between the carbon-carbon σ orbital of the alkyl substituent and the LP* orbital of the boron in **2** is 17.4 kcal mol^{-1}, so the stabilizing effect of this superconjugation is much smaller than the π donation from the alkoxy substituent seen in **1**. The sum of these stabilization energies is 89.6 kcal mol^{-1}, which is smaller than the total of 227.1 kcal mol^{-1} in **1**. This suggests that the boron in **2** is more Lewis acidic and highly electrophilic than that in **1**, contributing to the formation of the ate complex. Also, as with the simplified model results in section 3.1, the boat-shaped six-membered ring transition state of **2** with 9-BBN is more stable than **1**. As the results of the NBO analysis indicate, the stability of the Lewis pair that **2** forms with the aldehyde may also contribute to the stability of the transition state.

Table S8 Result of NBO interaction analysis for the π type interaction in the N–B, O1–B, and O2–B bonds in **1**. LP*(B) denotes unoccupied 2p orbital of the B atom.

1	Donor NBO	Acceptor NBO	D–A Interaction [kcal/mol]	sum [kcal/mol]
N	LP(N)	LP*(B)	53.14	53.14
O1	LP1(O1)	LP*(B)	64.28	65.02
	LP2(O1)	LP*(B)	0.74	
O2	LP1(O2)	LP*(B)	59.18	108.99
	LP2(O2)	LP*(B)	0.73	
	LP3(O2)	LP*(B)	49.08	
				Total 227.15

Table S9 Result of NBO interaction analysis for the π type interaction N–B, C1–B, and C2–B bonds in **2**. LP*(B) denotes unoccupied 2p orbital of the B atom.

2	Donor NBO	Acceptor NBO	D–A Interaction [kcal/mol]	sum [kcal/mol]
N	LP(N)	LP*(B)	72.18	72.18
C1	σ(C1-C3)	LP*(B)	2.84	8.78
	σ(C1-C4)	LP*(B)	5.94	
C2	σ(C2-C5)	LP*(B)	4.99	8.58

σ(C2-C6)	LP*(B)	3.59	
			Total 89.54

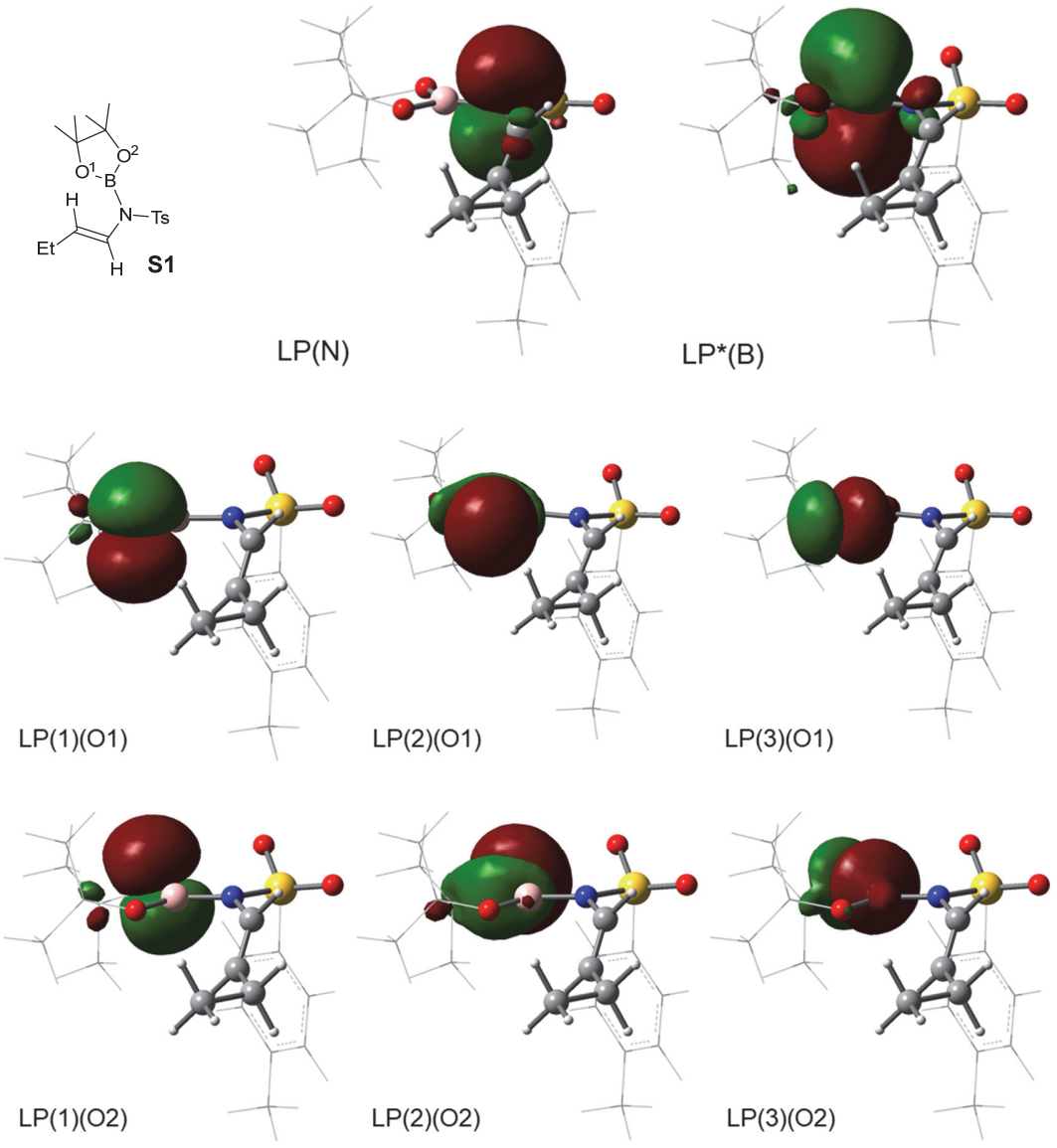


Figure S8. NBOs related the B atom of **1**.

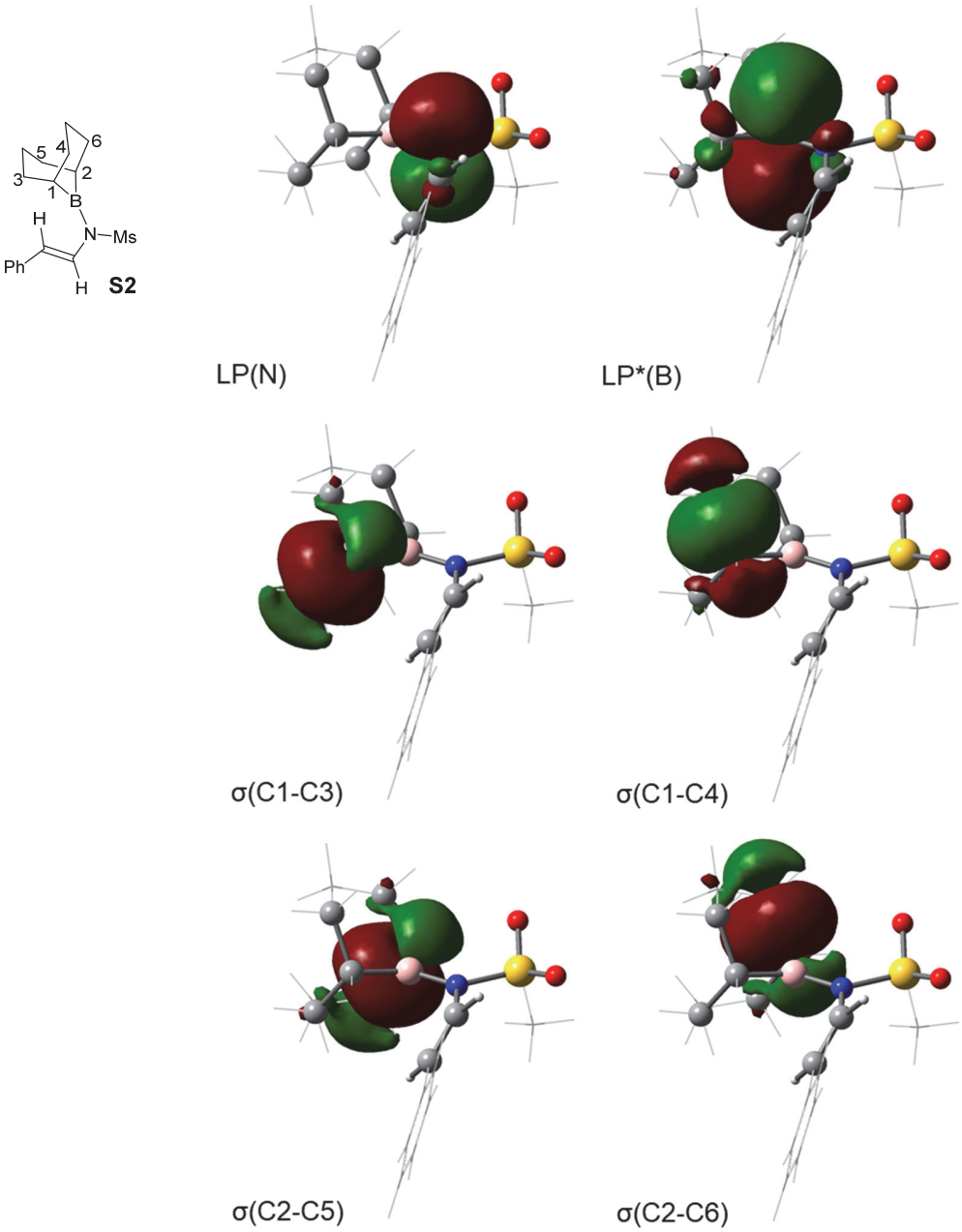
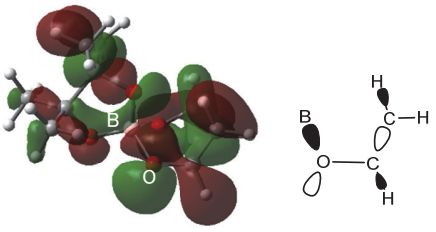


Figure S9. NBOs related the B atom of **2**.

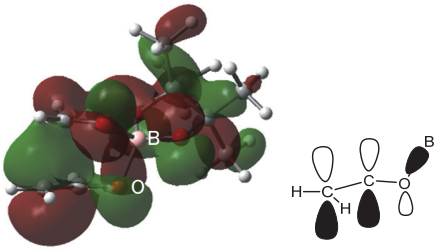
S9. Interaction between boron and carbonyl/imino group in the transition state of the aldol reaction of enolate/aza-enolate

Molecular orbitals shown below are related to the B-N interactions in the Boat-B type TS and chair type TS. In the boat case, a lone-pair (σ orbital) has a bonding interaction with the B atom. In the chair case, π orbital of the N=C moiety is involved in the interaction.

(a) Enolate with Bpin

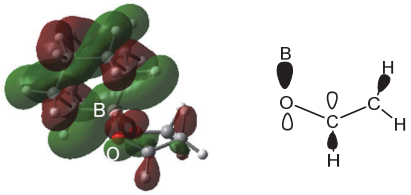


Boat-B form (HOMO-6)

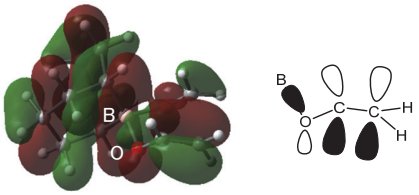


Chair form (HOMO)

(b) Enolate with 9-BBN

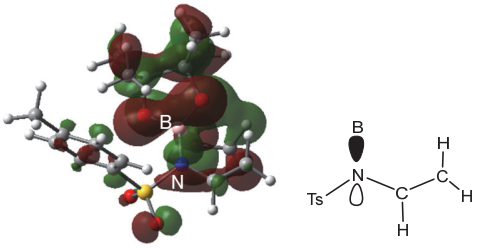


Boat-B form (HOMO-3)

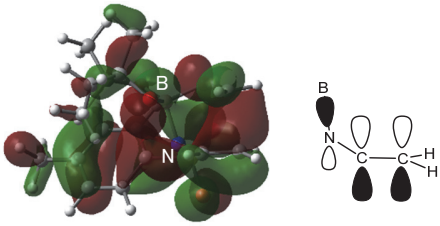


Chair form (HOMO-1)

(c) Aza-enolate with Bpin

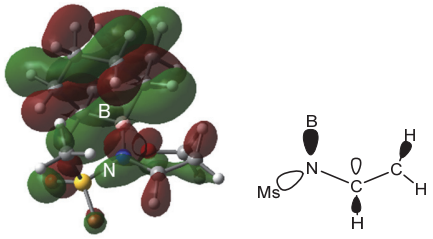


Boat-B form (HOMO-9)

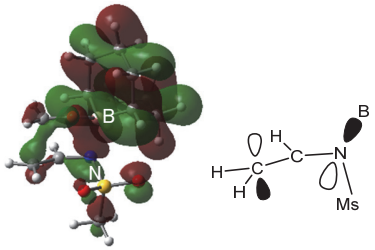


Chair form (HOMO)

(d) Aza-enolate with 9-BBN

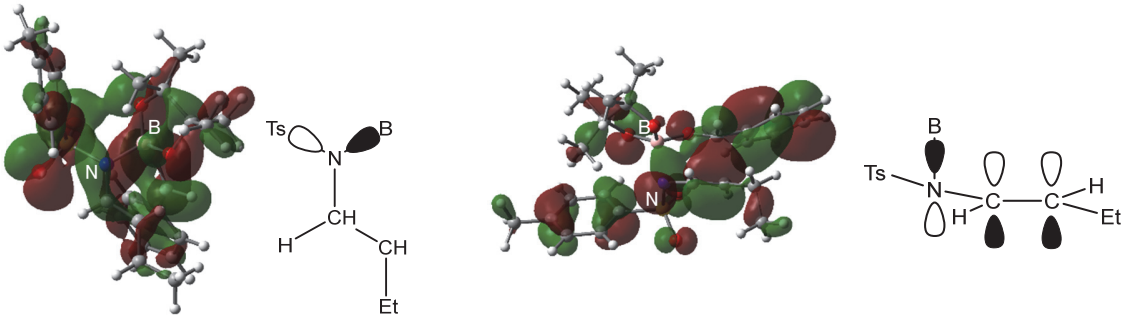


Boat-B form (HOMO-3)



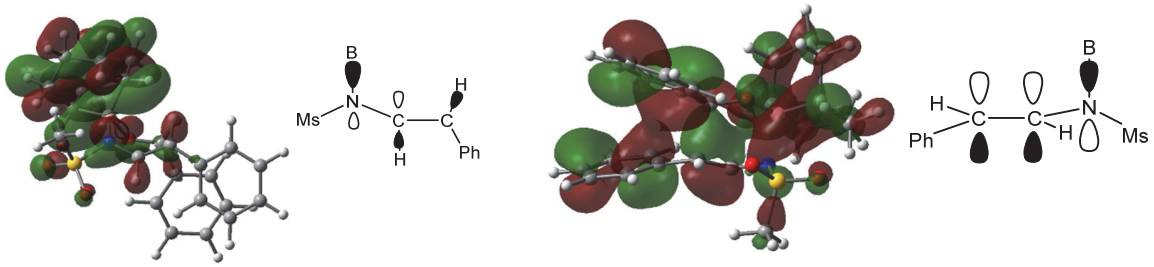
Chair form (HOMO-2)

(e) Case of **1**



Boat-B form (HOMO-9) Chair form (HOMO)

(f) Case of **2**



Boat-B form (HOMO-6) Chair form (HOMO-1)

Figure S10 Kohn-Sham orbitals that involve B–X (X = O for enolate or N for aza-enolate) bonding in the transition state. (a−d) The reactions in the simplified model systems and (e, f) the reactions with **1** and **2**. The orbitals for the Boat-B and Chair transition states are shown for each case.

S10. Aza-aldol reaction with a bulkier substituent.

In section 2.1, we employed simpler model compounds to exclude any steric effect from the substituent groups at the C1 position of aza-enolate and aldehyde. In contrast, an examination with a bulkier group would be useful for a more stable conclusion. For this purpose, aza-enolate **7** was employed.

In the same way as in the aza-enolate **1**, four types of TS was obtained. **TS1-7a** and **TS1-7b** adopt the Boat-B type transition state but produce syn- and anti-products, respectively. Calculated activation Gibbs energy was smallest for **TS1-7a** (23.4 kcal mol^{-1}) that gives syn product and second smallest for **TS1-7b** (25.8 kcal mol^{-1}). This result is very similar to that obtained for aza-enolate **1**. As the steric repulsion between the substituents at the C1 position and aldehyde determines the relative stability of **TS1-7a**, it would be reasonable for **TS1-7a** to be the most stable transition state. The activation energy for **TS1-7c** and **TS1-7d**, which are the Chair type TSs, were 37.0 kcal mol^{-1} and 30.6 kcal mol^{-1}, respectively, and this relative stability of the Chair TSs is also similar to that observed in **1**.

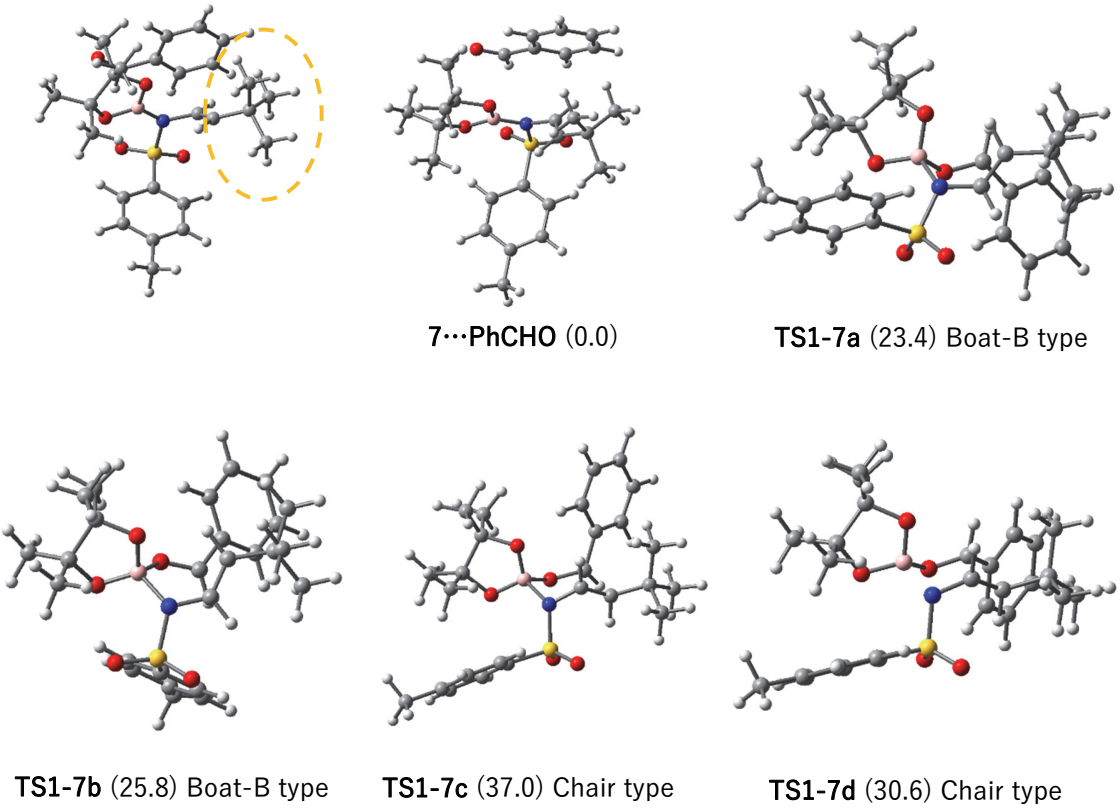


Figure S11 Structure of aza-enolate **7** with a ^{t}Bu group at the C1 position of aza-enolate. The number in parentheses is the Gibbs energy relative (in kcal mol^{-1}) to the **7···PhCHO** state.

S11. Steric repulsions between the substituents in Chair/Boat TSs

Here, we discuss the origin of the syn/anti selectivity in Boat-B/Chair TS in the simplified aza-enolate **5** and **6** in terms of the steric repulsions between the substituents in the 6-membered ring. As shown in Figure S12, the newly formed C-C bond in the Boat-B TS takes eclipsed conformation. The H-C-C-H dihedral angle in **5** and **6** is 25.6° and 16.6°, respectively. In these TS structures, flagpole-flagpole repulsion and flagpole-pseudoequatorial repulsion direct bulky substituent groups being in bowsprit and pseudoaxial positions, which results in syn selectivity. In contrast, the H-C-C-H angles of Chair TS in **5** and **6** are 47.6° and 42.5°, respectively, indicating the C-C bonds are in staggered conformation. The 1,3-diaxial repulsive interaction in this TS conformation leads the substituent group of aldehyde to an equatorial position and that of aza-enolate to an equatorial position, which causes anti selectivity. This interpretation was led by the present DFT calculations which reproduced the experimental syn/anti selectivity.

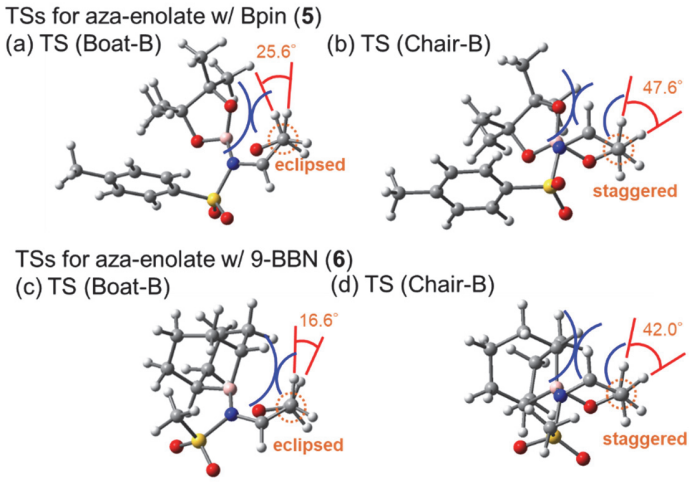


Figure S12 TS Structures of aza-enolates **5** and **6.**

S12. Atomic coordinate of the optimized structures

Atomic coordinates of the intermediates and transition states are given below. For the transition state, imaginary frequency is also given. Unit for energy is Hartree, and that for the frequency is cm^{-1}.

B = Bpin, O-enolate

Reactant
ωB97XD/6-311+G**
Potential Energy = -564.519466333
Gibbs Free Energy (T = 298.15K) = -564.327379
C 3.12485300 0.28577600 0.10067700
C 4.41531700 -0.00366200 0.03676200
B 0.84462000 -0.35267300 -0.09821600
H 2.74728700 1.26715300 0.37272900
O 0.34429500 0.85670800 0.31160200
O -0.11585500 -1.26377500 -0.43215300
C -1.07338600 0.83375500 0.02445600
C -1.37850800 -0.70750500 -0.00507000
C -1.80749400 1.60784800 1.10580800
H -2.88897400 1.52458700 0.96511400
H -1.55402700 1.24377100 2.10130400
H -1.53701300 2.66438100 1.04952900
C -2.45754400 -1.12136300 -0.99146800
H -2.18498800 -0.86352500 -2.01470600
H -2.60437700 -2.20216100 -0.94090300
H -3.40613600 -0.63544600 -0.74534900
C -1.67746300 -1.28301400 1.37812800
H -2.65367900 -0.95541200 1.74328300
H -1.67931800 -2.37267900 1.31195100
H -0.91658500 -0.98886200 2.10513300
C -1.26488800 1.50718400 -1.33287100
H -0.74935600 0.95923600 -2.12521500
H -2.32324200 1.58168800 -1.59319700
H -0.84764500 2.51520700 -1.28859800
H 4.75804000 -0.99391300 -0.23717200
H 5.14587100 0.76133500 0.26182900
O 2.16977500 -0.64994500 -0.17609900

Chair TS
ωB97XD/6-311+G**
Potential Energy = -679.001338480
Gibbs Free Energy (T = 298.15K) = -678.778836
Imaginary Frequency = 265.5291*i*
C 2.59315500 -0.72260900 0.85483300
C 3.76959600 -0.33973500 0.28029300
B 0.58460000 -0.27190600 -0.29085000
H 2.35884300 -0.42795900 1.88207800
O 0.05165200 0.47271500 0.79765100
O -0.44010000 -0.79170800 -1.07980900
C -1.33811400 0.67022600 0.51031600
C -1.66743100 -0.58447800 -0.37229900
C -2.10721700 0.74512500 1.82010500
H -3.18470500 0.77816600 1.63239100
H -1.88751900 -0.11224900 2.45656800
H -1.82862900 1.65265900 2.36152300
C -2.78686800 -0.37093100 -1.37978600
H -2.53412900 0.41464800 -2.09226900
H -2.95711000 -1.29360000 -1.93920700
H -3.71805600 -0.10278500 -0.87110800
C -1.94838700 -1.83299000 0.46655400
H -2.91492300 -1.76979100 0.97375500
H -1.95926200 -2.70146400 -0.19536900
H -1.16650600 -1.98696600 1.21351100
C -1.48786200 1.98461100 -0.25998100
H -0.96628300 1.94040300 -1.21874000
H -2.53789800 2.22525900 -0.44486200
H -1.05046800 2.79109200 0.33406200
H 4.03147600 -0.70751300 -0.70477300
C 2.45095500 1.25890700 -0.54357100
H 2.20761700 1.74484400 0.40305800
O 1.55833400 0.62531000 -1.17145500
H 3.29188500 1.64752000 -1.11703200
H 4.54454300 0.11336400 0.88768800
O 1.64025900 -1.26817300 0.15788800

Boat TS
ωB97XD/6-311+G**
Potential Energy = -679.004191524
Gibbs Free Energy (T = 298.15K) = -678.781678
Imaginary Frequency = 264.5760*i*
C 2.82151300 -1.02916300 0.48943800
C 3.13036500 0.17593600 1.04744800
B 0.60848800 -0.39166300 -0.32908600
H 3.60329700 -1.75724300 0.27194600
O 0.16969300 0.47653100 0.70447900
O -0.48542100 -0.93349500 -1.00582300
C -1.22360100 0.72308000 0.46963800
C -1.66261900 -0.58808200 -0.26968800

C -1.91162200 0.96357500 1.80417300
H -2.99491800 1.03867200 1.67005900
H -1.69929700 0.15930300 2.50859100
H -1.55747500 1.90113300 2.24001000
C -2.81902400 -0.40735300 -1.24132000
H -2.56114900 0.28850300 -2.03998500
H -3.06721600 -1.36833300 -1.69743500
H -3.70728100 -0.03689400 -0.72025300
C -1.96705800 -1.73252400 0.69946200
H -2.90190900 -1.56570300 1.24132400
H -2.05742100 -2.65790400 0.12685500
H -1.15819500 -1.85968600 1.42258800
C -1.34826800 1.96671700 -0.41420400
H -0.88476200 1.80508600 -1.39014200
H -2.39322000 2.24717800 -0.56836800
H -0.84067300 2.80054200 0.07801900
H 2.35436900 0.76496500 1.51644100
C 2.35125800 1.24335400 -0.88310700
H 1.98744600 1.97199500 -0.16021800
O 1.56135000 0.40579900 -1.37945700
H 3.28945700 1.43726600 -1.40436200
H 4.16110400 0.36961000 1.31750500
O 1.64934600 -1.38301200 0.05852700

B = Bpin, N-enolate

Reactant
ωB97XD/6-311+G**
Potential Energy = -1363.56072134
Gibbs Free Energy (T = 298.15K) = -1363.252021
C 1.02781900 2.83856200 -1.02457400
N 0.61683200 1.79806200 -0.15322900
C 2.12185200 2.85733100 -1.77896300
B 1.28215500 0.52570200 -0.00211300
H 0.33851900 3.67312700 -1.02851100
S -0.82810200 2.04786200 0.72177200
O -0.55547700 1.93748400 2.13530300
O -1.42081200 3.25651200 0.18606100
C -3.04550100 -1.31530900 0.79430000
C -2.26573100 -0.23618700 1.18871200
C -1.82318000 0.65528700 0.22607200
C -2.14282600 0.49126900 -1.11545000
C -2.90977200 -0.59918600 -1.49320900
C -3.36946700 -1.51854800 -0.54649100
H -3.40022900 -2.01606000 1.54297700
H -1.98467900 -0.08841900 2.22378500
H -1.79266800 1.20424700 -1.85348100
H -3.16130800 -0.73688800 -2.53965200
O 2.32128700 0.10679700 -0.78383700
O 0.87163800 -0.40803800 0.90680400
C 2.75997300 -1.16563600 -0.24420100
C 1.47702400 -1.65737200 0.50826500
C 3.20395500 -2.05340500 -1.39345400
H 3.44188500 -3.05611500 -1.02698400
H 2.43219200 -2.13293600 -2.15888900
H 4.10186200 -1.63762900 -1.85523300
C 1.74324800 -2.49012600 1.74938500
H 2.31532400 -1.93155000 2.48980000
H 0.79438100 -2.78413600 2.20286200
H 2.29363800 -3.39832600 1.48741600
C 0.47780700 -2.36373700 -0.40752100
H 0.83777000 -3.35276300 -0.70071400
H -0.46807200 -2.47802200 0.12569400
H 0.28346500 -1.78011000 -1.31088000
C 3.92922600 -0.87573200 0.69308000
H 3.62053600 -0.24507600 1.52992700
H 4.35516600 -1.79998800 1.09040500
H 4.70631000 -0.34809900 0.13658600
C -4.17330100 -2.71703100 -0.97388100
H -4.77527800 -3.10655200 -0.15086700
H -4.84209800 -2.47124400 -1.80148600
H -3.51123800 -3.52051000 -1.31206200
H 2.83890900 2.05041600 -1.81211400
H 2.29679800 3.73279200 -2.39082400

Chair TS
ωB97XD/6-311+G**
Potential Energy = -1478.04400763
Gibbs Free Energy (T = 298.15K) = -1477.701659
Imaginary Frequency = 244.0273*i*
C 1.89633600 -1.88254900 1.16305100
N 0.83548700 -1.22258800 0.61187600
C 2.52828200 -2.95861400 0.61054200
B 1.43584000 0.05358500 -0.17132400
H 2.38727100 -1.32426400 1.95623100
S -0.36846700 -2.17978000 -0.13318500
O -0.05830600 -2.45785100 -1.52258200
O -0.59643700 -3.28661300 0.77869200
C -3.28693500 0.38875300 -1.16592600
C -2.16925300 -0.43167100 -1.22105100
C -1.76895600 -1.09092100 -0.06977800
C -2.45895900 -0.94871900 1.12641400
C -3.56842000 -0.11903700 1.16475000
C -3.99574300 0.56257500 0.02285000
H -3.60996900 0.90653400 -2.06295200
H -1.60520300 -0.55636100 -2.13579300
H -2.13519900 -1.48978100 2.00735100
H -4.11531200 -0.00237200 2.09451000
O 2.22656600 0.83015100 0.72015100

O 0.52850200 0.87043600 -0.85568200
C 1.98053200 2.20438600 0.39071300
C 0.52797500 2.14096000 -0.19282300
C 2.12407700 3.04372800 1.65028000
H 1.82724100 4.07930200 1.45852900
H 1.51259000 2.64676100 2.46075900
H 3.16672000 3.04455000 1.97749200
C 0.20305600 3.21963800 -1.21389000
H 0.85822900 3.15381400 -2.08279000
H -0.82792200 3.09815400 -1.55510200
H 0.30129000 4.21458500 -0.76906300
C -0.53872100 2.12052000 0.90372700
H -0.61499600 3.08972500 1.40361000
H -1.50479200 1.88805800 0.45246400
H -0.32079100 1.35410400 1.65070000
C 3.01169300 2.64042800 -0.65251200
H 2.90149700 2.06844700 -1.57657100
H 2.92064100 3.70416700 -0.88706100
H 4.01317500 2.46195600 -0.25316100
C -5.17990800 1.48938400 0.08481500
H -5.64188900 1.61109500 -0.89674100
H -5.93816900 1.11894100 0.77797700
H -4.87023200 2.48020700 0.43232000
H 2.05526400 -3.55792300 -0.15906700
C 3.31243000 -1.38235100 -0.73257900
H 3.95233100 -0.91078500 0.01447000
O 2.31458600 -0.75092500 -1.19055900
H 3.74440200 -2.14996500 -1.37310600
H 3.38748700 -3.38294400 1.11778400

Boat TS
ωB97XD/6-311+G**
Potential Energy = -1478.05138032
Gibbs Free Energy (T = 298.15K) = -1477.710469
Imaginary Frequency = 255.8848*i*
C 1.55747100 -2.34418600 1.07679800
N 0.79189000 -1.44304400 0.40833400
C 2.74775300 -2.03803800 1.66597700
B 1.43744300 -0.12610100 -0.12907700
H 1.21962300 -3.37481500 1.03126800
S -0.53439400 -2.12524500 -0.44784700
O -0.25332000 -2.13327500 -1.86400700
O -0.83664200 -3.37128300 0.23420900
C -3.53919900 0.48542600 -0.96927800
C -2.44910500 -0.34104700 -1.20556000
C -1.85510100 -0.98343600 -0.13169900
C -2.32308800 -0.81776200 1.16459900
C -3.40026400 0.02528500 1.38357100
C -4.02334700 0.68759200 0.32261300
H -4.01472600 0.98891700 -1.80442600
H -2.05096100 -0.48482400 -2.20183600
H -1.85226100 -1.34208100 1.98792600
H -3.76988000 0.16648800 2.39381400
O 2.06326900 0.67862300 0.85833200
O 0.64524300 0.67149000 -0.96196400
C 1.99841700 2.02964800 0.38104800
C 0.66878400 2.01020800 -0.44489800
C 1.99635900 2.96760200 1.57821500
H 1.82334200 3.99947500 1.25833100
H 1.22756900 2.68811400 2.29837100
H 2.96587400 2.92624000 2.08069500
C 0.63113400 2.98235300 -1.61390200
H 1.41193400 2.76011700 -2.34137600
H -0.33408000 2.90631400 -2.12001300
H 0.75322300 4.01204300 -1.26393000
C -0.55872900 2.21462200 0.44259500
H -0.61029400 3.24035200 0.81693000
H -1.45858100 2.01580100 -0.14025700
H -0.54738200 1.53047900 1.29335100
C 3.22913600 2.30417700 -0.48793300
H 3.24115000 1.66910200 -1.37602800
H 3.26430700 3.34824000 -0.80871600
H 4.12857200 2.09922900 0.09883800
C -5.17348000 1.62387500 0.57757500
H -5.79801800 1.73815700 -0.31035600
H -5.80205900 1.26676500 1.39610400
H -4.80245600 2.61587000 0.85410500
H 2.96727800 -1.02409800 1.96678200
C 3.60449500 -1.29042000 -0.38695000
H 4.13916600 -0.60403300 0.26769900
O 2.58526100 -0.90456600 -1.00674300
H 4.11415700 -2.18560800 -0.74515000
H 3.30645700 -2.84381800 2.12524100

B = 9-BBN, O-enolate
Reactant
ωB97XD/6-311+G**
Potential Energy = -491.389006354
Gibbs Free Energy (T = 298.15K) = -491.167271
C -2.91604700 0.00239700 0.28534400
C -4.17335600 -0.00133100 -0.13022900
B -0.55292600 -0.00023700 -0.24777200
H -2.64722000 0.00821600 1.33725000
H -4.41616000 -0.00710800 -1.18582700
C 0.54430200 -0.00437300 -1.36879300
H 0.10174600 -0.00719800 -2.37007000
C 0.06732800 0.00418000 1.19986100
H -0.66212400 0.00683600 2.01623300

C 0.89614800 1.30928400 1.32813400
H 1.41872500 1.31823300 2.29238000
H 0.19052500 2.14961700 1.35924600
C 0.89537800 -1.30065800 1.33641500
H 0.18908700 -2.14018400 1.37341400
H 1.41829100 -1.30351100 2.30051700
C 1.36664500 -1.30690400 -1.20558800
H 2.20021100 -1.31319700 -1.91847400
H 0.71967000 -2.14664500 -1.48959900
C 1.36825700 1.29815100 -1.21373100
H 0.72243700 2.13680500 -1.50351700
H 2.20214500 1.29875300 -1.92627700
C 1.90978000 -1.56291900 0.21033500
H 2.24309700 -2.60383400 0.27699900
H 2.80467900 -0.96152900 0.37612500
C 1.91117500 1.56301000 0.20068600
H 2.80535800 0.96179100 0.37092700
H 2.24557900 2.60399800 0.26040500
H -4.97763100 0.00141700 0.59295900
O -1.87643100 -0.00078700 -0.59730400

Chair TS
ωB97XD/6-311+G**
Potential Energy = -605.886714280
Gibbs Free Energy (T = 298.15K) = -605.632604
Imaginary Frequency = 214.4667*i*
C 2.40720300 -1.04740500 0.23660500
C 3.57039500 -0.43203500 -0.11395300
B 0.32678900 0.00390300 -0.28466900
H 2.26891400 -1.40694800 1.26213900
H 3.74259000 -0.15480800 -1.14728300
C 2.26422300 1.42541700 0.23588500
H 2.15170400 1.27542400 1.31092400
O 1.29678800 1.24877600 -0.54379700
C -0.84234100 -0.01446400 -1.35396100
H -0.43804100 -0.00074000 -2.37385200
C -0.29874100 0.00216300 1.19357600
H 0.44737600 0.02494500 2.00265700
C -1.06370900 -1.33108200 1.35303000
H -1.56141500 -1.36708000 2.33062700
H -0.32354000 -2.14159300 1.35730100
C -1.16890400 1.26640500 1.36130800
H -0.49892300 2.13655600 1.38651600
H -1.67620600 1.25080400 2.33454600
C -1.69705900 1.25654500 -1.17252100
H -2.55130500 1.24353400 -1.86139400
H -1.08151100 2.11515000 -1.46846100
C -1.61235700 -1.34075300 -1.17825200
H -0.94313000 -2.15207300 -1.48728000
H -2.47255600 -1.37527000 -1.85900600
C -2.21509500 1.49657100 0.25629400
H -2.58431900 2.52538700 0.33175400
H -3.08453300 0.86366500 0.44242900
C -2.09888600 -1.62871100 0.25356300
H -3.01227600 -1.06515100 0.45301700
H -2.38827100 -2.68306600 0.32296600
H 3.08484400 2.05648200 -0.10482900
H 4.40991500 -0.42910400 0.57151200
O 1.37925700 -1.08021900 -0.55750100

Boat TS
ωB97XD/6-311+G**
Potential Energy = -605.886050156
Gibbs Free Energy (T = 298.15K) = -605.631967
Imaginary Frequency = 131.1108*i*
C 2.61226600 -1.05629100 -0.38817200
C 3.16543400 -0.50751400 0.72385700
B 0.34216300 -0.01118500 -0.35863800
H 3.26464300 -1.50845900 -1.13661700
H 2.57563700 -0.25977500 1.59304400
C 2.15502400 1.67064300 0.00025400
H 1.97943100 1.72347100 1.07476200
O 1.26934400 1.28000400 -0.77474200
C -0.91454700 -0.07439500 -1.32801600
H -0.58813200 -0.08961700 -2.37544500
C -0.17102300 0.04607600 1.16007700
H 0.62056000 0.11931100 1.91723500
C -0.87724500 -1.30524200 1.42180000
H -1.28984200 -1.32154000 2.43851600
H -0.11048300 -2.08928400 1.38970000
C -1.07331500 1.28597300 1.35126500
H -0.43766400 2.18131100 1.30289000
H -1.50331200 1.28281900 2.36102100
C -1.78691500 1.17939300 -1.12791300
H -2.68660600 1.12281400 -1.75373100
H -1.21813900 2.04373500 -1.49385100
C -1.63375200 -1.41286700 -1.05118700
H -0.97107800 -2.21678700 -1.39192200
H -2.54542900 -1.48841300 -1.65742600
C -2.20730800 1.45049400 0.32555400
H -2.60246600 2.46971800 0.39925500
H -3.03938100 0.79790600 0.59494100
C -1.99121200 -1.66826800 0.42408000
H -2.90205400 -1.12532000 0.68332600
H -2.23994900 -2.72772600 0.54941700
H 4.23897500 -0.57455200 0.84779700
H 3.03292700 2.16715600 -0.41663400
O 1.36154500 -1.04236100 -0.75059500

B = 9-BBN, N-enolate

Reactant
ωB97XD/6-311+G**
Potential Energy = -1059.40766397
Gibbs Free Energy (T = 298.15K) = -1059.139184
C -1.49736000 1.89759900 0.60017100
N -1.04494400 0.59799100 0.20275600
C -1.09171700 3.01123100 0.01173700
B 0.33464200 0.20646000 0.11789200
H -2.20798100 1.91279900 1.41829200
S -2.31880400 -0.47546000 -0.18955700
O -3.55085500 0.24240300 0.06093900
O -2.06284700 -1.05859400 -1.48779100
H -0.41638700 2.99497200 -0.83564200
C 0.87022900 -1.17353400 -0.43231300
H 0.09479200 -1.87443500 -0.74557000
C 1.52555900 1.14476300 0.55237800
H 1.19013300 2.09772100 0.96748100
C 2.34865300 1.46147200 -0.72120700
H 3.24468500 2.03171600 -0.44790400
H 1.74641800 2.13001900 -1.34967800
C 2.32081800 0.41935800 1.66467200
H 1.67789800 0.36287400 2.55333900
H 3.18161900 1.03299600 1.95632300
C 1.72444000 -1.86768400 0.65424500
H 2.19123400 -2.76635300 0.23365600
H 1.04516400 -2.22440600 1.44128700
C 1.64544800 -0.80810300 -1.72786500
H 0.91047400 -0.44377000 -2.45585900
H 2.07167800 -1.72091700 -2.16028600
C 2.80174500 -0.99443200 1.31394000
H 3.14841100 -1.48896300 2.22731600
H 3.67708100 -0.93427600 0.66590500
C 2.75573800 0.24018900 -1.56232200
H 3.64054200 -0.22832000 -1.12885500
H 3.06475900 0.58336700 -2.55496800
C -2.18111000 -1.75229500 1.05153600
H -2.28391800 -1.28745100 2.03067100
H -3.00531500 -2.44087400 0.86568900
H -1.22575100 -2.26145600 0.94785100
H -1.42831200 3.97201600 0.38010400

Chair TS
ωB97XD/6-311+G**
Potential Energy = -1173.89894712
Gibbs Free Energy (T = 298.15K) = -1173.597602
Imaginary Frequency = 294.3185*i*
C 1.30929000 1.18750500 1.20858900
N 0.97918600 0.02653200 0.58207500
C 2.04165400 2.22351300 0.68114600
B -0.51604000 0.30142300 -0.11314600
H 0.71209400 1.38496200 2.09479300
S 2.20199200 -0.74195000 -0.32976400
O 1.65224800 -1.97709200 -0.83535000
O 2.87361600 0.16790400 -1.24467900
H 2.72619100 2.06672500 -0.14275900
C 0.33889100 2.56276500 -0.52824500
H -0.27637600 3.02155700 0.24739800
O -0.01465800 1.45110500 -1.03895700
C -1.14562400 -0.88725600 -0.96841900
H -0.45549000 -1.25520800 -1.73098500
C -1.60635400 0.76356500 0.98431100
H -1.29474000 1.59649400 1.63016600
C -1.86367400 -0.43211800 1.92502700
H -2.62286200 -0.16642300 2.67176200
H -0.93803400 -0.62427500 2.48387100
C -2.85910100 1.27741400 0.23838800
H -2.59369100 2.22305600 -0.25378700
H -3.64369600 1.52856000 0.96352900
C -2.37550400 -0.32659900 -1.71572500
H -2.84716900 -1.12590000 -2.30073600
H -2.01633700 0.41155900 -2.44292500
C -1.45977000 -2.07247400 -0.03181000
H -0.50405200 -2.50278400 0.28141900
H -1.97704600 -2.86114800 -0.59252600
C -3.43835200 0.33261100 -0.82593800
H -4.13491600 0.89725200 -1.45548000
H -4.04249400 -0.43716100 -0.34275500
C -2.28555200 -1.73104500 1.22062800
H -3.34535000 -1.67248000 0.96547700
H -2.20501500 -2.55861400 1.93404600
C 3.35385200 -1.15076300 0.97531400
H 2.84063600 -1.77544200 1.70369800
H 4.16041900 -1.70187000 0.49213000
H 3.73618200 -0.23579200 1.42519200
H 0.89516600 3.23442700 -1.18052300
H 2.17241400 3.11283000 1.28871900

Boat TS
ωB97XD/6-311+G**
Potential Energy = -1173.90210290
Gibbs Free Energy (T = 298.15K) = -1173.600908
Imaginary Frequency = 20.2059*i*
C 1.63202700 1.70538700 0.62900100
N 1.09134900 0.52273600 0.16139000
C 1.02004000 2.73140600 1.25756500

B -0.44644200 0.36892500 -0.18943300
H 2.68009800 1.83252400 0.37950000
S 2.29478000 -0.58573100 -0.33819800
O 1.83311300 -1.34379800 -1.47647100
O 3.56326500 0.11586000 -0.42345400
H 0.04336700 2.67483800 1.70667700
C -0.59190100 2.83542900 -0.80710400
H -1.22984800 3.06050700 0.04719500
O -0.45012300 1.68359800 -1.21895000
C -0.98815800 -0.85585300 -1.07347200
H -0.36434500 -1.02818100 -1.95098400
C -1.45566900 0.53019800 1.05910400
H -1.22917500 1.35732100 1.73726300
C -1.25018000 -0.74714100 1.90661400
H -1.86873900 -0.69462700 2.81086000
H -0.21006300 -0.74724000 2.25694200
C -2.91562200 0.74504700 0.59883600
H -3.01045200 1.77156600 0.21970200
H -3.58503100 0.69445200 1.46701700
C -2.39533300 -0.48396900 -1.59071300
H -2.76729300 -1.29156600 -2.23275700
H -2.31092400 0.39736100 -2.23750100
C -0.99878900 -2.16707100 -0.25718700
H 0.02286700 -2.55354700 -0.23339800
H -1.57230300 -2.92791100 -0.80105500
C -3.42649100 -0.20784500 -0.49231900
H -4.33240400 0.21607600 -0.93898700
H -3.73896300 -1.15279100 -0.04371100
C -1.55146500 -2.06771400 1.18014800
H -2.63236800 -2.21958400 1.17075700
H -1.15345000 -2.89745600 1.77599600
C 2.39609000 -1.66883200 1.07831600
H 1.42746700 -2.13380100 1.24751200
H 3.15174000 -2.41688400 0.83871100
H 2.70115200 -1.07112600 1.93597900
H 1.62227200 3.60045000 1.49036300
H -0.18465600 3.65801400 -1.39921100

Boat-A TS
ωB97XD/6-311+G**
Potential Energy = -1173.883942
Gibbs Free Energy (T = 298.15K) = -1173.582956
Imaginary Frequency = 359.4*i*
C 1.40350000 1.19420900 1.19155300
N 0.99862600 0.03715400 0.65089800
C 2.22182400 2.17018500 0.62980000
B -0.57939900 0.44130300 0.06205600
H 0.72606600 1.53492700 1.97271300
S 2.14012700 -0.81862300 -0.30014200
O 1.57489700 -2.10734700 -0.61153200
O 2.66156600 0.01122200 -1.37830300
H 3.02136500 1.91988200 -0.05626400
C 0.79196300 2.40423800 -0.71238600
H 1.36390200 1.86940300 -1.47357600
O -0.35841400 1.90711100 -0.36492300
C -1.13216500 -0.49364500 -1.11962700
H -0.41975900 -0.61032300 -1.94564300
C -1.64964600 0.43999000 1.25545100
H -1.33047700 1.04859900 2.11412900
C -1.84770700 -0.99836600 1.76413100
H -2.56765900 -1.01032600 2.59245600
H -0.89289200 -1.34587400 2.17912300
C -2.93104000 1.11397900 0.70791500
H -2.71215400 2.18089000 0.59527900
H -3.73626200 1.04050000 1.45007500
C -2.35617600 0.27127200 -1.68177900
H -2.80134700 -0.31125600 -2.49780400
H -2.00767700 1.20943500 -2.12545400
C -1.49950500 -1.90969900 -0.62157500
H -0.57377900 -2.46774200 -0.48650700
H -2.05640400 -2.43008700 -1.41153100
C -3.44861700 0.58060900 -0.64347100
H -4.13877100 1.31866300 -1.06671400
H -4.04900400 -0.31593900 -0.48039900
C -2.30733900 -1.98735900 0.68622100
H -3.37036500 -1.83421100 0.49046600
H -2.22872000 -3.00580200 1.08217600
C 3.44697900 -1.08068200 0.89165000
H 3.03245300 -1.62882500 1.73556700
H 4.19133100 -1.68278700 0.37079400
H 3.87418300 -0.12788900 1.19800200
H 2.35762800 3.07152200 1.21754800
H 0.80610400 3.49233600 -0.76795800

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ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1441.91307164
Gibbs Free Energy (T = 323K) = -1441.553571
C 0.25374600 2.35845200 0.64204600
N 0.30292000 1.00770100 1.11930100
C 0.17876500 2.65435100 -0.65306700
B 1.23635900 0.04886700 0.56778000
C 0.22359000 4.04938700 -1.19882100
C 1.47069300 4.28341600 -2.06026000
H 2.38080500 4.14931100 -1.46686000
H 1.47393700 5.29721800 -2.47271200
H 1.50800100 3.57679400 -2.89666600
H 0.19627300 4.77262900 -0.37584300

H -0.67238600 4.22405900 -1.80842600
H 0.28976400 3.12323900 1.41148700
S -1.05562400 0.49560800 1.97508400
O -0.65113100 -0.55498900 2.89427600
O -1.68848700 1.70335900 2.48854200
C -2.78026500 -2.07323800 -0.60622300
C -2.01429100 -1.55848100 0.43181700
C -2.09931200 -0.19878600 0.72022800
C -2.92928400 0.64594000 -0.01314900
C -3.68618700 0.11116300 -1.04860000
C -3.62456000 -1.25078400 -1.35962800
H -2.72026800 -3.13346100 -0.83626100
H -1.34938100 -2.19371500 1.00528500
H -2.98424500 1.70188800 0.22751900
H -4.33675000 0.76370800 -1.62399700
O 2.25550800 0.42818900 -0.26026900
O 1.16486000 -1.29841400 0.78912000
C 3.06904900 -0.75288000 -0.47071900
C 2.05264600 -1.91025200 -0.17952000
C 3.60895500 -0.72360400 -1.89239800
H 4.14730500 -1.65098600 -2.11394600
H 2.80703400 -0.60052400 -2.62357200
H 4.30678500 0.11126300 -2.00523900
C 2.66475700 -3.15831400 0.43635100
H 3.14503900 -2.94036200 1.39241100
H 1.88444700 -3.90566700 0.60777500
H 3.40845000 -3.59053300 -0.24134600
C 1.19638300 -2.27927700 -1.39156600
H 1.78591500 -2.80120800 -2.15099200
H 0.38726400 -2.93960100 -1.06677400
H 0.74531900 -1.39164900 -1.84710400
C 4.21614600 -0.69158400 0.53734600
H 3.84449100 -0.72107600 1.56638600
H 4.91493000 -1.52110400 0.39477400
H 4.76057500 0.24659200 0.39744700
C -4.47097300 -1.82737800 -2.46446000
H -3.96995000 -2.66925700 -2.95096500
H -5.42266200 -2.19664000 -2.06476800
H -4.70138300 -1.07537000 -3.22428800
H 0.13329600 1.84254000 -1.37828600

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1442.25018448
Gibbs Free Energy (T = 323K) = -1441.896037
C 0.20895200 2.32723700 0.64660800
N 0.28223900 0.97622500 1.11428700
C 0.14744700 2.63474400 -0.63899100
B 1.23549600 0.04416900 0.56127700
C 0.16783200 4.03287800 -1.16768700
C 1.41575100 4.30355300 -2.01118400
H 2.32027300 4.18421300 -1.41095300
H 1.40132400 5.31826700 -2.41343800
H 1.47771400 3.60741300 -2.85132500
H 0.11455500 4.74307300 -0.33847100
H -0.72316100 4.19281300 -1.78374300
H 0.21573800 3.08470300 1.42073800
S -1.04964100 0.44237600 1.96873600
O -0.62978000 -0.61727300 2.84072200
O -1.67300800 1.61893100 2.51544900
C -2.79123300 -2.06633900 -0.63736000
C -2.00589200 -1.56863900 0.38637400
C -2.10353800 -0.22426600 0.71800600
C -2.97281000 0.61858000 0.04192800
C -3.75117400 0.10246400 -0.98148400
C -3.67019200 -1.24100400 -1.33869300
H -2.72419800 -3.11726900 -0.89575500
H -1.31554800 -2.20541200 0.92248800
H -3.04403600 1.66134200 0.32154200
H -4.43734500 0.75592200 -1.50793800
O 2.25545200 0.45699000 -0.24411500
O 1.19149800 -1.30430500 0.75642700
C 3.09749500 -0.70119100 -0.46788400
C 2.10412700 -1.88205700 -0.20957500
C 3.65085100 -0.63527700 -1.87850100
H 4.20602400 -1.54703000 -2.11026900
H 2.85748200 -0.51180600 -2.61448300
H 4.33442500 0.21077600 -1.96557100
C 2.73441700 -3.12315200 0.39112000
H 3.19090100 -2.91273800 1.35712800
H 1.97202700 -3.89098900 0.53201600
H 3.49879500 -3.52102600 -0.28027600
C 1.27272300 -2.24617400 -1.43542100
H 1.88021300 -2.74549100 -2.19194100
H 0.47380400 -2.92370500 -1.13065100
H 0.81427100 -1.36172800 -1.88295300
C 4.22799200 -0.63503700 0.55250900
H 3.84620300 -0.69575500 1.57336500
H 4.94552900 -1.44289900 0.40006000
H 4.74983100 0.31608500 0.43802100
C -4.49708100 -1.79307400 -2.46626000
H -3.89060100 -1.89223100 -3.37063900
H -4.88362400 -2.78382900 -2.22164800
H -5.33909700 -1.14065400 -2.69884100
H 0.13232100 1.83130100 -1.37153100

PhCHO
ωB97XD/6-31G*
Solvent = THF
Potential Energy = -345.457990203

Gibbs Free Energy (T = 323K) = -345.380240
C 2.21068200 -0.24735000 0.00000000
C 1.72906500 1.06009800 0.00000000
C 0.35678700 1.28900300 0.00000100
C -0.53148200 0.21097300 0.00000000
C -0.04357200 -1.10038300 0.00000000
C 1.32557100 -1.32760800 0.00000000
H 3.28143300 -0.42787200 0.00000000
H 2.42099400 1.89621800 0.00000000
H -0.02878700 2.30581200 0.00000100
H -0.74968800 -1.92490100 0.00000000
H 1.70879900 -2.34316200 0.00000000
C -1.98690300 0.46869600 0.00000000
H -2.27177900 1.54054300 0.00000400
O -2.84023300 -0.39590100 -0.00000300

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -345.549236475
Gibbs Free Energy (T = 323K) = -345.472400
C -2.20429000 -0.24280200 -0.00000800
C -1.72168400 1.05846200 -0.00000600
C -0.35337800 1.28276700 0.00000400
C 0.52907100 0.20697700 0.00001000
C 0.03981700 -1.09853000 0.00001000
C -1.32458100 -1.32153100 0.00000300
H -3.27312500 -0.42066400 -0.00001600
H -2.41030700 1.89421300 -0.00001300
H 0.03531000 2.29584700 0.00000600
H 0.74365700 -1.92202800 0.00001700
H -1.70981100 -2.33377600 0.00000300
C 1.98384300 0.46482700 0.00000700
H 2.26649300 1.53638400 0.00002600
O 2.83187400 -0.39387500 -0.00001800

1···PhCHO

ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.38863554
Gibbs Free Energy (T = 323K) = -1786.928668
C 1.27873500 -1.25094500 1.12838600
N 0.31482300 -0.71523800 0.22218700
C 1.31172800 -0.95002300 2.42323100
B -0.06865500 0.67859600 0.19514600
C 2.42157600 -1.38674700 3.33307600
C 3.21178100 -0.19145300 3.87852600
H 3.65993000 0.37823400 3.05806600
H 4.01225900 -0.52264300 4.54794500
H 2.55949900 0.48713700 4.43928000
H 3.09633600 -2.06245600 2.79421200
H 2.00374100 -1.95499400 4.17445000
H 2.02691700 -1.88996300 0.67178000
S -0.45492800 -1.80253900 -0.80615900
O -0.27292000 -1.40046100 -2.19513600
O -0.00755800 -3.12857100 -0.39527600
C -4.40047200 -0.97721000 -0.96957400
C -3.07012400 -1.15615000 -1.33491800
C -2.16546000 -1.59518200 -0.37844800
C -2.56252500 -1.85313100 0.93254200
C -3.89108500 -1.65937500 1.28124900
C -4.82877000 -1.22119300 0.33717400
H -5.11364000 -0.63063100 -1.71208400
H -2.73100600 -0.93913500 -2.34121300
H -1.84058800 -2.18816600 1.67119400
H -4.20804900 -1.84998900 2.30274200
O 0.31072700 1.57839900 1.14821400
O -0.90035200 1.18027100 -0.76172300
C -0.19892900 2.86920300 0.72395900
C -1.34333600 2.46994300 -0.27850800
C -0.67476100 3.62362200 1.95718800
H -1.14850500 4.56700600 1.66625000
H -1.38977300 3.03755300 2.53871600
H 0.18044500 3.85590700 2.59876800
C -1.49412200 3.40202500 -1.47043800
H -0.58131700 3.42256100 -2.06940100
H -2.31451700 3.05554600 -2.10598500
H -1.72684700 4.41835100 -1.13575200
C -2.69352700 2.23743900 0.40092500
H -3.12933600 3.17556900 0.75725300
H -3.37842100 1.78478200 -0.32146600
H -2.60043900 1.54878800 1.24741900
C 0.95937900 3.61290400 0.06284800
H 1.31437500 3.08767100 -0.82835100
H 0.66478200 4.62808400 -0.22072300
H 1.78433900 3.68296100 0.77875900
C -6.27232300 -1.03779400 0.72668000
H -6.79927100 -0.39529300 0.01614600
H -6.78936900 -2.00407900 0.75017800
H -6.36005200 -0.59560100 1.72367600
H 0.54657500 -0.30212900 2.84586800
C 4.75299900 -1.28871600 -0.03578800
C 4.14652900 -2.02697900 -1.05075700
C 3.24514600 -1.40694100 -1.91103600
C 2.95403700 -0.04907000 -1.75971800
C 3.55850100 0.68587800 -0.73502400
C 4.45577100 0.06561300 0.12422300
H 5.45681500 -1.77010400 0.63654400
H 4.37379700 -3.08155200 -1.16919800
H 2.76030800 -1.97514600 -2.70052400
H 3.31910600 1.73876000 -0.62556800

H 4.93059000 0.63508900 0.91701700
C 2.02229000 0.59993300 -2.70839500
H 1.59688100 -0.06771500 -3.47862400
O 1.73317300 1.78111200 -2.68661200

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.81612476
Gibbs Free Energy (T = 323K) = -1787.362693
C 1.06146300 -1.42183700 1.03137900
N 0.24243700 -0.70149100 0.11412000
C 1.03914300 -1.23967500 2.34173600
B -0.02467300 0.71120600 0.23092700
C 2.01229800 -1.89732000 3.26924600
C 2.94376900 -0.87880900 3.93000200
H 3.52775100 -0.34930200 3.17417500
H 3.63458500 -1.36805200 4.61977500
H 2.37372900 -0.13505600 4.49229700
H 2.60159500 -2.63667600 2.71957400
H 1.46376400 -2.43946500 4.04657300
H 1.75085000 -2.11539400 0.56881600
S -0.55166600 -1.59755300 -1.05131100
O -0.37619300 -0.97655300 -2.33587700
O -0.12481700 -2.96043600 -0.86314700
C -4.43618300 -0.56490400 -0.94265100
C -3.11739000 -0.69397600 -1.34965500
C -2.25069200 -1.45508300 -0.58634500
C -2.67886000 -2.08249000 0.57709300
C -3.99468500 -1.93696800 0.97265500
C -4.89289300 -1.17833400 0.21967700
H -5.11879900 0.03205400 -1.53664600
H -2.75566600 -0.19848800 -2.23993100
H -1.98757000 -2.67287800 1.16565600
H -4.33432900 -2.41987600 1.88189900
O 0.41826000 1.46688900 1.27325800
O -0.78301900 1.38915300 -0.67207900
C 0.05680000 2.84076500 0.97823200
C -1.09842800 2.66656300 -0.07001600
C -0.36111000 3.51324500 2.27294100
H -0.72654800 4.52324900 2.07436600
H -1.14266600 2.95295300 2.78444700
H 0.49981000 3.58850000 2.93930700
C -1.12365700 3.71817600 -1.16267900
H -0.20537600 3.69753400 -1.74781400
H -1.96303000 3.52767600 -1.83363200
H -1.25087200 4.71380700 -0.73162400
C -2.47587700 2.51737500 0.56717000
H -2.81656900 3.45827800 1.00248600
H -3.18685900 2.21069300 -0.20117200
H -2.47270600 1.75151600 1.34591900
C 1.29616000 3.51650500 0.40649000
H 1.60637500 3.05381300 -0.53136100
H 1.11657300 4.57877900 0.23041300
H 2.10939300 3.42199100 1.12861000
C -6.32702400 -1.04984300 0.65097300
H -6.80809400 -0.19187200 0.18058800
H -6.89056700 -1.94418000 0.37155300
H -6.40353300 -0.94026300 1.73406600
H 0.33921300 -0.53165600 2.77451200
C 4.54937900 -1.59650500 -0.01809500
C 3.92216600 -2.17973200 -1.11071500
C 3.14322900 -1.40036800 -1.95272700
C 2.99936900 -0.03841300 -1.70752700
C 3.62504900 0.54156200 -0.60572100
C 4.39670500 -0.23761200 0.23720900
H 5.15582300 -2.20384400 0.64335000
H 4.03536100 -3.23960200 -1.30193900
H 2.63912300 -1.84667900 -2.80285500
H 3.49928500 1.60189800 -0.42540200
H 4.88515400 0.21052800 1.09384100
C 2.19328500 0.77924300 -2.63899700
H 1.72081300 0.21763100 -3.46375200
O 2.04887600 1.97572600 -2.54548400

***syn-E*-P1**
ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.41290232
Gibbs Free Energy (T = 323K) = -1786.948182
C 0.53994300 -1.31668000 0.45983300
N -0.48636500 -0.76126300 -0.05940900
C 1.44405800 -0.52397900 1.35053700
B 1.31253200 1.91207600 -0.40802100
C 1.90449700 -1.36804700 2.54886500
C 2.61027900 -0.55127300 3.63092300
H 3.55452200 -0.12411800 3.27924000
H 2.83723800 -1.18121400 4.49604000
H 1.97738000 0.27580000 3.97067500
H 2.55166000 -2.18328500 2.20436800
H 1.01764500 -1.84007100 2.98831400
H 0.79041300 -2.36359200 0.25497600
S -1.38968700 -1.71404000 -1.14030900
O -1.36138600 -0.99924400 -2.41128900
O -0.97267800 -3.11556100 -1.10019600
C -5.00722400 -0.30454100 -0.08859800
C -3.75236000 -0.42319000 -0.67014900
C -3.00218300 -1.57106400 -0.42456000
C -3.48788100 -2.59434700 0.38318500
C -4.74748000 -2.45810100 0.95450600
C -5.52098100 -1.31473400 0.73265000

H -5.60108000 0.58462300 -0.28025000
H -3.36369300 0.35644600 -1.31653100
H -2.89354600 -3.48583900 0.55176200
H -5.13741100 -3.25613000 1.57973700
O 1.02198900 2.48389500 0.80731200
O 0.74630200 2.55528300 -1.47631100
C 0.32639600 3.72096200 0.52152800
C -0.23611700 3.45899200 -0.92080500
C -0.73580500 3.94259400 1.58770200
H -1.34246200 4.82117400 1.34439900
H -1.39465800 3.07662100 1.68169600
H -0.25735000 4.11690700 2.55620000
C -0.32582000 4.69608700 -1.80117900
H 0.65338300 5.15691100 -1.94843400
H -0.72619200 4.42180000 -2.78164700
H -0.99841800 5.43494700 -1.35272000
C -1.57128400 2.71185600 -0.91340100
H -2.38765100 3.35319400 -0.56747000
H -1.79312700 2.38377500 -1.93338500
H -1.52145700 1.82287500 -0.27658000
C 1.36762300 4.83916700 0.56609600
H 2.13382500 4.69921400 -0.20294300
H 0.90471300 5.81996100 0.42236200
H 1.85818500 4.82902200 1.54377200
C -6.87209500 -1.16214800 1.38078000
H -6.77914100 -0.63668200 2.33845100
H -7.55182000 -0.58112400 0.75110200
H -7.33059000 -2.13463500 1.58019500
H 0.87189800 0.33456700 1.71501500
C 5.18021600 -3.03306000 -1.04609000
C 4.03838000 -2.65271200 -1.74867400
C 3.22118200 -1.63800000 -1.26051300
C 3.53487800 -0.99307300 -0.06122800
C 4.68648500 -1.36979400 0.62994600
C 5.50442000 -2.38701200 0.14354300
H 5.81783800 -3.82436800 -1.42851200
H 3.78381900 -3.14519800 -2.68229900
H 2.34286200 -1.33105700 -1.82037100
H 4.95321100 -0.86231900 1.55348000
H 6.39836900 -2.66819000 0.69204500
C 2.61472200 0.06945100 0.50281600
H 3.18281100 0.73312600 1.16457500
O 2.09609900 0.81635900 -0.58484500

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.83778007
Gibbs Free Energy (T = 323K) = -1787.378433
C 0.60043300 -1.30109300 0.40162800
N -0.42112700 -0.76154100 -0.12528500
C 1.46186200 -0.51722500 1.33766400
B 1.21525900 1.95383300 -0.35225000
C 1.94424500 -1.39745200 2.49576700
C 2.59887100 -0.60914500 3.62519800
H 3.52432700 -0.12512400 3.30850700
H 2.84326500 -1.26895800 4.45909000
H 1.92738600 0.16923000 3.99586100
H 2.62844200 -2.16364800 2.12010000
H 1.07562200 -1.92838700 2.89586700
H 0.87638800 -2.33486400 0.17343000
S -1.29707600 -1.69327900 -1.21977200
O -1.32293100 -0.93566200 -2.44356600
O -0.83261800 -3.06088400 -1.24380300
C -4.97978900 -0.52796300 -0.14023300
C -3.74086700 -0.58107300 -0.75450400
C -2.88991100 -1.63689400 -0.46405100
C -3.26266800 -2.63621900 0.42206600
C -4.50559600 -2.56819400 1.02678000
C -5.37836400 -1.51439700 0.76033200
H -5.65189400 0.29122500 -0.36868900
H -3.43698100 0.18088800 -1.46039500
H -2.59077100 -3.45992000 0.62572300
H -4.80616800 -3.35045000 1.71428400
O 0.80879000 2.45096800 0.85831000
O 0.66395600 2.59356400 -1.42628300
C 0.02623200 3.63670400 0.57800600
C -0.42066400 3.39449600 -0.90493800
C -1.11334000 3.71848700 1.57607800
H -1.77808800 4.54827400 1.32496700
H -1.69499100 2.79771900 1.59398700
H -0.71451300 3.89358300 2.57682200
C -0.55104300 4.65461700 -1.73891700
H 0.39602200 5.18787600 -1.81067900
H -0.87517500 4.39399400 -2.74776400
H -1.29768900 5.32256900 -1.30317100
C -1.68582500 2.54824700 -1.01311200
H -2.56838400 3.10867000 -0.69897500
H -1.81528400 2.24752000 -2.05398300
H -1.60352700 1.64203300 -0.41055600
C 0.95819300 4.83287300 0.73472300
H 1.77681000 4.79410600 0.01359000
H 0.42086700 5.77333900 0.60133900
H 1.38476300 4.81896600 1.73890200
C -6.71347800 -1.43300400 1.44561000
H -6.62474400 -0.87796000 2.38362000
H -7.44639100 -0.91678100 0.82450100
H -7.09710300 -2.42559600 1.68436300
H 0.84902100 0.29328400 1.73585400
C 5.37524400 -2.71642100 -1.05052400
C 4.21910000 -2.39618700 -1.74989500

C 3.33839000 -1.45153500 -1.24638300
C 3.60156500 -0.81756200 -0.03516300
C 4.76709400 -1.13294700 0.65247300
C 5.64944300 -2.07987000 0.15069900
H 6.06372900 -3.45387700 -1.44544400
H 4.00324500 -2.88157900 -2.69417800
H 2.44785100 -1.18897000 -1.80487800
H 4.99403400 -0.63160700 1.58700700
H 6.55525300 -2.31432700 0.69699500
C 2.61386200 0.16928300 0.54386100
H 3.13263400 0.83116500 1.24250500
O 2.08891600 0.93408000 -0.52753400

***anti-E*-P1**

ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.41194594
Gibbs Free Energy (T = 323K) = -1786.947058
C 0.35952800 0.08779500 1.00081300
N 1.06311900 -0.26704600 -0.00453100
C -0.60289200 1.23106600 0.94141900
B -2.10515900 -0.72827500 -0.71288000
C 0.06051700 2.45405100 1.62776400
C 1.29046600 3.02236400 0.91978000
H 2.06198200 2.26050300 0.76560100
H 1.72683400 3.82473400 1.52212400
H 1.04111300 3.44659000 -0.05770000
H 0.33210100 2.15655500 2.64754000
H -0.70421300 3.23104800 1.72892800
H 0.47554600 -0.39904400 1.97531400
S 2.15867000 -1.53338600 0.27602900
O 2.11004500 -1.98975300 1.66621400
O 1.93790300 -2.50066200 -0.79329600
C 5.55447300 0.55041300 0.85349900
C 4.37600800 -0.14782600 1.08507500
C 3.69254800 -0.69184300 0.00105000
C 4.16502800 -0.54729500 -1.30049700
C 5.34584200 0.15282500 -1.51119000
C 6.05607400 0.70989400 -0.44240000
H 6.09463500 0.97691100 1.69388800
H 3.99357800 -0.27409800 2.09234700
H 3.61867700 -0.97936000 -2.13192600
H 5.72199200 0.26947700 -2.52354600
O -2.19917600 -1.07707800 0.61702700
O -2.57585900 -1.69514200 -1.56399600
C -2.94711600 -2.31352600 0.67533900
C -2.75199000 -2.89122800 -0.77213300
C -2.36951800 -3.17466500 1.78850600
H -2.84441000 -4.16124000 1.79502800
H -1.29100600 -3.30430800 1.67273500
H -2.55572700 -2.70066900 2.75706900
C -3.94642900 -3.66738800 -1.30775100
H -4.84235900 -3.04491500 -1.35916600
H -3.72579100 -4.03285300 -2.31501400
H -4.15543500 -4.53275400 -0.66991500
C -1.47496300 -3.71848400 -0.92131700
H -1.55007700 -4.66864300 -0.38400000
H -1.31676300 -3.93378200 -1.98204200
H -0.59613800 -3.17780600 -0.55708200
C -4.39577800 -1.93688600 0.98508700
H -4.82229200 -1.31658300 0.19007600
H -5.02252400 -2.82498800 1.10847400
H -4.42142300 -1.36444800 1.91718600
C 7.35048800 1.44229000 -0.68058100
H 7.35312900 1.93848300 -1.65515500
H 7.53053300 2.19477100 0.09218900
H 8.19392600 0.74219400 -0.66411000
H -1.45251300 0.94364100 1.56756000
C -4.20251400 4.56408700 -0.25552600
C -2.97455700 4.86646100 -0.83581500
C -1.98220700 3.89084500 -0.91633500
C -2.20491200 2.61114400 -0.41210000
C -3.44117700 2.31408700 0.16899500
C -4.43475300 3.28330000 0.24532900
H -4.97840000 5.32127100 -0.19500100
H -2.78825900 5.85974000 -1.23295900
H -1.02770500 4.12847900 -1.37949300
H -3.62710300 1.31759900 0.56325200
H -5.39232000 3.04059900 0.69632600
C -1.12040500 1.55303800 -0.47457300
H -0.28691100 1.93026200 -1.07345500
O -1.59891300 0.42643500 -1.20095500

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.83649303
Gibbs Free Energy (T = 323K) = -1787.377736
C 0.38648100 0.05938600 0.99988200
N 1.05854900 -0.32685400 -0.00604900
C -0.55074400 1.21941600 0.94398100
B -2.11941700 -0.69897700 -0.70461400
C 0.15010000 2.42536200 1.61746300
C 1.38384100 2.95674100 0.89359900
H 2.12637700 2.17306000 0.72610000
H 1.85374100 3.74133100 1.48882600
H 1.13337900 3.38925500 -0.07661300
H 0.42517400 2.12345300 2.63198900
H -0.59065300 3.22040900 1.72645200
H 0.51223900 -0.41647600 1.97642600
S 2.13505900 -1.58912300 0.25905600

O 2.08619700 -2.05451700 1.62699600
O 1.91170300 -2.53000900 -0.80775800
C 5.51108600 0.49382400 0.86036600
C 4.33599700 -0.20330600 1.07984100
C 3.66296200 -0.74658200 -0.00429400
C 4.14630000 -0.60114200 -1.29577300
C 5.32323600 0.09836300 -1.49708100
C 6.02167900 0.65444000 -0.42669700
H 6.04205200 0.92044800 1.70360600
H 3.94467400 -0.33003900 2.08099000
H 3.60721900 -1.03261800 -2.12903800
H 5.70609600 0.21607200 -2.50433400
O -2.24825200 -1.03833000 0.62077700
O -2.59796300 -1.65570500 -1.55761800
C -3.03214300 -2.25292400 0.67171900
C -2.82399900 -2.84299200 -0.76568400
C -2.50502300 -3.12334800 1.79670900
H -3.00612900 -4.09391900 1.79335200
H -1.43123900 -3.28295900 1.70596500
H -2.70139000 -2.64286000 2.75686500
C -4.02476700 -3.58605000 -1.32102500
H -4.89809600 -2.93956000 -1.39679500
H -3.79151600 -3.96484100 -2.31745000
H -4.27225400 -4.43774400 -0.68313700
C -1.56918900 -3.70189100 -0.88232500
H -1.68349900 -4.64680400 -0.34829900
H -1.39186200 -3.92083500 -1.93632500
H -0.68875800 -3.18492400 -0.49666600
C -4.47229400 -1.83518200 0.94740300
H -4.86462500 -1.21086300 0.14204500
H -5.12275700 -2.70367300 1.06308000
H -4.50074400 -1.25852700 1.87353000
C 7.31354400 1.38822600 -0.65284100
H 7.32946200 1.86822600 -1.63200900
H 7.47513000 2.14974300 0.11097300
H 8.15665800 0.69316700 -0.61129800
H -1.39828400 0.95765100 1.57950800
C -4.05325900 4.64007300 -0.24957700
C -2.82635800 4.90038200 -0.83976500
C -1.86675700 3.89895800 -0.91834700
C -2.12149800 2.63525700 -0.40359300
C -3.35663300 2.38076800 0.18813700
C -4.31774200 3.37527200 0.26233500
H -4.80480900 5.41819900 -0.19031400
H -2.61513300 5.88238400 -1.24593800
H -0.91131400 4.10342400 -1.38957200
H -3.56891900 1.39564500 0.59118600
H -5.27662900 3.16533100 0.72123000
C -1.06890000 1.54993500 -0.46501500
H -0.23251400 1.90382000 -1.06915700
O -1.57797400 0.43555100 -1.19004100

***syn-Z*-P1**

ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.41184968
Gibbs Free Energy (T = 323K) = -1786.946596
C -1.14311700 -1.98579900 0.74990100
N 0.08108800 -2.34256900 0.82828300
C -1.88410700 -0.76478700 1.22304500
B -0.50221000 1.66724000 -0.36549800
C -3.08711000 -1.20662400 2.07171300
C -2.66042400 -1.87550100 3.37791500
H -2.08569900 -2.79004400 3.19232000
H -3.53452400 -2.14705400 3.97699600
H -2.03327600 -1.20465300 3.97498600
H -3.72553700 -1.88472300 1.49273100
H -3.69146000 -0.31853000 2.29155200
H -1.77346700 -2.72253900 0.24132900
S 1.28225000 -1.42758100 1.59450100
O 0.96028500 -0.00868900 1.75663700
O 1.64631100 -2.19540300 2.78169600
C 3.75844600 -0.63821500 -1.47501900
C 2.74800700 -0.52315600 -0.52705100
C 2.56913600 -1.55778600 0.38598400
C 3.37564900 -2.69334000 0.36757800
C 4.37945200 -2.78681400 -0.58667200
C 4.58665500 -1.76320000 -1.51888800
H 3.90338000 0.16375500 -2.19362900
H 2.10966600 0.35495300 -0.50411100
H 3.22205300 -3.48622500 1.09183100
H 5.01407100 -3.66828200 -0.60851800
O -1.01980900 2.61344800 0.47921600
O 0.69164000 2.01991100 -0.93951400
C 0.00760600 3.61863500 0.66011300
C 0.91711400 3.40933400 -0.60951700
C -0.65918100 4.98465300 0.74148400
H 0.09673100 5.77493300 0.79700800
H -1.30152200 5.17425200 -0.12114800
H -1.27406500 5.03904000 1.64479800
C 2.40542400 3.61075000 -0.36405200
H 2.78228900 2.91933800 0.39285900
H 2.95718900 3.43603400 -1.29283500
H 2.60610400 4.63589700 -0.03596700
C 0.46304000 4.22808900 -1.81828000
H 0.64877200 5.29600600 -1.67048200
H 1.02135100 3.89854500 -2.69922800
H -0.60339200 4.08353300 -2.01825800
C 0.71911300 3.30227300 1.97447500
H 1.18824900 2.31597600 1.94597100

H 1.47944500 4.05550200 2.20240100
H -0.01833400 3.30314000 2.78282500
C 5.69896900 -1.86319700 -2.52989400
H 5.48227000 -1.26779400 -3.42114400
H 6.63833200 -1.49219000 -2.10339000
H 5.86466700 -2.89974800 -2.83752700
H -1.23490900 -0.13383200 1.83061400
C -4.92421700 -1.94903600 -2.74154100
C -5.44668900 -1.20642700 -1.68582000
C -4.59174200 -0.53461400 -0.81605400
C -3.20797900 -0.60417000 -0.98526000
C -2.69077400 -1.34305300 -2.05157100
C -3.54443600 -2.01222300 -2.92383000
H -5.58919500 -2.47024700 -3.42355100
H -6.52109400 -1.14189400 -1.54253600
H -5.00556100 0.05314000 -0.00038600
H -1.61666700 -1.38246500 -2.20312100
H -3.12988900 -2.58223900 -3.74994200
C -2.29138600 0.09583200 -0.00318900
H -2.80555100 0.97719700 0.39694700
O -1.10688900 0.49130000 -0.67869800

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.83613903
Gibbs Free Energy (T = 323K) = -1787.376125
C -1.12631900 -1.98020100 0.74178300
N 0.08738600 -2.34067700 0.83818300
C -1.86574500 -0.76239800 1.21477600
B -0.50497300 1.67476800 -0.36714300
C -3.06086500 -1.20348400 2.06908800
C -2.62894200 -1.85934300 3.37615300
H -2.05183900 -2.77007000 3.19629400
H -3.49733000 -2.13006700 3.97861700
H -2.00441700 -1.18304900 3.96462600
H -3.69579900 -1.88698700 1.49779200
H -3.66771200 -0.31908300 2.28262200
H -1.75670000 -2.70752300 0.22222300
S 1.28590700 -1.45366500 1.60233400
O 0.97590300 -0.05417600 1.79172500
O 1.65157400 -2.23734100 2.75559100
C 3.72778500 -0.62636500 -1.46991700
C 2.72937300 -0.52674400 -0.51439100
C 2.55428500 -1.56953400 0.38111800
C 3.35651900 -2.70132500 0.33570100
C 4.34896300 -2.78160000 -0.62351000
C 4.55067300 -1.74735900 -1.53831900
H 3.86689400 0.18497000 -2.17552000
H 2.09470700 0.34975100 -0.47167300
H 3.20655500 -3.50329600 1.04689600
H 4.98012000 -3.66210000 -0.66453200
O -1.00598800 2.60456400 0.49975600
O 0.67572100 2.03781900 -0.95325700
C 0.02109200 3.61170100 0.67657300
C 0.90519500 3.42352100 -0.61041500
C -0.64580600 4.97019500 0.79046500
H 0.10766900 5.75986100 0.83390800
H -1.30983700 5.16611300 -0.05031400
H -1.23370000 5.01191200 1.70892800
C 2.39294700 3.62655100 -0.39005000
H 2.78712100 2.92344900 0.34266600
H 2.92523400 3.47668200 -1.33110300
H 2.59286600 4.64310800 -0.04425100
C 0.42633100 4.25579800 -1.79509600
H 0.61685700 5.31865200 -1.63726600
H 0.96460600 3.93729600 -2.68901700
H -0.64166800 4.11569800 -1.97273500
C 0.75923800 3.27722000 1.96674000
H 1.23741800 2.29967200 1.90894600
H 1.51345800 4.03280600 2.19390400
H 0.03904800 3.25407300 2.78640900
C 5.65132000 -1.83662200 -2.55805200
H 5.46318000 -1.17497100 -3.40408300
H 6.60680100 -1.54585500 -2.11288300
H 5.76061800 -2.85597900 -2.93151500
H -1.21534400 -0.13278100 1.81704900
C -4.91522400 -1.93688900 -2.73300600
C -5.43256200 -1.20097400 -1.67671500
C -4.57796900 -0.53486900 -0.81022700
C -3.19981300 -0.60294700 -0.98325000
C -2.68795900 -1.33458500 -2.05035000
C -3.54104200 -1.99859400 -2.91929500
H -5.58079900 -2.45428700 -3.41353200
H -6.50426600 -1.13737600 -1.53074700
H -4.98826000 0.04841200 0.00717900
H -1.61662400 -1.37285700 -2.20501900
H -3.13025800 -2.56383700 -3.74743700
C -2.28366300 0.09529300 -0.00420500
H -2.80185500 0.97003800 0.39810600
O -1.10658100 0.50394300 -0.68469500

***anti-Z*-P1**
ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.40677261
Gibbs Free Energy (T = 323K) = -1786.945686
C -1.27764300 1.77571500 0.27748100
N -2.41599700 1.22423800 0.08844300
C -0.12885600 1.38910100 1.17221400
B 2.95807900 -0.53577100 0.78228600

C 0.39292300 2.64225700 1.88981600
C -0.64061000 3.22557600 2.85279500
H -1.54567700 3.55083100 2.32619700
H -0.23263100 4.09311400 3.37986400
H -0.94191800 2.48308700 3.59941100
H 0.68573400 3.39726600 1.14973500
H 1.29865300 2.36305900 2.43537900
H -1.11771600 2.67986900 -0.31724800
S -2.79116300 -0.19138700 0.95588100
O -1.81790800 -1.23615600 0.63854400
O -3.03030800 0.16653600 2.35250200
C -5.56966500 -1.82383300 -1.45707400
C -4.35210600 -1.50151400 -0.86926500
C -4.33702500 -0.61829400 0.20529500
C -5.51246600 -0.05922500 0.69987400
C -6.71882600 -0.39293300 0.09902500
C -6.76640900 -1.27780500 -0.98403800
H -5.58916200 -2.51315400 -2.29631400
H -3.42703800 -1.93341800 -1.23534700
H -5.48285500 0.62101400 1.54428200
H -7.64035200 0.03902600 0.47883600
O 2.86486700 -1.27593900 -0.36839600
O 4.14105900 -0.68740400 1.45415300
C 4.20407000 -1.74617600 -0.64494200
C 4.85030400 -1.75869000 0.78628400
C 4.12311900 -3.10683400 -1.31933500
H 5.12561600 -3.52742700 -1.45081300
H 3.52246200 -3.80826500 -0.73632400
H 3.66524900 -3.00236400 -2.30746600
C 6.33993800 -1.45074900 0.80972200
H 6.55024500 -0.45822600 0.40538000
H 6.70969000 -1.48709400 1.83879800
H 6.89133400 -2.19280200 0.22274600
C 4.55994200 -3.04364800 1.56190100
H 5.11748200 -3.89095200 1.15174600
H 4.86062900 -2.90450000 2.60427600
H 3.49279000 -3.28645200 1.54340600
C 4.84226600 -0.72154800 -1.58492400
H 4.91740500 0.26203000 -1.10995600
H 5.84137400 -1.03600600 -1.90110700
H 4.21187700 -0.61736900 -2.47278700
C -8.08570200 -1.65541700 -1.60545400
H -7.95945800 -1.98720000 -2.63965100
H -8.55001200 -2.47678100 -1.04729600
H -8.78490000 -0.81425400 -1.59427800
H -0.46062400 0.66871200 1.92542600
C 2.41860500 2.94939200 -3.01674600
C 3.01712700 3.08431800 -1.76614500
C 2.54665200 2.34915900 -0.68161900
C 1.47588000 1.46671300 -0.83807300
C 0.88574200 1.33070700 -2.09530700
C 1.34942700 2.07157500 -3.17884300
H 2.78734800 3.52163400 -3.86261300
H 3.85390600 3.76358100 -1.63333000
H 3.02141600 2.44978800 0.28977400
H 0.06377800 0.63132000 -2.23028800
H 0.88342100 1.95282100 -4.15236100
C 0.94586800 0.65545600 0.32995400
H 0.48140000 -0.25737200 -0.05862500
O 1.98671400 0.30646900 1.23199100

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.83148687
Gibbs Free Energy (T = 323K) = -1787.375305
C 1.27721600 1.81679600 -0.31767000
N 2.39580800 1.24209700 -0.13393900
C 0.11130100 1.43648700 -1.18757500
B -2.92723200 -0.53373700 -0.75433400
C -0.41089700 2.68211500 -1.90948500
C 0.59796800 3.22871800 -2.91391000
H 1.53009000 3.52803300 -2.42630000
H 0.19776300 4.10318500 -3.42931200
H 0.84651800 2.47547400 -3.66512700
H -0.66462100 3.45262300 -1.17504100
H -1.33732200 2.41265500 -2.41866700
H 1.14401300 2.73715600 0.25628200
S 2.73603800 -0.18658600 -0.96018900
O 1.75381100 -1.19068700 -0.62526100
O 2.98103400 0.13417600 -2.34503600
C 5.46838400 -1.81575100 1.48727700
C 4.26358900 -1.47936600 0.89288200
C 4.26663600 -0.62582700 -0.19840700
C 5.45146500 -0.10966600 -0.70222600
C 6.64575700 -0.45537200 -0.09640200
C 6.67340900 -1.31187600 1.00383800
H 5.47129600 -2.48316800 2.34134700
H 3.33004700 -1.87848100 1.26719500
H 5.43614900 0.54971800 -1.56027000
H 7.57493900 -0.05473900 -0.48528800
O -2.80402000 -1.25640800 0.40054000
O -4.09248800 -0.75572200 -1.43051300
C -4.11172400 -1.81370400 0.66706700
C -4.74468400 -1.86513100 -0.76663100
C -3.94826900 -3.16390400 1.33759400
H -4.92039700 -3.64735700 1.45825000
H -3.29938300 -3.82140200 0.76064800
H -3.50931100 -3.03107300 2.32783100
C -6.24511900 -1.64445500 -0.80085900
H -6.51492300 -0.66814100 -0.40031600

H -6.60243600 -1.70404500 -1.83026700
H -6.75493800 -2.41544500 -0.21853600
C -4.37532100 -3.12879700 -1.53590800
H -4.88690600 -4.00315000 -1.12998400
H -4.67444800 -3.00700600 -2.57796800
H -3.29923200 -3.31050200 -1.50782000
C -4.82094400 -0.83688200 1.60009000
H -4.95557500 0.13777900 1.12633900
H -5.79765100 -1.21584600 1.90565500
H -4.20805800 -0.69665300 2.49177200
C 7.98089300 -1.70287300 1.63379800
H 7.84409100 -2.02010000 2.66804800
H 8.43218300 -2.53521700 1.08686600
H 8.69053400 -0.87445000 1.61507700
H 0.42685600 0.70351000 -1.93186100
C -2.39966300 3.08600700 2.97092900
C -3.01239200 3.18342100 1.72926000
C -2.55153700 2.42601400 0.66237600
C -1.47598600 1.55969900 0.82740600
C -0.87267900 1.46003200 2.07607800
C -1.32680200 2.22260400 3.14211300
H -2.76140700 3.67627100 3.80428600
H -3.85417200 3.85138100 1.59017000
H -3.03658800 2.49759700 -0.30378900
H -0.04729800 0.76999400 2.21865600
H -0.84996700 2.13234600 4.11080200
C -0.95357900 0.72450600 -0.32269000
H -0.48708800 -0.17540500 0.08519200
O -2.00033600 0.34827600 -1.20663800

R-1a

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.81330025
Gibbs Free Energy (T = 323K) = -1787.359061
C 0.97684700 -0.61625100 1.60147700
N 0.05435200 -0.44323600 0.52987500
C 1.92067800 0.26404300 1.89058500
B -0.56230000 0.82709500 0.21862600
C 2.87392900 0.11007700 3.03340000
C 4.32840000 0.09772500 2.56015200
H 4.50508900 -0.73106800 1.87111100
H 5.01416100 -0.00024300 3.40443900
H 4.57371000 1.02183200 2.03060200
H 2.64952900 -0.81038700 3.57973900
H 2.73302900 0.93654100 3.73864600
H 0.84957000 -1.52850600 2.17015900
S -0.42683100 -1.80429000 -0.30625400
O -0.10988100 -1.66033100 -1.70189900
O 0.11466400 -2.92873300 0.41614600
C -4.36662500 -1.78998200 -1.10460600
C -2.98899800 -1.78803400 -1.25841400
C -2.18777600 -1.79555400 -0.13195300
C -2.73984900 -1.80525500 1.14172000
C -4.11455000 -1.79524100 1.27844300
C -4.94832900 -1.78334300 0.15904200
H -4.99866900 -1.78483600 -1.98519900
H -2.53718600 -1.76713200 -2.24076000
H -2.10250600 -1.81088000 2.01759800
H -4.55131900 -1.79706400 2.27056500
O -0.55840700 1.87708000 1.08405500
O -1.28868200 1.03086800 -0.91299800
C -1.22958300 2.97268600 0.41089500
C -2.07174300 2.22717000 -0.68300500
C -2.05673900 3.73067000 1.43248200
H -2.64783600 4.50574500 0.93929700
H -2.73036300 3.06971400 1.97618900
H -1.39506300 4.21466600 2.15264600
C -2.20939100 2.97567300 -1.99438900
H -1.23753300 3.16427400 -2.44806000
H -2.80636400 2.38569500 -2.69172500
H -2.71530300 3.93051700 -1.83429400
C -3.43790400 1.76731900 -0.18433000
H -4.11048900 2.61345500 -0.03395100
H -3.87691000 1.10039700 -0.92715100
H -3.35508600 1.21307800 0.75291200
C -0.14601300 3.87336900 -0.16830300
H 0.47628100 3.33741800 -0.88544900
H -0.58171600 4.74905700 -0.65281100
H 0.49465500 4.21657100 0.64615600
C -6.44141600 -1.73478000 0.32365500
H -6.76741100 -0.71067100 0.52538000
H -6.95231300 -2.07584400 -0.57711800
H -6.76584100 -2.35289200 1.16226900
H 2.03125500 1.14706200 1.26788000
C 5.27860700 -2.14178700 -0.64923100
C 3.90102100 -2.09711400 -0.84226400
C 3.27812400 -0.88693900 -1.08268300
C 4.03358800 0.28312200 -1.12567700
C 5.41207000 0.23505200 -0.94035900
C 6.03602500 -0.97899100 -0.70027800
H 5.76436600 -3.09152000 -0.45848600
H 3.31529400 -3.00714400 -0.80158100
H 2.20870700 -0.82931400 -1.24153400
H 5.99195900 1.15159500 -0.97680600
H 7.10772100 -1.02067800 -0.55056500
C 3.37905200 1.58443100 -1.34399600
H 4.06624200 2.45053300 -1.41179800
O 2.18407100 1.74329700 -1.43838900

R-1b

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.81684797
Gibbs Free Energy (T = 323K) = -1787.360870
C -0.09397200 -0.69820300 1.99131100
N 0.97109700 0.12543600 1.53030400
C -0.48515100 -1.81838900 1.40004200
B 1.97802100 -0.34853200 0.59142400
C -1.58223300 -2.71052700 1.89753100
C -2.39572400 -2.16884100 3.06424400
H -1.77868100 -2.01959400 3.95376000
H -3.19399700 -2.86539800 3.32590200
H -2.85717500 -1.21173400 2.80751100
H -1.14703300 -3.67955000 2.16859000
H -2.25014600 -2.91803800 1.05487600
H -0.56331300 -0.32862200 2.89244000
S 0.88005800 1.74575600 1.89369300
O 0.19223000 1.85551100 3.15359100
O 2.20694600 2.27523600 1.74902000
C -2.33443800 3.11588400 -0.08856700
C -1.51174400 2.61762500 0.90992700
C -0.16088500 2.44926500 0.64975700
C 0.37707600 2.78125800 -0.58690700
C -0.45873800 3.27541000 -1.57125200
C -1.82436600 3.44651700 -1.34110600
H -3.39223400 3.24525700 0.11034900
H -1.91214100 2.36239300 1.88230800
H 1.43054400 2.62750400 -0.77587400
H -0.04577800 3.52523200 -2.54181800
O 2.51013000 -1.59573200 0.68249200
O 2.43356800 0.38014800 -0.45798800
C 3.24843400 -1.82599700 -0.54496800
C 3.52599100 -0.36498300 -1.05036800
C 4.49408600 -2.62775200 -0.21860800
H 5.11645500 -2.73692500 -1.10967100
H 5.08438200 -2.15442900 0.56467000
H 4.20881400 -3.62466200 0.12107600
C 3.45381900 -0.19680300 -2.55622500
H 2.45983400 -0.43933200 -2.92976800
H 3.67902000 0.83773800 -2.82073100
H 4.18668100 -0.84119700 -3.04688200
C 4.81393000 0.23387500 -0.49931100
H 5.69162000 -0.24053000 -0.94123400
H 4.83741400 1.29768200 -0.73923400
H 4.86782000 0.12974600 0.58582700
C 2.33131500 -2.62218200 -1.46568500
H 1.42958700 -2.06186900 -1.71756400
H 2.84225800 -2.89208000 -2.39149600
H 2.03812400 -3.54173100 -0.95592300
C -2.71546700 3.99436000 -2.41979900
H -2.61737600 5.08162300 -2.47903200
H -2.44477200 3.58736100 -3.39531700
H -3.76305500 3.76310200 -2.22559800
H 0.02362200 -2.15367900 0.50144500
C -4.76632800 -2.54269500 -0.45086700
C -4.52434100 -1.28958900 0.09543000
C -3.39141900 -0.58493900 -0.27966200
C -2.50291700 -1.13232800 -1.19979300
C -2.74941500 -2.38980100 -1.74698900
C -3.88012000 -3.09304600 -1.37225000
H -5.64904400 -3.09753300 -0.15610800
H -5.21409000 -0.86778300 0.81586700
H -3.18262000 0.38944200 0.14764200
H -2.04350100 -2.80055400 -2.45860100
H -4.07502900 -4.07222300 -1.79199000
C -1.28782000 -0.37627400 -1.56079700
H -1.17872900 0.60235800 -1.06110000
O -0.44707700 -0.76522900 -2.33876300

R-1c

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.81100352
Gibbs Free Energy (T = 323K) = -1787.357647
C -0.94719800 -1.24849400 -0.69138700
N 0.04079900 -0.73024500 0.19807500
C -1.97826400 -1.97681900 -0.30057200
B 0.37448600 0.66942900 0.11701200
C -3.02978000 -2.49840100 -1.22469500
C -3.12725100 -4.02423300 -1.20008600
H -2.19000100 -4.47881200 -1.52816400
H -3.92648300 -4.37437600 -1.85642000
H -3.33723700 -4.38535900 -0.19026200
H -2.83292900 -2.14937900 -2.24210400
H -3.99218300 -2.06829800 -0.92485700
H -0.81476500 -0.96249000 -1.73008100
S 1.02538800 -1.75812000 1.07089900
O 1.04791400 -1.33081200 2.44330700
O 0.61964900 -3.10267200 0.75820900
C 4.89565500 -0.75563000 0.60153400
C 3.64959900 -0.98112800 1.16755500
C 2.63077100 -1.47562100 0.37595800
C 2.83721000 -1.74609800 -0.97059800
C 4.08000300 -1.50448400 -1.52297400
C 5.12696100 -1.00248900 -0.74710000
H 5.69722400 -0.36903700 1.22054200
H 3.46226100 -0.76241000 2.20996000
H 2.03255200 -2.13840800 -1.58088800

H 4.24529700 -1.71009100 -2.57459700
O -0.14103400 1.46221500 -0.86860600
O 1.29570200 1.28369800 0.90717500
C 0.37006100 2.79965800 -0.63054400
C 1.64916500 2.51362400 0.22962900
C 0.64440700 3.45609400 -1.97034200
H 1.12177900 4.42781200 -1.82461200
H 1.28895200 2.83995300 -2.59580200
H -0.29663700 3.61640300 -2.49924500
C 1.96307000 3.56968900 1.27106300
H 1.14831600 3.67939700 1.98525000
H 2.86380500 3.28660600 1.81814800
H 2.14416200 4.53410200 0.79102400
C 2.88459100 2.21201600 -0.61314700
H 3.24649400 3.10821200 -1.11985700
H 3.67323500 1.83774400 0.04025700
H 2.67958300 1.44354100 -1.36178600
C -0.70356400 3.56904200 0.12903200
H -0.93588900 3.08753200 1.07894600
H -0.39078900 4.59844300 0.31194600
H -1.61482600 3.59281000 -0.47138200
C 6.46427000 -0.71697400 -1.37139800
H 7.23530600 -0.57537800 -0.61374800
H 6.77203900 -1.53098900 -2.03023800
H 6.41630500 0.19259800 -1.97621800
H -2.08339100 -2.21907800 0.75356100
C -5.69117700 0.41352200 -1.37248700
C -4.41603500 0.95430700 -1.51675600
C -3.55775800 1.00098600 -0.43469300
C -3.97527300 0.50497700 0.79973100
C -5.24794200 -0.03884200 0.94037300
C -6.10890400 -0.08401700 -0.14657100
H -6.35967100 0.37648200 -2.22453700
H -4.09481400 1.33164600 -2.48004500
H -2.55177300 1.38975900 -0.53334300
H -5.56209300 -0.42824700 1.90329700
H -7.09970000 -0.50769600 -0.03930800
C -3.07337800 0.52687200 1.96736200
H -3.49847300 0.08600600 2.89076000
O -1.95289600 0.97758800 1.96922800

R-1d

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.81127153
Gibbs Free Energy (T = 323K) = -1787.356679
C 0.94143200 -0.96988900 0.79560000
N -0.03964600 -0.54506600 -0.14843600
C 2.04108100 -1.62754900 0.46473000
B -0.55876500 0.79694300 -0.05932300
C 3.05170400 -2.12219700 1.44721700
C 3.12351400 -3.65027600 1.47590400
H 2.16761400 -4.07828800 1.78509000
H 3.89386600 -3.99009100 2.17109300
H 3.36253300 -4.04696400 0.48620200
H 2.81939900 -1.73850900 2.44471700
H 4.03244000 -1.72218600 1.17000700
H 0.72730600 -0.69855800 1.82461500
S -0.85493800 -1.66549500 -1.08819300
O -0.87154200 -1.20319200 -2.44871800
O -0.30113400 -2.95849500 -0.78748200
C -4.83918500 -1.18608100 -0.77525300
C -3.55154100 -1.23595000 -1.28906100
C -2.51002000 -1.60213500 -0.45839700
C -2.73430000 -1.91737000 0.87564900
C -4.01986600 -1.85067200 1.37588100
C -5.09140900 -1.48162200 0.55958000
H -5.65861000 -0.90009000 -1.42475800
H -3.35217300 -0.97979000 -2.32071300
H -1.91062500 -2.20826600 1.51664200
H -4.20002300 -2.09101200 2.41767300
O -0.19230500 1.63023900 0.95768400
O -1.50868300 1.30495400 -0.88969700
C -0.85648700 2.89748700 0.70851600
C -2.04727800 2.46868800 -0.21623000
C -1.27493200 3.49396100 2.03885500
H -1.85959900 4.40257200 1.87777100
H -1.87011200 2.79446300 2.62428500
H -0.38831900 3.75904000 2.61722600
C -2.44261600 3.49535400 -1.25908000
H -1.61656500 3.71775300 -1.93294500
H -3.27572800 3.11301000 -1.85097300
H -2.76352000 4.42140600 -0.77658000
C -3.27260200 1.99769100 0.56111900
H -3.77190900 2.83165100 1.05715300
H -3.97337500 1.53474400 -0.13431200
H -3.00630200 1.25054800 1.31208700
C 0.14813300 3.80440000 0.00911300
H 0.49680200 3.35940200 -0.92393800
H -0.28475400 4.78418200 -0.19822800
H 1.01023100 3.94779000 0.66320600
C -6.47993500 -1.39242900 1.12834200
H -6.72759800 -2.29004600 1.69836600
H -6.56022500 -0.54119700 1.80945200
H -7.22503600 -1.26685300 0.34260400
H 2.22076400 -1.85797600 -0.58136700
C 6.54124300 -0.40651800 0.09084600
C 5.85005600 -0.59480000 -1.10301600
C 4.63146600 0.02795600 -1.30046500
C 4.09482300 0.83224800 -0.29732000

C 4.78434300 1.01386200 0.89645300
C 6.01266500 0.39944200 1.08931700
H 7.49622800 -0.89546300 0.24215300
H 6.26738500 -1.22917900 -1.87531500
H 4.07328400 -0.10639000 -2.21915300
H 4.35263400 1.63350400 1.67550300
H 6.55259100 0.54078700 2.01733400
C 2.77601600 1.47384400 -0.46941900
H 2.38367400 1.98781300 0.42748500
O 2.13369300 1.45601800 -1.49289800

TS1-1a

ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.36801404
Gibbs Free Energy (T = 323K) = -1786.900313
Imaginary Frequency = 300.2738*i*
C 1.12550700 -0.83846200 1.36466800
N 0.03852300 -0.57826300 0.59756600
C 1.97724800 0.14339200 1.81003600
B 0.01513200 0.79601700 -0.21935300
C 3.20992400 -0.20242100 2.61193500
C 3.91676700 1.04246100 3.14603000
H 4.21357900 1.71240800 2.33146200
H 4.81900000 0.77301600 3.70280000
H 3.25946700 1.60760300 3.81571500
H 3.90566800 -0.78499200 1.99382400
H 2.93390200 -0.85141200 3.45291900
H 1.37670500 -1.88641300 1.51431500
S -0.69330000 -1.95539800 -0.09677000
O -0.35844100 -2.03786700 -1.51216200
O -0.34625000 -3.08386100 0.76454600
C -4.59360300 -1.44991800 -0.91294800
C -3.22166000 -1.62207600 -1.06095800
C -2.42248800 -1.63132200 0.07434800
C -2.96415900 -1.47888900 1.34801900
C -4.33286500 -1.29341000 1.47462400
C -5.16626700 -1.27482600 0.34925500
H -5.22663800 -1.44335400 -1.79554900
H -2.77324900 -1.73754800 -2.04081000
H -2.32621700 -1.49704900 2.22581300
H -4.76442300 -1.16501400 2.46313800
O 0.02997700 1.93840700 0.63452100
O -1.03311300 0.92205500 -1.15387400
C -0.67241300 2.96813200 -0.06942100
C -1.73608800 2.13989900 -0.86557700
C -1.24934800 3.94580300 0.94671800
H -1.89333300 4.68236600 0.45386900
H -1.83117400 3.42736800 1.71201600
H -0.43618500 4.48489500 1.44358000
C -2.17674800 2.76871000 -2.18177900
H -1.33530800 2.89126400 -2.86772000
H -2.91946200 2.12623700 -2.66564600
H -2.63531000 3.74876200 -2.00876800
C -2.96249800 1.81156800 -0.01212800
H -3.56543900 2.70531300 0.17936900
H -3.58388000 1.08328600 -0.53888100
H -2.66720600 1.37477300 0.94591400
C 0.31694800 3.70161900 -0.98324400
H 0.72541700 3.03418200 -1.74744400
H -0.15347500 4.55564200 -1.48104200
H 1.14750200 4.07447000 -0.37485400
C -6.64657100 -1.04229300 0.50175900
H -6.85495800 0.02854300 0.60970400
H -7.19988700 -1.40270200 -0.36959000
H -7.03742800 -1.54368500 1.39211200
H 1.57625200 1.14642100 1.91116800
C 5.79312200 -1.70334900 -1.34138900
C 4.49840300 -2.11480600 -1.66415500
C 3.41083400 -1.32038700 -1.32930800
C 3.61550300 -0.10525200 -0.66456900
C 4.91184200 0.30340900 -0.34091900
C 5.99981100 -0.49452600 -0.68172000
H 6.64107000 -2.32801200 -1.60513800
H 4.34055000 -3.05808200 -2.17749300
H 2.39772100 -1.62814200 -1.57151300
H 5.06922600 1.24987500 0.16947300
H 7.00607400 -0.17265600 -0.43317800
C 2.46735000 0.73057500 -0.29065800
H 2.66731500 1.70744600 0.15186100
O 1.36786400 0.57845600 -0.94565900

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.79132650
Gibbs Free Energy (T = 323K) = -1787.328883
Imaginary Frequency = 316.6954*i*
C 1.12191700 -0.83451100 1.35675200
N 0.03940200 -0.57917800 0.59533400
C 1.97516900 0.14230000 1.79793500
B 0.01390900 0.79697200 -0.21524400
C 3.20236400 -0.20973600 2.59962000
C 3.92660500 1.02755000 3.11866400
H 4.22989500 1.68373500 2.29929800
H 4.82386400 0.75267300 3.67519000
H 3.27978000 1.60665800 3.78212800
H 3.88550800 -0.80872500 1.98819600
H 2.91716900 -0.84354000 3.44529600
H 1.37159100 -1.88023700 1.50856000
S -0.68439500 -1.94789800 -0.09442200

O -0.34892600 -2.01936200 -1.49045400
O -0.34258700 -3.06177000 0.75728800
C -4.57173900 -1.45078700 -0.91624500
C -3.20331300 -1.61517300 -1.06016500
C -2.40852300 -1.63148700 0.07119000
C -2.95397700 -1.48602900 1.33856700
C -4.31783700 -1.30627400 1.46329800
C -5.14647700 -1.28554200 0.34026900
H -5.20077200 -1.44081900 -1.79884200
H -2.75280500 -1.72279900 -2.03718800
H -2.31967600 -1.50810800 2.21592400
H -4.75107500 -1.18423100 2.44938400
O 0.01711100 1.93250100 0.64430300
O -1.02833700 0.92871000 -1.15214500
C -0.68043000 2.96558600 -0.05819500
C -1.73771000 2.14102400 -0.85982000
C -1.26170200 3.93873200 0.95334100
H -1.90704200 4.66891600 0.45869000
H -1.84037600 3.41960000 1.71633900
H -0.45349000 4.48175700 1.44786900
C -2.17613000 2.77527300 -2.16927300
H -1.33677600 2.89778900 -2.85309200
H -2.92000500 2.13885100 -2.65315300
H -2.63034300 3.75341700 -1.99088300
C -2.96122300 1.80493700 -0.01165400
H -3.56802900 2.69322900 0.17677000
H -3.57432400 1.07536300 -0.54023200
H -2.66718900 1.37195000 0.94515100
C 0.31038000 3.69741300 -0.96571400
H 0.71830700 3.03229200 -1.72809900
H -0.15778700 4.55054000 -1.46096600
H 1.13674000 4.06747400 -0.35503800
C -6.62467900 -1.06088900 0.49110900
H -6.83408300 0.00399900 0.62461200
H -7.17070600 -1.40047000 -0.38934800
H -7.01536500 -1.58359900 1.36562200
H 1.57688200 1.14303900 1.90255900
C 5.77039000 -1.69652900 -1.34818600
C 4.47808400 -2.10896700 -1.65840100
C 3.39625100 -1.31803800 -1.31767800
C 3.60347500 -0.10614400 -0.65871700
C 4.89677200 0.30334700 -0.34823700
C 5.97966800 -0.49025900 -0.69588000
H 6.61524000 -2.31908800 -1.61719000
H 4.31816000 -3.05145900 -2.16760600
H 2.38356100 -1.62536500 -1.55223600
H 5.05604700 1.24875700 0.15823100
H 6.98547700 -0.16695900 -0.45774300
C 2.45834800 0.72829100 -0.27683200
H 2.66586000 1.70207700 0.16397500
O 1.36356400 0.58673500 -0.93611900

TS1-1b

ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.36229744
Gibbs Free Energy (T = 323K) = -1786.894437
Imaginary Frequency = 325.8465*i*
C -0.24769700 -0.05094000 2.04244500
N 0.85755100 0.34148800 1.34780400
C -0.88220000 -1.25827100 1.87671900
B 1.26446800 -0.52411700 0.08396500
C -2.09989300 -1.65173300 2.67070600
C -2.91543500 -0.49927100 3.25350200
H -2.36269000 0.04441300 4.02680800
H -3.83200300 -0.87996900 3.71267100
H -3.20337300 0.21850200 2.47646400
H -1.78414900 -2.32623200 3.47755100
H -2.74107100 -2.25765600 2.01795800
H -0.69186000 0.70517800 2.68380600
S 1.19173600 2.00716600 1.43081200
O 0.68593500 2.46822900 2.72045100
O 2.58961200 2.20499800 1.10228000
C -1.92738300 3.69658300 -0.47012300
C -1.06796900 3.25113600 0.52716000
C 0.15779200 2.69792300 0.16289100
C 0.53612700 2.58877400 -1.17330000
C -0.33835600 3.04018500 -2.15298400
C -1.57840100 3.59604600 -1.82048600
H -2.88419900 4.13012100 -0.19327100
H -1.34145500 3.33241500 1.57344100
H 1.47963000 2.12242200 -1.43387400
H -0.05493600 2.95171400 -3.19795700
O 1.70751700 -1.81605400 0.49070400
O 2.19887500 0.02934200 -0.81477500
C 2.72612800 -2.21235700 -0.43201400
C 3.34253900 -0.83330600 -0.84603900
C 3.69190400 -3.15135900 0.28059000
H 4.54726400 -3.38741700 -0.36217200
H 4.06221900 -2.71145700 1.20928000
H 3.18302500 -4.08908400 0.52643800
C 3.93741300 -0.79884500 -2.24831900
H 3.18204300 -1.01634300 -3.00709400
H 4.34885500 0.19525800 -2.45089900
H 4.74981300 -1.52802500 -2.34188900
C 4.36880100 -0.32074800 0.16703200
H 5.29534300 -0.90297600 0.12623700
H 4.59882900 0.72326500 -0.06008000
H 3.96910200 -0.35904100 1.18420300
C 2.06839400 -2.94560100 -1.60737000

H 1.38801100 -2.28764800 -2.15512200
H 2.81437000 -3.34113900 -2.30445400
H 1.48824200 -3.78710500 -1.21428900
C -2.50552800 4.09838000 -2.89598900
H -2.24094500 5.12335800 -3.18076700
H -2.44032800 3.48027100 -3.79609000
H -3.54476900 4.10682800 -2.55583400
H -0.33512600 -2.07041600 1.40814000
C -4.38531800 -3.26413100 -1.13094500
C -4.70166100 -1.99744900 -0.64555700
C -3.68384100 -1.10047400 -0.33843700
C -2.34869300 -1.47097000 -0.51988500
C -2.03328300 -2.74260100 -1.01127400
C -3.05158100 -3.63520700 -1.31408800
H -5.17887900 -3.96553400 -1.36939800
H -5.73855300 -1.70874500 -0.50731300
H -3.92320100 -0.10954800 0.03880100
H -0.99070900 -3.01272100 -1.14701700
H -2.81047600 -4.62267900 -1.69461800
C -1.28433000 -0.51820200 -0.17876400
H -1.61440300 0.49459000 0.07690800
O -0.11340800 -0.66832200 -0.68451600

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.78659255
Gibbs Free Energy (T = 323K) = -1787.324494
Imaginary Frequency = 344.2404*i*
C -0.22864500 -0.01614400 2.00961600
N 0.85285500 0.42523100 1.31926100
C -0.78674700 -1.25961400 1.87028400
B 1.30413100 -0.44241300 0.06931500
C -1.97260100 -1.70998200 2.67495900
C -2.85210300 -0.60209700 3.24141900
H -2.32935800 -0.00890000 3.99500800
H -3.73609100 -1.02861400 3.71703700
H -3.19158400 0.07706500 2.45450100
H -1.61142500 -2.34851100 3.48830000
H -2.57635000 -2.36520700 2.03860600
H -0.71901200 0.72180000 2.63445500
S 1.08491800 2.09473000 1.37635200
O 0.59908900 2.53689200 2.65991900
O 2.43956500 2.36239800 1.00074500
C -2.18301600 3.53383100 -0.45230300
C -1.26907900 3.17107200 0.52328700
C -0.02437100 2.69508100 0.13739900
C 0.31897500 2.58409700 -1.20307900
C -0.60807500 2.94932000 -2.16200500
C -1.86988600 3.42441900 -1.80516500
H -3.15654500 3.90712500 -0.15592300
H -1.51612800 3.25491600 1.57343800
H 1.28363700 2.18040300 -1.48076300
H -0.35048100 2.85523500 -3.21081600
O 1.82818600 -1.69012100 0.51178500
O 2.20111200 0.13567600 -0.84765900
C 2.86694200 -2.05208000 -0.40092700
C 3.39625200 -0.65303600 -0.85482400
C 3.88702900 -2.90750400 0.33174200
H 4.75434300 -3.10189100 -0.30438800
H 4.22532100 -2.42376100 1.24730700
H 3.43992300 -3.86781900 0.59755600
C 3.98983500 -0.62553300 -2.25342100
H 3.25148800 -0.90500400 -3.00436000
H 4.34637500 0.38093700 -2.48229400
H 4.83925300 -1.30978600 -2.32399100
C 4.38519500 -0.05132300 0.14084400
H 5.34214400 -0.57736800 0.11663500
H 4.55267000 0.99442300 -0.11763700
H 3.98796800 -0.08360000 1.15618000
C 2.25302300 -2.85280500 -1.55107800
H 1.53723600 -2.25175100 -2.11318900
H 3.01921400 -3.22176100 -2.23629100
H 1.72521200 -3.71316800 -1.13368900
C -2.85836900 3.83131600 -2.86149500
H -2.63365300 4.83775200 -3.22479700
H -2.81745300 3.15705200 -3.71830500
H -3.87684400 3.83720200 -2.47204500
H -0.18936200 -2.04317200 1.42096500
C -4.17510200 -3.49747200 -1.06752400
C -4.55439200 -2.24373000 -0.60946800
C -3.58692500 -1.29412000 -0.32004600
C -2.23976200 -1.59842800 -0.49228500
C -1.86104500 -2.85700500 -0.95686500
C -2.82858000 -3.80259400 -1.24187400
H -4.93006100 -4.24113000 -1.29231900
H -5.60265900 -2.00610700 -0.47816000
H -3.87497600 -0.31148300 0.03748400
H -0.80779800 -3.07476300 -1.08675000
H -2.53800900 -4.78166800 -1.60244000
C -1.22726700 -0.58653100 -0.16878100
H -1.61625500 0.41023300 0.05613900
O -0.05642300 -0.68281400 -0.68340900

TS1-1c

ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.35247638
Gibbs Free Energy (T = 323K) = -1786.883276
Imaginary Frequency = 246.7404*i*
C 1.12531500 -1.26366200 0.85812600

N -0.10058600 -0.84739900 0.47671000
C 1.94919100 -2.10114800 0.12175700
B 0.13195200 0.64098100 -0.21657800
C 3.24377400 -2.61811200 0.68772500
C 3.02141300 -3.93257900 1.44407500
H 2.34539900 -3.78492500 2.29248200
H 3.97181800 -4.31895200 1.82411100
H 2.58023300 -4.69332200 0.79177200
H 3.68780600 -1.86933700 1.35275500
H 3.95599700 -2.78070200 -0.12815800
H 1.57322600 -0.65415800 1.64384400
S -1.05724200 -1.99263000 -0.36397100
O -0.73381600 -2.03549100 -1.78676700
O -0.95837700 -3.22808100 0.40970300
C -4.64789200 -0.34842100 -1.11648000
C -3.33824400 -0.78852900 -1.26380500
C -2.69001000 -1.34200100 -0.16672300
C -3.32355900 -1.46548600 1.06638700
C -4.62825700 -1.01033200 1.19788600
C -5.30782700 -0.44562100 0.11241800
H -5.16379500 0.08169400 -1.97022000
H -2.82011700 -0.69969700 -2.21069900
H -2.80694200 -1.91450000 1.90796400
H -5.13034500 -1.10038900 2.15687600
O 0.57168700 1.53556200 0.80203800
O -0.99778200 1.18008800 -0.85822300
C -0.04027800 2.80021500 0.52028200
C -1.38921800 2.35499800 -0.13555300
C -0.18359900 3.57511900 1.82329600
H -0.75620900 4.49557800 1.66472400
H -0.68456800 2.97784200 2.58835100
H 0.80628400 3.85252600 2.20032200
C -1.98211900 3.35200400 -1.12267000
H -1.30283200 3.53867900 -1.95770400
H -2.91828200 2.95338700 -1.52714300
H -2.20205000 4.30429900 -0.62747900
C -2.43873400 1.97339700 0.91091500
H -2.79954100 2.85509800 1.45070000
H -3.28990100 1.50479900 0.41137800
H -2.03202500 1.25981600 1.63326300
C 0.85995000 3.57499900 -0.44904800
H 0.96580800 3.04563000 -1.40058900
H 0.46577300 4.57701000 -0.64686300
H 1.85568100 3.68052200 -0.00692800
C -6.71217900 0.07395400 0.27560600
H -7.25484100 0.06324600 -0.67365600
H -7.27420600 -0.51882400 1.00302200
H -6.69539000 1.10912000 0.63642600
H 1.48478500 -2.73799400 -0.62784900
C 5.98317300 1.17041000 0.22940800
C 4.79877300 1.62634100 0.80686300
C 3.57177500 1.11403400 0.40077100
C 3.52023500 0.13091200 -0.59255200
C 4.71119300 -0.31821200 -1.17247000
C 5.93733700 0.19768900 -0.76502100
H 6.93772900 1.57532100 0.55159300
H 4.83051500 2.38868800 1.57955900
H 2.64837600 1.47336800 0.84255300
H 4.67907000 -1.07293600 -1.95444200
H 6.85318700 -0.15862400 -1.22605600
C 2.25346600 -0.47820000 -1.09615900
H 2.42920000 -1.15299900 -1.93888100
O 1.15057300 0.21530800 -1.25622100

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.77485382
Gibbs Free Energy (T = 323K) = -1787.311445
Imaginary Frequency = 249.7451*i*
C 1.10718800 -1.26312300 0.83855600
N -0.11042600 -0.84626800 0.45310300
C 1.93000500 -2.10153500 0.11102700
B 0.14010500 0.64614300 -0.23743700
C 3.21022700 -2.63042100 0.68758000
C 2.96889400 -3.94500700 1.43100700
H 2.28657300 -3.79759300 2.27090200
H 3.90855100 -4.34268800 1.81758900
H 2.52825000 -4.69462500 0.77011300
H 3.65071100 -1.89032300 1.36016400
H 3.92870100 -2.79306100 -0.11899600
H 1.55218800 -0.66143300 1.62958800
S -1.05973300 -1.97072400 -0.39506800
O -0.75509500 -1.98316800 -1.80302400
O -0.95312900 -3.20539600 0.34492500
C -4.66831100 -0.36610000 -1.07889300
C -3.36165300 -0.79279900 -1.24905800
C -2.68538700 -1.32945900 -0.16833700
C -3.28998200 -1.44450500 1.07474100
C -4.59023400 -1.00295600 1.23135700
C -5.29803800 -0.45792200 0.15959900
H -5.20485600 0.05134100 -1.92317200
H -2.86449400 -0.70495600 -2.20447000
H -2.75069300 -1.87897700 1.90659700
H -5.06867700 -1.08793700 2.20029900
O 0.56541300 1.53079900 0.79217600
O -0.97506300 1.19610400 -0.88992700
C -0.03299500 2.80068400 0.50912000
C -1.37256900 2.36728600 -0.16536400
C -0.18994800 3.57104900 1.80836300
H -0.75902400 4.48953700 1.64403300

H -0.69850000 2.97423400 2.56449200
H 0.79360100 3.84728500 2.19460500
C -1.94657900 3.37259900 -1.14864200
H -1.26148900 3.55441800 -1.97613200
H -2.88322700 2.98854700 -1.55854000
H -2.15720200 4.32225300 -0.65019700
C -2.43226800 1.98226300 0.86406400
H -2.80044500 2.86061600 1.39851500
H -3.27314800 1.51376200 0.35324600
H -2.03360000 1.27093400 1.58868900
C 0.88237200 3.56956300 -0.44490300
H 0.99360600 3.04308100 -1.39416500
H 0.49899900 4.57269100 -0.64255700
H 1.87054100 3.66460100 0.00933900
C -6.70089100 0.04603800 0.35067000
H -7.24523800 0.07440900 -0.59366900
H -7.25363300 -0.58055400 1.05221600
H -6.68598900 1.06100300 0.75753800
H 1.46614700 -2.72735600 -0.64405600
C 5.97533300 1.14052300 0.27005400
C 4.79337500 1.59828200 0.83903500
C 3.57150000 1.09365800 0.42474300
C 3.52185000 0.11699500 -0.56752100
C 4.71017300 -0.33314600 -1.13902400
C 5.93162800 0.17478000 -0.72407400
H 6.92747400 1.53968500 0.59855400
H 4.82343300 2.35713900 1.61194300
H 2.64872700 1.45670700 0.85824100
H 4.67877100 -1.08371900 -1.92162200
H 6.84708300 -0.18241200 -1.17966800
C 2.25664700 -0.48441000 -1.08039100
H 2.44191300 -1.15470000 -1.92169800
O 1.16551200 0.22026200 -1.25958000

TS1-1d

ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.36004723
Gibbs Free Energy (T = 323K) = -1786.895752
Imaginary Frequency = 288.3411*i*
C 1.00159800 -0.46743900 1.69313600
N -0.12301000 -0.46328100 0.94468500
C 2.22973500 -0.97199400 1.28972900
B -0.05290600 1.01906000 0.13541400
C 3.39683600 -1.00799000 2.23990300
C 3.37909100 -2.27999600 3.09470900
H 2.47823500 -2.32179300 3.71535300
H 4.25278100 -2.31082500 3.75256000
H 3.39529000 -3.17492600 2.46418000
H 3.37647700 -0.12213200 2.88675500
H 4.32737800 -0.96744000 1.66497000
H 0.98294300 0.25052800 2.51302400
S -0.45433000 -1.86891400 0.03982500
O 0.21709900 -1.87817100 -1.25739600
O -0.22202900 -2.99151300 0.94634400
C -4.03644200 -1.24653900 -1.68702200
C -2.66487200 -1.33893900 -1.48372600
C -2.19628100 -1.70348900 -0.22761200
C -3.06903000 -1.97834800 0.82108900
C -4.43576600 -1.87379700 0.60208200
C -4.93878400 -1.50439600 -0.65062100
H -4.41126900 -0.96548100 -2.66714500
H -1.96533200 -1.12396300 -2.28211200
H -2.68514900 -2.27316500 1.79191400
H -5.12413700 -2.08632700 1.41504000
O -0.01427200 2.03580500 1.12969000
O -1.11058700 1.24448300 -0.75943200
C -0.89725800 3.07164200 0.67935100
C -1.93129800 2.26909900 -0.18160900
C -1.48928100 3.77571100 1.89335700
H -2.25238300 4.49965100 1.58684000
H -1.94165500 3.06130100 2.58499500
H -0.70272500 4.31790200 2.42818200
C -2.57608800 3.06307300 -1.31019600
H -1.82936700 3.42538200 -2.02067500
H -3.28015400 2.42304600 -1.85195400
H -3.13016700 3.92087300 -0.91324500
C -3.01609100 1.61145100 0.67575300
H -3.70153600 2.35749900 1.09107900
H -3.59250900 0.92143500 0.05403100
H -2.57584700 1.03991100 1.49785000
C -0.08089900 4.06481700 -0.15422300
H 0.33017000 3.58463300 -1.04744700
H -0.68422900 4.92404100 -0.46470900
H 0.75391900 4.43146200 0.45138500
C -6.42229700 -1.35924500 -0.86813100
H -6.98714900 -2.05580700 -0.24198000
H -6.74774600 -0.34475700 -0.60937600
H -6.69152900 -1.53610100 -1.91317400
H 2.23864900 -1.72030800 0.49925100
C 5.80132500 -0.36142200 -2.18134500
C 4.54663000 -0.84040700 -2.56106400
C 3.41929300 -0.51174200 -1.81943300
C 3.54631400 0.30115000 -0.68903900
C 4.80090300 0.77951200 -0.30845200
C 5.92791200 0.44891100 -1.05635400
H 6.67976800 -0.62060600 -2.76442700
H 4.44951800 -1.47302400 -3.43790500
H 2.43699300 -0.88215300 -2.09587900
H 4.89497700 1.41618600 0.56746300

H 6.90184500 0.82648400 -0.76127800
C 2.34578900 0.67145200 0.10353300
H 2.50988800 1.41280700 0.89074500
O 1.23512600 0.78308500 -0.58348800

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.78287224
Gibbs Free Energy (T = 323K) = -1787.321032
Imaginary Frequency = 299.4980*i*
C 0.98433600 -0.48924000 1.67100900
N -0.12980500 -0.47262000 0.91916400
C 2.20886600 -0.99698300 1.27641100
B -0.03863300 1.02712900 0.12451200
C 3.35986600 -1.05404200 2.23855900
C 3.32588400 -2.33825700 3.06810300
H 2.41883400 -2.38759800 3.67425100
H 4.18809000 -2.38654300 3.73515400
H 3.34564700 -3.21894800 2.42250300
H 3.33245200 -0.18116300 2.89794700
H 4.29632400 -1.00654400 1.67923200
H 0.96569700 0.21553900 2.50003000
S -0.45851900 -1.84609300 -0.00973200
O 0.18178800 -1.81371300 -1.30093300
O -0.20875900 -2.97759700 0.85166600
C -4.06772200 -1.26779500 -1.66600400
C -2.69583700 -1.34786100 -1.48793600
C -2.19968800 -1.68569500 -0.24204500
C -3.04891600 -1.94416800 0.82433300
C -4.41424400 -1.85233600 0.63301400
C -4.94395400 -1.51130800 -0.61231500
H -4.46216300 -1.00628300 -2.64117000
H -2.01482900 -1.14253300 -2.30165500
H -2.64395200 -2.21651800 1.79052000
H -5.08350200 -2.05236300 1.46201600
O -0.01452200 2.02745700 1.13155800
O -1.08321500 1.26719200 -0.77705800
C -0.88607100 3.07330300 0.68356200
C -1.90975800 2.28571600 -0.19737900
C -1.48977800 3.76552300 1.89313000
H -2.24600000 4.49122800 1.58331900
H -1.95015000 3.04786400 2.57129600
H -0.71012100 4.30099700 2.43899400
C -2.53894600 3.09497100 -1.31811400
H -1.78671700 3.45631100 -2.01865200
H -3.24558300 2.46957100 -1.86788800
H -3.08498200 3.95146800 -0.91456900
C -3.00067900 1.61954100 0.63864500
H -3.68837300 2.35944400 1.05363700
H -3.56858600 0.93907200 0.00356900
H -2.56958300 1.04057100 1.45659200
C -0.05756800 4.06780700 -0.12936600
H 0.36009300 3.59449800 -1.01973000
H -0.65287700 4.92984300 -0.43757300
H 0.76875900 4.42416000 0.48878100
C -6.43020800 -1.38617200 -0.79764200
H -6.96204300 -2.17090800 -0.25713100
H -6.78128300 -0.42570500 -0.41041000
H -6.70598700 -1.44230400 -1.85098300
H 2.21698200 -1.73388200 0.47917700
C 5.80902800 -0.35986500 -2.13613700
C 4.56054300 -0.83202100 -2.52709300
C 3.43327600 -0.50904800 -1.79255700
C 3.55304200 0.29022500 -0.65810800
C 4.80075300 0.76150900 -0.26679600
C 5.92847300 0.43761600 -1.00770800
H 6.68907700 -0.61439300 -2.71445200
H 4.46883800 -1.45508400 -3.40842900
H 2.45344000 -0.87188800 -2.07899700
H 4.88903400 1.38856600 0.61359700
H 6.89887800 0.81082800 -0.70419600
C 2.34826800 0.65449200 0.12759200
H 2.51377000 1.38134400 0.92485400
O 1.25159900 0.79242000 -0.57293100

TS2-*syn*-P1
ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.37302588
Gibbs Free Energy (T = 323K) = -1786.909989
Imaginary Frequency = 276.2765*i*
C 0.81144000 1.11921600 2.00278000
N 0.74437000 -0.12336400 2.16536200
C -0.27959000 1.94777500 1.37510200
B -1.70911900 0.12468800 -0.69550000
C -0.25662200 3.37863500 1.93035100
C -1.42807100 4.24213300 1.46253700
H -1.36676500 4.48307400 0.39635100
H -1.44535500 5.18889400 2.01025800
H -2.38281300 3.73290800 1.63342200
H 0.69491500 3.86094300 1.67335300
H -0.28073600 3.31150200 3.02463600
H 1.72418400 1.65955300 2.29661300
S 0.74548200 -1.71270800 2.26270200
O 1.49336400 -2.13947800 3.44474500
O -0.60396500 -2.25732100 2.12641400
C 3.77510100 -2.16277900 -0.34167100
C 3.05821700 -1.98735600 0.83414800
C 1.66747100 -2.05807000 0.79133400
C 0.98849700 -2.30804600 -0.39643100

C 1.72473800 -2.47973400 -1.56294600
C 3.12025800 -2.39885600 -1.55665300
H 4.85998900 -2.11075000 -0.31827100
H 3.56772800 -1.79549500 1.77263300
H -0.09537500 -2.33623400 -0.41622600
H 1.20183500 -2.66568000 -2.49667200
O -2.79679500 0.83983300 -0.26139500
O -2.01981600 -1.09579300 -1.23526500
C -3.96706100 0.13024000 -0.73513700
C -3.41763700 -1.32899900 -0.93463200
C -5.06937900 0.25683800 0.30517000
H -5.93571000 -0.34816700 0.01815600
H -4.72777400 -0.06583000 1.29091400
H -5.39102100 1.30016400 0.37725800
C -4.04676600 -2.08757000 -2.09375000
H -3.88257000 -1.57812400 -3.04577400
H -3.60817100 -3.08765100 -2.15984100
H -5.12472800 -2.19842200 -1.93599700
C -3.46887900 -2.16936400 0.34008600
H -4.49926500 -2.42587500 0.60405300
H -2.91194100 -3.09608300 0.17578300
H -3.00199100 -1.65070100 1.18182600
C -4.39010400 0.79911600 -2.04302700
H -3.60879100 0.71320400 -2.80493400
H -5.31044500 0.35794300 -2.43678600
H -4.56916800 1.86183700 -1.85584500
C 3.90417400 -2.52457500 -2.83655400
H 4.04300000 -1.53760800 -3.29375200
H 4.89637400 -2.94836800 -2.65728700
H 3.38381800 -3.15439600 -3.56342200
H -1.24158800 1.48193700 1.61332600
C 3.83906000 2.95734000 -1.44750300
C 3.51976100 1.62319100 -1.20300900
C 2.23150800 1.27145800 -0.81337700
C 1.24717300 2.25081900 -0.66099500
C 1.56864700 3.58379300 -0.91936900
C 2.85914000 3.93692100 -1.30750000
H 4.84435400 3.23189400 -1.75264400
H 4.27320900 0.84872000 -1.31612600
H 1.98035400 0.23085400 -0.64165100
H 0.80554700 4.35274700 -0.82554100
H 3.09541300 4.97772800 -1.50742700
C -0.13891500 1.87669800 -0.17689000
H -0.87442800 2.56932500 -0.59945700
O -0.42500900 0.56108700 -0.62407000

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.80253502
Gibbs Free Energy (T = 323K) = -1787.340514

Imaginary Frequency = 280.3693*i*
C 0.83621500 1.08663100 1.99518400
N 0.74665900 -0.14473200 2.17953000
C -0.25317100 1.93149000 1.39734800
B -1.70763600 0.13487300 -0.68892300
C -0.20851600 3.35287400 1.96470100
C -1.37873500 4.22879600 1.52971100
H -1.34860200 4.45934700 0.46291900
H -1.36472200 5.17745200 2.06846200
H -2.33228700 3.73667200 1.73569900
H 0.73973200 3.82833300 1.69501600
H -0.21059200 3.27480900 3.05572100
H 1.77023700 1.61001500 2.24459000
S 0.72749500 -1.72625900 2.24962000
O 1.44294700 -2.16366400 3.42537600
O -0.60791900 -2.24964500 2.08622800
C 3.76729600 -2.16098900 -0.32579100
C 3.04382300 -1.98678400 0.83961600
C 1.65844200 -2.05961000 0.78913700
C 0.99333800 -2.31323000 -0.39909600
C 1.73442600 -2.48353400 -1.55702000
C 3.12441500 -2.39984900 -1.54127900
H 4.84955000 -2.10641800 -0.29471400
H 3.54385200 -1.79209000 1.77976900
H -0.08798300 -2.34405900 -0.42366200
H 1.21923700 -2.67134900 -2.49199400
O -2.79331100 0.84207600 -0.24849700
O -2.01753100 -1.07370900 -1.24600900
C -3.96531800 0.14034800 -0.73091300
C -3.41634300 -1.31291000 -0.95554900
C -5.06282700 0.24747000 0.31032200
H -5.92471900 -0.35556700 0.01594800
H -4.71940900 -0.08742000 1.28804800
H -5.38766900 1.28583000 0.39614200
C -4.04037900 -2.04686100 -2.12754500
H -3.86850100 -1.52387500 -3.06743500
H -3.60724200 -3.04538900 -2.20588100
H -5.11706900 -2.15450200 -1.97758800
C -3.47112800 -2.17358600 0.30058000
H -4.49990400 -2.43326200 0.55624600
H -2.91664700 -3.09548800 0.11976000
H -3.00654800 -1.67189600 1.15026000
C -4.38965600 0.82803400 -2.02383200
H -3.61212800 0.75440500 -2.78670600
H -5.30854100 0.39342800 -2.42068300
H -4.56884200 1.88450700 -1.81848200
C 3.91654200 -2.52737400 -2.81196300
H 4.06364600 -1.54242500 -3.26423600
H 4.90205700 -2.95534900 -2.62389700
H 3.39908600 -3.15144900 -3.54135100

H -1.21357800 1.47168800 1.64157500
C 3.80787200 2.97052300 -1.48304800
C 3.50121400 1.63974800 -1.23202100
C 2.22591200 1.28283400 -0.82218600
C 1.24243200 2.25351800 -0.65516100
C 1.55165700 3.58279700 -0.91918300
C 2.82875400 3.94132400 -1.32853300
H 4.80410800 3.24935400 -1.80499500
H 4.25591900 0.87153700 -1.35611200
H 1.98538000 0.24283600 -0.64395900
H 0.78795700 4.34598900 -0.81239600
H 3.05588700 4.98067200 -1.53362700
C -0.13283200 1.87541600 -0.15329500
H -0.86934400 2.57235300 -0.55966200
O -0.42684300 0.56591200 -0.61083400

TS2-*anti*-P1

ωB97XD/6-31G*
Solvent = THF
Potential Energy = -1787.37791542
Gibbs Free Energy (T = 323K) = -1786.913420
Imaginary Frequency = 250.5921*i*
C -0.71828300 -0.93155600 -1.81788200
N 0.43212200 -1.39158100 -1.61028800
C -1.90293100 -1.08501400 -0.90025100
B -0.22971100 1.55756700 0.06068600
C -3.07035800 -1.67073500 -1.71488500
C -2.73814300 -3.03054700 -2.32959500
H -1.91999700 -2.96432200 -3.05538800
H -3.60997500 -3.43996100 -2.84795500
H -2.43642000 -3.74447000 -1.55557300
H -3.35725000 -0.95967300 -2.50110600
H -3.93431000 -1.76799700 -1.05105000
H -0.91657000 -0.38217100 -2.74989100
S 1.79077800 -2.18531800 -1.39269600
O 1.45905800 -3.60560800 -1.49415100
O 2.85031500 -1.69134200 -2.26777200
C 1.74952000 -1.07323200 2.50405300
C 1.32480400 -1.43286600 1.23095200
C 2.27037100 -1.73752000 0.25950000
C 3.63284800 -1.69880900 0.55224600
C 4.03993100 -1.35275100 1.83341600
C 3.10784400 -1.03136300 2.82665600
H 1.00932300 -0.80834300 3.25334400
H 0.26806100 -1.43062900 0.99454900
H 4.36319100 -1.91321300 -0.21983700
H 5.10137300 -1.31593100 2.06206900
O -0.21053800 2.00695000 -1.23643800
O 0.78053900 2.04519000 0.84056100
C 0.79265700 3.05162800 -1.28978500
C 1.70623800 2.70050200 -0.05921200
C 1.49147300 2.98820500 -2.63932500
H 2.32041200 3.70271400 -2.67259400
H 1.88161700 1.98862500 -2.84267900
H 0.78534800 3.24917400 -3.43334700
C 2.30714400 3.90470600 0.65002300
H 1.53392000 4.56774200 1.04418400
H 2.92709300 3.56606300 1.48549800
H 2.94250600 4.47381300 -0.03660400
C 2.79837700 1.68744400 -0.39621900
H 3.59512400 2.14472000 -0.99066800
H 3.22915800 1.30590300 0.53411300
H 2.39954500 0.83608900 -0.95432900
C 0.05574000 4.38117100 -1.13164800
H -0.45041500 4.44259900 -0.16298300
H 0.74163300 5.22872400 -1.22060200
H -0.69987300 4.46464100 -1.91811900
C 3.56112000 -0.66331700 4.21507900
H 4.51473600 -0.12793200 4.19303300
H 2.82302700 -0.03505200 4.72125600
H 3.70336400 -1.56441400 4.82313500
H -1.63749300 -1.78000600 -0.09523300
C -5.77764700 -0.04250600 2.19800800
C -4.56238800 -0.56079800 2.64397800
C -3.42294700 -0.44676600 1.85505000
C -3.48604100 0.18972100 0.61339700
C -4.70203200 0.71138400 0.17486800
C -5.84566000 0.59420200 0.96226000
H -6.66689600 -0.13228300 2.81458600
H -4.50295700 -1.05421200 3.60947300
H -2.47463600 -0.84141800 2.20830700
H -4.75731700 1.21209600 -0.78858800
H -6.78715600 1.00526100 0.61073000
C -2.25416000 0.27866600 -0.25762600
H -2.42541500 1.01129500 -1.05568100
O -1.15891700 0.69503300 0.55171500

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1787.80587249
Gibbs Free Energy (T = 323K) = -1787.348697
Imaginary Frequency = 270.2390*i*
C -0.07250300 -0.51021100 -2.20195100
N 1.14801500 -0.38736300 -1.97655100
C -0.96956300 -1.45434600 -1.45285300
B -0.92943100 1.41323400 0.38745900
C -1.78561300 -2.29151900 -2.44334500
C -0.90814900 -3.14339500 -3.35462800
H -0.25627700 -2.53033500 -3.98223900
H -1.52080100 -3.75866700 -4.01516700

H -0.27100700 -3.80893600 -2.76702600
H -2.41825000 -1.62714500 -3.04266500
H -2.46140700 -2.93510500 -1.87751800
H -0.55416400 0.08690200 -2.98947700
S 2.66476300 -0.06148900 -1.69832900
O 3.43249500 -0.80566300 -2.66077500
O 2.83037400 1.36450900 -1.59679000
C 3.84044700 -2.45622200 1.31679000
C 3.66198600 -1.91961500 0.04942500
C 2.96361900 -0.73333200 -0.08797400
C 2.44092600 -0.07989700 1.02095700
C 2.62035900 -0.63185500 2.27452400
C 3.32383900 -1.82583600 2.44364100
H 4.39058000 -3.38387700 1.42687300
H 4.06173400 -2.41647100 -0.82477700
H 1.88704200 0.84359400 0.90927900
H 2.20469300 -0.12709300 3.13957400
O -1.47140600 2.21050500 -0.58301400
O -0.26103400 2.09687500 1.36347900
C -1.36081800 3.57380700 -0.10576500
C -0.17992000 3.47569600 0.92585600
C -1.09269900 4.48533600 -1.28787600
H -0.91392200 5.50707300 -0.94551600
H -0.22902300 4.15228200 -1.86167100
H -1.96186200 4.49544400 -1.94780000
C -0.32489700 4.37982800 2.13581600
H -1.22719900 4.15392200 2.70242600
H 0.53547300 4.24863200 2.79406300
H -0.35808000 5.42644400 1.82479100
C 1.19021100 3.66285600 0.28750900
H 1.34171100 4.69738400 -0.02523200
H 1.95806200 3.41384900 1.02246700
H 1.32865100 3.00973600 -0.57503200
C -2.69648400 3.92235500 0.54177000
H -2.90625700 3.27458600 1.39521500
H -2.71392400 4.95972700 0.87959100
H -3.49071400 3.78589000 -0.19370900
C 3.52532800 -2.39991600 3.81865300
H 2.58711800 -2.41560600 4.37686600
H 3.91575700 -3.41687300 3.77236300
H 4.23330400 -1.79258300 4.38858400
H -0.33918700 -2.10328500 -0.83871300
C -4.54790200 -3.16570000 1.68597100
C -3.19637400 -3.13653700 2.00810700
C -2.33174900 -2.31073400 1.30823100
C -2.81048400 -1.50295400 0.28079900
C -4.16277900 -1.53107600 -0.03308700
C -5.03009700 -2.36138600 0.66466600
H -5.22303000 -3.81204800 2.23399200
H -2.81633500 -3.75978300 2.80886500
H -1.27929000 -2.28057300 1.56566700
H -4.54197600 -0.89987900 -0.82975000
H -6.08363300 -2.37497400 0.41217500
C -1.86107300 -0.62996700 -0.50188100
H -2.43900400 0.08996300 -1.08928100
O -1.01513100 0.06311400 0.41015800

2

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1290.20361443
Gibbs Free Energy (T = 213K) = -1289.839181
C -0.92208500 0.78764500 -0.44818300
N 0.48407700 0.89890700 -0.22941200
C -1.68611400 -0.00818300 0.30412800
B 1.37816100 -0.22967100 -0.13239900
H -1.31788400 1.39441400 -1.25453000
S 1.01915300 2.50266800 -0.02355200
O 2.38119400 2.60506100 -0.51942900
O -0.01318900 3.36766400 -0.57466500
H -1.21955600 -0.52566700 1.14132100
C 2.83615000 -0.21620500 0.47290800
H 3.17015800 0.75760600 0.84154400
C 0.97638300 -1.66933700 -0.64049400
H -0.03438700 -1.71405700 -1.05948300
C 1.03474500 -2.66971700 0.53768700
H 0.89991200 -3.69370400 0.16329500
H 0.16960500 -2.47057100 1.18641200
C 1.96318100 -1.98225500 -1.79821700
H 1.75468300 -1.27777800 -2.61617300
H 1.74880500 -2.98293700 -2.19765100
C 3.82881500 -0.62486600 -0.64292600
H 4.83369100 -0.74892000 -0.21658600
H 3.89157900 0.22278600 -1.33748600
C 2.79239500 -1.17667700 1.69233500
H 2.12734900 -0.73330000 2.44996100
H 3.78752200 -1.22071400 2.15517100
C 3.45371800 -1.88969700 -1.43582900
H 4.04333500 -1.91308100 -2.36039300
H 3.74952000 -2.78247700 -0.87862900
C 2.31098300 -2.60493400 1.39530300
H 3.11466300 -3.16454800 0.91058600
H 2.12663800 -3.12129700 2.34541500
C 1.01898700 2.69080800 1.75007900
H 1.74219900 1.99685200 2.18055500
H 1.29868400 3.72264500 1.97127800
H 0.01116800 2.48247000 2.11298000
C -3.12152300 -0.25724200 0.10976800
C -3.85533600 -0.82744000 1.15745000
C -3.79066900 0.05152300 -1.08255800

C -5.22029400 -1.06121500 1.03033800
H -3.34849700 -1.08442000 2.08439600
C -5.15500400 -0.17853200 -1.20870600
H -3.23955900 0.45906500 -1.92473300
C -5.87611200 -0.73353500 -0.15294600
H -5.77122500 -1.50128900 1.85613900
H -5.65642900 0.06703300 -2.14003400
H -6.94111300 -0.91745300 -0.25671100

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1290.49171461
Gibbs Free Energy (T = 213K) = -1290.130027
C -0.91377000 0.78947800 -0.45357300
N 0.48979100 0.90488200 -0.23576600
C -1.67196600 -0.00663300 0.29214300
B 1.37579600 -0.22333800 -0.13429600
H -1.31259400 1.39672300 -1.25466900
S 1.01580400 2.49284400 -0.01473700
O 2.37814900 2.58716600 -0.45546300
O 0.01841200 3.34664600 -0.60039000
H -1.20280000 -0.52927100 1.12179400
C 2.81415300 -0.22448900 0.50309100
H 3.13265600 0.74165000 0.89473900
C 0.98389700 -1.64851800 -0.67509500
H -0.01485900 -1.68055000 -1.11588500
C 1.01478300 -2.67238200 0.47971200
H 0.89130200 -3.68520700 0.08037200
H 0.13529800 -2.48934000 1.10876700
C 1.99458700 -1.93813000 -1.81503700
H 1.80773400 -1.21641500 -2.61955700
H 1.78551400 -2.92583300 -2.24055500
C 3.83337100 -0.61527300 -0.59052900
H 4.82299000 -0.75239000 -0.14054400
H 3.91908000 0.24307900 -1.26504300
C 2.73833700 -1.20404300 1.70244400
H 2.05541300 -0.77455100 2.44812800
H 3.71853400 -1.25435000 2.18898600
C 3.47319300 -1.85973600 -1.41602900
H 4.08318600 -1.86715400 -2.32402200
H 3.75084700 -2.76259900 -0.87162800
C 2.26711600 -2.62371400 1.36761000
H 3.08081900 -3.17164200 0.89288200
H 2.06070900 -3.15729000 2.30014500
C 0.95698200 2.69146100 1.74689800
H 1.66218100 1.99673500 2.19835500
H 1.23609500 3.72161300 1.96241100
H -0.06199100 2.49252200 2.07348000
C -3.10567500 -0.25576000 0.10277200
C -3.82450900 -0.85851300 1.13581300
C -3.78581100 0.08548100 -1.06889000
C -5.18484000 -1.09469000 1.01500300
H -3.30814700 -1.14049500 2.04728900
C -5.14466000 -0.14799900 -1.18875300
H -3.24746100 0.52279700 -1.90123500
C -5.85071500 -0.73658700 -0.14728300
H -5.72496100 -1.56139800 1.83010900
H -5.65590000 0.12261300 -2.10492100
H -6.91333300 -0.92245000 -0.24671700

PhCHO

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -345.455708864
Gibbs Free Energy (T = 213K) = -345.364491
C 2.21054800 -0.24813300 -0.00028400
C 1.32472300 -1.32731300 -0.00015500
C -0.04420800 -1.09945800 0.00001700
C -0.53101800 0.21173300 0.00006300
C 0.35777600 1.28856500 -0.00006600
C 1.72979000 1.05929800 -0.00024000
H 3.28129800 -0.42929200 -0.00041800
H 1.70723900 -2.34324100 -0.00019000
H -0.75272800 -1.92191200 0.00011900
H -0.02761700 2.30568200 -0.00002900
H 2.42229500 1.89509200 -0.00034000
C -1.98799800 0.46822900 0.00025400
H -2.27271100 1.54132900 0.00027900
O -2.83943200 -0.39564800 0.00038100

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -345.546956259
Gibbs Free Energy (T = 213K) = -345.456648
C 2.20414900 -0.24372900 0.00000300
C 1.32360300 -1.32126700 -0.00000100
C -0.04054800 -1.09748600 -0.00000400
C -0.52859800 0.20790800 -0.00000400
C 0.35452200 1.28237800 -0.00000200
C 1.72255000 1.05754100 0.00000200
H 3.27294500 -0.42234600 0.00000700
H 1.70798800 -2.33392500 0.00000000
H -0.74701500 -1.91875400 -0.00000700
H -0.03374800 2.29584200 -0.00000200
H 2.41184900 1.89286300 0.00000500
C -1.98506600 0.46436700 -0.00000300
H -2.26780000 1.53720400 -0.00000800
O -2.83098600 -0.39364500 0.00000700

2···PhCHO

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.67402225
Gibbs Free Energy (T = 213K) = -1635.203338
C 2.40743700 -0.63665800 -0.65417100
N 0.98008200 -0.61541500 -0.55557200
C 3.18037500 -0.09579300 0.28933000
B 0.20833700 0.59061500 -0.39405100
H 2.80729000 -1.10539800 -1.54613100
S 0.28981000 -2.17238500 -0.53433100
O -1.03874000 -2.11342300 -1.12627900
O 1.27991300 -3.07655200 -1.10107100
H 2.69540000 0.36434700 1.14926900
C -1.30318300 0.66977600 0.03918800
H -1.77142600 -0.30273100 0.18539300
C 0.82155300 2.02986500 -0.60588600
H 1.87455400 2.01597100 -0.90718400
C 0.73322400 2.80479500 0.73224900
H 1.03621700 3.84925900 0.57587500
H 1.47955500 2.37439500 1.41606300
C 0.02045500 2.66836900 -1.77177100
H 0.25221900 2.10186400 -2.68507700
H 0.38488100 3.68978600 -1.94803700
C -2.10439900 1.37627300 -1.07895600
H -3.13512200 1.54582800 -0.73985400
H -2.17262400 0.67210000 -1.91882700
C -1.31942100 1.39461200 1.40879100
H -0.82413400 0.74377800 2.14505900
H -2.35859600 1.49388100 1.75024800
C -1.50542700 2.69987400 -1.58575000
H -1.97197700 2.95432800 -2.54544900
H -1.77351200 3.51406400 -0.90719200
C -0.63941600 2.77226100 1.42931900
H -1.30303700 3.51207400 0.97480700
H -0.51440700 3.09181300 2.47122300
C 0.14576900 -2.51617200 1.20849500
H -0.58105700 -1.83775200 1.65862800
H -0.19184300 -3.54971300 1.30995300
H 1.13265700 -2.39489500 1.65855700
C 4.64824800 -0.00916800 0.24754200
C 5.29072000 0.96943100 1.01503900
C 5.43178300 -0.87568600 -0.52637200
C 6.67564400 1.09694400 0.99438100
H 4.69479400 1.64243200 1.62680500
C 6.81523900 -0.74876400 -0.54637700
H 4.95888800 -1.66737900 -1.10012300
C 7.44249400 0.23945200 0.21062900
H 7.15553500 1.86584300 1.59238900
H 7.40798200 -1.43056200 -1.14884000
H 8.52402200 0.33393200 0.19516000
C -6.08835400 0.75236800 -0.74430200
C -5.82302400 0.97038700 0.60934100
C -4.95158700 0.12926500 1.28715800
C -4.34715300 -0.93464200 0.61051900
C -4.61204300 -1.14935700 -0.74324400
C -5.48361300 -0.30408300 -1.42160900
H -6.76813600 1.41369200 -1.27333300
H -6.29676400 1.79732600 1.12913900
H -4.72461600 0.27946700 2.33813600
H -4.11557600 -1.96374400 -1.26463600
H -5.68655900 -0.46357300 -2.47574700
C -3.38279300 -1.81241200 1.30361700
H -2.98573800 -2.64450200 0.68901000
O -3.00158000 -1.65109600 2.44738700

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.05321363
Gibbs Free Energy (T = 213K) = -1635.587325
C 2.38134500 -0.67669300 -0.59089300
N 0.96029200 -0.61235100 -0.48795200
C 3.17134800 -0.10352200 0.30929400
B 0.23126700 0.61340600 -0.31428400
H 2.76344400 -1.20911000 -1.45112200
S 0.20932600 -2.12345300 -0.48538900
O -1.10176600 -1.98055100 -1.05711000
O 1.13674100 -3.04788900 -1.08060700
H 2.70457100 0.41241900 1.14450200
C -1.25436900 0.74953300 0.17892000
H -1.73031100 -0.19532800 0.43343900
C 0.86255300 2.01849600 -0.63817500
H 1.90096100 1.95761000 -0.97129200
C 0.83027400 2.90651800 0.62364700
H 1.14284900 3.92531000 0.36830900
H 1.58940900 2.52477900 1.31768600
C 0.03385200 2.56490200 -1.83021700
H 0.23116400 1.92008600 -2.69522900
H 0.40557700 3.55884200 -2.10332300
C -2.08067600 1.36828300 -0.97025700
H -3.09480500 1.58103900 -0.61823500
H -2.18185200 0.59703000 -1.74114400
C -1.21320200 1.59487300 1.47511900
H -0.70181700 1.00408100 2.24675800
H -2.23678200 1.74002700 1.83805000
C -1.48192800 2.63288900 -1.60304800
H -1.97295600 2.81133100 -2.56438000
H -1.71923100 3.50286300 -0.99006900
C -0.51805000 2.95612700 1.35704300
H -1.18351800 3.66155900 0.85959600
H -0.35991200 3.36178000 2.36083500

C 0.06571500 -2.49678500 1.23944700
H -0.57725400 -1.75381500 1.70562500
H -0.39004600 -3.48184400 1.31966400
H 1.06837500 -2.49209000 1.66288700
C 4.63775400 -0.04653200 0.25487200
C 5.30084800 0.91800100 1.01358900
C 5.39958900 -0.92300500 -0.52147900
C 6.68308400 1.02076600 0.98513200
H 4.72200100 1.59960200 1.62795500
C 6.77949400 -0.82166000 -0.54836000
H 4.91244700 -1.70293000 -1.09481500
C 7.42719800 0.15232500 0.20146800
H 7.17907000 1.77991600 1.57815200
H 7.35565400 -1.51209800 -1.15282500
H 8.50772800 0.22714600 0.17931300
C -5.91670100 1.16728100 -0.25854500
C -5.40144700 1.03587900 1.02782700
C -4.63870700 -0.06948900 1.35481400
C -4.39025800 -1.04912100 0.39545700
C -4.90145900 -0.91196700 -0.88990500
C -5.66574100 0.19747000 -1.21810000
H -6.51366900 2.03508900 -0.51300900
H -5.59789500 1.79972900 1.77036600
H -4.22368900 -0.19463300 2.34764100
H -4.69196200 -1.67400900 -1.63306900
H -6.06230800 0.30790500 -2.21973700
C -3.57938300 -2.23788800 0.73161700
H -3.46846000 -2.97596100 -0.08362100
O -3.05887000 -2.42178000 1.80631400

***syn-E*-P2**

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.69685765
Gibbs Free Energy (T = 213K) = -1635.221933
C 0.57044100 1.28758900 -0.10116900
N -0.44696400 1.99106700 -0.41389600
C 0.78941000 -0.03401000 -0.77161400
B -1.91069800 -1.18658400 0.28662300
H 1.27941000 1.62113700 0.66339600
S -0.63746600 3.43378200 0.47667100
O -1.94624900 3.35530700 1.11104400
O 0.53831600 3.71512500 1.29782100
H 0.00652600 -0.12739600 -1.52923700
C 3.68769500 -1.45154500 3.17836700
C 2.58572300 -0.63148000 3.40967800
C 1.55373700 -0.56598200 2.47807300
C 1.61820100 -1.31665300 1.30261300
C 2.71841600 -2.14543800 1.08281100
C 3.75003400 -2.21254300 2.01410000
H 4.49170200 -1.50208600 3.90652600
H 2.52591300 -0.04232600 4.31978700
H 0.68674300 0.05885900 2.66879900
H 2.77547200 -2.73190600 0.16939600
H 4.60181800 -2.86012000 1.82949900
C 0.54370000 -1.19775100 0.24593200
H 0.51926800 -2.12024700 -0.34679100
O -0.70068700 -0.98308000 0.88410500
C -3.23377600 -0.84982200 1.06456800
H -3.03240900 -0.48123900 2.07786300
C -2.18818000 -1.73023500 -1.17025000
H -1.28859900 -1.99383900 -1.74384000
C -2.90226400 -0.58253700 -1.93454100
H -3.19719000 -0.93215800 -2.93387200
H -2.17100300 0.22274100 -2.09221400
C -3.02531800 -3.02738400 -1.02390000
H -2.36921000 -3.79998300 -0.59754700
H -3.31840000 -3.39301200 -2.01790600
C -4.05926900 -2.15482500 1.18251300
H -5.03497100 -1.94201100 1.64118300
H -3.53392000 -2.82125900 1.88145900
C -3.93132600 0.28990100 0.27743500
H -3.32378300 1.19598200 0.39759600
H -4.90694900 0.51254900 0.73191000
C -4.28055400 -2.91093400 -0.14037300
H -4.64254000 -3.92151500 0.08622600
H -5.08424600 -2.43457100 -0.70723600
C -4.12911600 0.02213100 -1.22618900
H -4.99658000 -0.62555000 -1.37794200
H -4.38174900 0.96868100 -1.71989700
C -0.70442600 4.60435400 -0.86190800
H -1.50973600 4.31425000 -1.53718600
H -0.90668700 5.58187200 -0.41994800
H 0.25751500 4.60930400 -1.37623300
C 2.13528700 -0.12834900 -1.46437700
C 2.19671400 -0.72170400 -2.72706900
C 3.31960200 0.32173200 -0.87346300
C 3.41284700 -0.86755200 -3.38768900
H 1.28160100 -1.07330900 -3.19789000
C 4.53491300 0.18461500 -1.53649800
H 3.30758600 0.76306700 0.11852800
C 4.58616300 -0.41106500 -2.79387600
H 3.44145800 -1.33328900 -4.36812300
H 5.44544500 0.53947100 -1.06350200
H 5.53625500 -0.51904200 -3.30819400

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.07339487
Gibbs Free Energy (T = 213K) = -1635.602279

C 0.56214100 1.28636300 -0.08517300
N -0.45356600 1.98786600 -0.37656900
C 0.78076800 -0.02751700 -0.76543400
B -1.90703900 -1.19817500 0.28526500
H 1.27587400 1.61933600 0.67248500
S -0.63681700 3.41769800 0.50601800
O -1.93947100 3.35207600 1.11117600
O 0.51419600 3.67831900 1.33687000
H 0.00076800 -0.11608800 -1.52230100
C 3.69266600 -1.50061500 3.13719900
C 2.61032300 -0.66455700 3.37447700
C 1.57615100 -0.58408700 2.45420000
C 1.61816900 -1.33564800 1.28434100
C 2.69786100 -2.18085200 1.05938500
C 3.73229400 -2.26292800 1.97906000
H 4.49967200 -1.56292100 3.85749500
H 2.56833800 -0.07382700 4.28171100
H 0.72439600 0.05615400 2.64913400
H 2.73710500 -2.76974300 0.14928900
H 4.56968000 -2.92391600 1.79028200
C 0.54133100 -1.20071500 0.23655700
H 0.51735300 -2.11492200 -0.36405100
O -0.70136000 -0.99798400 0.88092800
C -3.22554400 -0.85651300 1.06006800
H -3.02165500 -0.50345800 2.07535900
C -2.18511600 -1.72728400 -1.17205500
H -1.28691200 -1.99476900 -1.73958600
C -2.88339200 -0.56952700 -1.93087800
H -3.18441300 -0.91260600 -2.92742900
H -2.14274300 0.22311600 -2.08849100
C -3.03560600 -3.01359100 -1.03852000
H -2.39428800 -3.79320600 -0.60932100
H -3.32127900 -3.37113800 -2.03441200
C -4.07613000 -2.14291400 1.15853600
H -5.04981600 -1.91431200 1.60680500
H -3.57310400 -2.82222100 1.85718200
C -3.89284700 0.30480800 0.28277200
H -3.26339900 1.19182600 0.40807800
H -4.85921200 0.54834600 0.73903500
C -4.29545600 -2.88382500 -0.16968600
H -4.67572300 -3.88714400 0.04468100
H -5.08218600 -2.39080000 -0.74049600
C -4.09661300 0.05095200 -1.21897000
H -4.97346800 -0.57825400 -1.37302900
H -4.33182600 1.00269400 -1.70481600
C -0.66705200 4.58742300 -0.82313600
H -1.47597500 4.31715800 -1.49743300
H -0.84551500 5.56317700 -0.37395700
H 0.29650300 4.56525400 -1.32745700
C 2.12356100 -0.10912000 -1.45903600
C 2.18544200 -0.67008300 -2.73076500
C 3.30315900 0.32663600 -0.85978200
C 3.39806400 -0.80143300 -3.39069300
H 1.27210000 -1.00730000 -3.20994900
C 4.51487100 0.20326000 -1.52132800
H 3.28955400 0.74579500 0.13924700
C 4.56691400 -0.36245800 -2.78695800
H 3.42785900 -1.24317600 -4.37953000
H 5.42340900 0.54572500 -1.04089900
H 5.51546700 -0.46007600 -3.30113400

***anti-E*-P2**

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.69527765
Gibbs Free Energy (T = 213K) = -1635.219490
C 1.52132200 -0.78110400 -0.44364400
N 1.52000800 -1.74893300 0.38621700
C 1.09220000 0.59185900 -0.00391300
B -1.77799400 -0.53913900 -0.49893700
H 1.86210500 -0.90659800 -1.47749500
S 2.03366500 -3.25111300 -0.23302800
O 0.94932800 -4.19087200 0.01787500
O 2.56915300 -3.11844700 -1.58605000
H 0.66610200 0.48753700 0.99764200
C -2.33223100 4.53962800 0.22153000
C -1.23999900 4.16149200 0.99407200
C -0.46397000 3.06360900 0.62744700
C -0.77376000 2.32796000 -0.51501400
C -1.86820200 2.72164900 -1.29242100
C -2.64325200 3.81599200 -0.92805200
H -2.93761100 5.39319000 0.51095800
H -0.98723200 4.71881400 1.89102900
H 0.38326600 2.79137500 1.24692400
H -2.12049400 2.15302100 -2.18305200
H -3.49198800 4.10322500 -1.54144900
C 0.01042700 1.10872500 -0.97509300
H 0.50177300 1.36919100 -1.91924000
O -0.85913300 0.03783100 -1.33539200
C -2.71325700 -1.66539000 -1.07240600
H -2.49604800 -1.88117300 -2.12618800
C -2.07632900 -0.22872200 1.02005800
H -1.45020600 0.55491300 1.46035300
C -1.80612600 -1.53805900 1.80704900
H -2.07852400 -1.39343700 2.86219100
H -0.72276400 -1.71948400 1.78897900
C -3.53891500 0.28284700 1.09310600
H -3.56167800 1.28174700 0.63523500
H -3.82688500 0.42213100 2.14446300
C -4.16191300 -1.11924000 -0.98954100

H -4.87253100 -1.88885400 -1.32213200
H -4.25012200 -0.29231300 -1.70965300
C -2.45568800 -2.95718900 -0.25835200
H -1.45681700 -3.32687700 -0.52352500
H -3.16381700 -3.74029300 -0.56454600
C -4.58682200 -0.60535800 0.39761400
H -5.51733400 -0.03332300 0.29268900
H -4.83625200 -1.45305800 1.04081100
C -2.51636600 -2.79464400 1.27164000
H -3.55747400 -2.79922800 1.60612700
H -2.05415600 -3.67645400 1.73168000
C 3.37231000 -3.59278100 0.88930900
H 2.98536600 -3.57364500 1.90841000
H 3.75080700 -4.58604200 0.64030600
H 4.15085900 -2.84140100 0.74975100
C 2.34400500 1.45619400 0.07487300
C 2.89547000 1.74639000 1.32554600
C 2.99579800 1.91686400 -1.07154500
C 4.05752800 2.50289400 1.43202300
H 2.40664600 1.37735500 2.22389600
C 4.16019800 2.67265400 -0.96644800
H 2.60474000 1.68886400 -2.05915500
C 4.69227700 2.97098200 0.28434200
H 4.46736000 2.72546400 2.41247400
H 4.65218400 3.02720900 -1.86691000
H 5.59898500 3.56256500 0.36449600

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.07161457
Gibbs Free Energy (T = 213K) = -1635.600291
C 1.52008100 -0.90294000 -0.42273300
N 1.37631200 -1.88037100 0.37058000
C 1.17533100 0.49036900 0.01640200
B -1.76884600 -0.44470500 -0.48352100
H 1.91263500 -1.03994900 -1.43475700
S 1.77438500 -3.40135300 -0.24536000
O 0.59449000 -4.21101300 -0.10395100
O 2.41408400 -3.30166700 -1.53488500
H 0.74390200 0.40840400 1.01417300
C -2.00997400 4.62407700 0.19352300
C -1.04940900 4.11071800 1.04919100
C -0.33195700 2.97486200 0.69742900
C -0.56914100 2.33766600 -0.51243000
C -1.52891200 2.86859100 -1.37269600
C -2.24653500 3.99960800 -1.02406900
H -2.57180300 5.50761400 0.47159300
H -0.85585700 4.59150500 2.00059900
H 0.40885100 2.59264000 1.38721800
H -1.72437000 2.37439400 -2.31779300
H -2.99326700 4.39426100 -1.70266400
C 0.13213900 1.06757200 -0.95740700
H 0.64090900 1.28789400 -1.89945900
O -0.81344900 0.06168200 -1.31500100
C -2.82175800 -1.44668400 -1.07184200
H -2.61418600 -1.68342400 -2.12006300
C -2.03827300 -0.12216800 1.03403500
H -1.31994500 0.56123900 1.49042000
C -1.96181100 -1.45844400 1.81089500
H -2.21725500 -1.28373700 2.86269300
H -0.91704400 -1.78879800 1.79610000
C -3.41516900 0.58588300 1.08869100
H -3.28985200 1.58188000 0.64695600
H -3.70025800 0.75020100 2.13419100
C -4.17981300 -0.70298500 -1.01628300
H -4.98059900 -1.36330300 -1.36853900
H -4.13487700 0.12787600 -1.73163500
C -2.76508400 -2.76149100 -0.26380200
H -1.82244900 -3.26176500 -0.50877900
H -3.56578200 -3.43569800 -0.58995900
C -4.55872600 -0.14002600 0.36218300
H -5.39324700 0.55725400 0.23993000
H -4.94073600 -0.94414800 0.99109300
C -2.83647000 -2.59429500 1.26149600
H -3.87102100 -2.44416200 1.57243300
H -2.52168100 -3.53191400 1.72896600
C 2.97479100 -3.90361500 0.95585900
H 2.50718600 -3.87990700 1.93704400
H 3.27279700 -4.91717300 0.69205800
H 3.82376700 -3.22559400 0.90219500
C 2.46137100 1.29540400 0.09443800
C 2.99505400 1.61280500 1.33999000
C 3.15417900 1.68154100 -1.04964300
C 4.18205100 2.32063700 1.44320000
H 2.47227600 1.30345500 2.23888300
C 4.34326200 2.38808700 -0.94832200
H 2.77386900 1.43121900 -2.03341500
C 4.85865100 2.71283600 0.29733400
H 4.57908400 2.56568200 2.42094400
H 4.86863600 2.68445500 -1.84810200
H 5.78592900 3.26731600 0.37502900

***syn-Z*-P2**
ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.69540589
Gibbs Free Energy (T = 213K) = -1635.220512
C -1.87681600 -0.99007900 -1.34052800
N -2.49999200 -2.09116300 -1.15490600
C -1.60474900 0.13298800 -0.37115400

B 2.03046500 -0.55935100 -0.56630500
H -1.46702200 -0.86890700 -2.34483800
S -3.19093200 -2.40537000 0.36609000
O -2.14085800 -2.49384600 1.38133200
O -4.31857400 -1.50556800 0.59098300
H -2.31619000 0.07555200 0.45637100
C 0.56951200 2.89654500 3.26227800
C 0.99646200 3.10573900 1.95332400
C 0.75616400 2.14406000 0.97630500
C 0.09294000 0.96200000 1.30560200
C -0.33685700 0.75719200 2.61686100
C -0.10099000 1.72101600 3.59214200
H 0.75948800 3.64715400 4.02366600
H 1.51590700 4.02219800 1.68967900
H 1.08257900 2.31029500 -0.04555200
H -0.85548300 -0.16459500 2.87087100
H -0.43397100 1.55021500 4.61148800
C -0.20459100 -0.09475900 0.26649900
H -0.23946100 -1.07382600 0.75428700
O 0.75621700 -0.11521700 -0.77813900
C 3.09637300 -0.45216300 -1.71707500
H 2.66703900 -0.06172800 -2.64895500
C 2.63095800 -1.14907000 0.76657700
H 1.90735000 -1.24541300 1.58517700
C 3.71831300 -0.14655900 1.23829900
H 4.24918000 -0.56056500 2.10667900
H 3.20082400 0.75337700 1.59699000
C 3.16004900 -2.56885400 0.43960300
H 2.29083200 -3.21285800 0.24214500
H 3.65545500 -2.99239300 1.32410900
C 3.65840700 -1.86599900 -2.00201700
H 4.49012000 -1.80449200 -2.71783100
H 2.86752300 -2.44080400 -2.50459200
C 4.14587600 0.57476400 -1.21410800
H 3.65684200 1.55903600 -1.17366800
H 4.95877300 0.66943700 -1.94754200
C 4.11858200 -2.65482400 -0.76156800
H 4.23847300 -3.70910300 -1.04027100
H 5.11386800 -2.31985700 -0.45879500
C 4.74785600 0.26988700 0.16999100
H 5.51361100 -0.50378100 0.07189200
H 5.27861700 1.16170300 0.52563500
C -3.81207300 -4.03915000 0.05082500
H -2.97606200 -4.69037400 -0.20578900
H -4.29423700 -4.37642100 0.97019400
H -4.53269800 -3.99015200 -0.76586600
C -1.76321900 1.48665000 -1.03682300
C -2.64866100 2.41193000 -0.48152800
C -1.03367600 1.84900900 -2.17372900
C -2.80000100 3.67679000 -1.04115600
H -3.22030800 2.14149500 0.40220400
C -1.18651300 3.11307600 -2.73518200
H -0.32266000 1.15334300 -2.60656100
C -2.06889400 4.03081500 -2.17120800
H -3.49056300 4.38466800 -0.59287900
H -0.61038600 3.38185000 -3.61569500
H -2.18588800 5.01678800 -2.61092900

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.07151030
Gibbs Free Energy (T = 213K) = -1635.601008
C -1.89142300 -0.98348300 -1.33590600
N -2.52328200 -2.06833700 -1.14012600
C -1.60664400 0.13889100 -0.37489100
B 2.01638900 -0.57971000 -0.57263000
H -1.48395400 -0.86885300 -2.34049900
S -3.21101200 -2.37501200 0.36591700
O -2.17625800 -2.47120800 1.36919100
O -4.31610900 -1.47589500 0.58412700
H -2.31408200 0.08718100 0.45252400
C 0.60460300 2.87510400 3.24403900
C 1.00268300 3.09123700 1.93244600
C 0.74905400 2.13547400 0.96038200
C 0.09858900 0.95380500 1.29532100
C -0.30167500 0.74221000 2.60916800
C -0.05065900 1.69899400 3.58078100
H 0.80607400 3.62136400 4.00331900
H 1.51157600 4.00921100 1.66343800
H 1.05608300 2.30533400 -0.06445300
H -0.80865900 -0.18156200 2.86934700
H -0.36042900 1.52242000 4.60391800
C -0.21005100 -0.09799600 0.25849800
H -0.25104000 -1.07368400 0.74682900
O 0.75188800 -0.12446900 -0.78443300
C 3.08936400 -0.45807400 -1.70953400
H 2.66614900 -0.05872000 -2.63696000
C 2.60445800 -1.18699900 0.75288300
H 1.87287000 -1.29760400 1.55826500
C 3.68088800 -0.18914600 1.25060600
H 4.20442200 -0.61542600 2.11378400
H 3.15734300 0.69960400 1.62008600
C 3.14246200 -2.59711800 0.41272500
H 2.28062800 -3.23998100 0.19512700
H 3.62597200 -3.02978100 1.29578800
C 3.66480100 -1.86025800 -2.00700800
H 4.50204700 -1.78172600 -2.71014500
H 2.88662600 -2.43253000 -2.52613300
C 4.12386100 0.56895700 -1.18286200
H 3.62723800 1.54588000 -1.13301500

H 4.93948400 0.68023000 -1.90639400
C 4.11490300 -2.66029100 -0.77415700
H 4.24624800 -3.70707800 -1.06420100
H 5.10079900 -2.32221400 -0.45504300
C 4.71444600 0.24857700 0.19919300
H 5.48384000 -0.51669700 0.09662300
H 5.23482300 1.13620000 0.57126900
C -3.84406300 -3.99707400 0.05345800
H -3.01120300 -4.64827500 -0.20068500
H -4.32625100 -4.32246900 0.97371600
H -4.56069900 -3.93572200 -0.76183100
C -1.75270800 1.49197700 -1.03719100
C -2.58946900 2.43805200 -0.45485600
C -1.04768000 1.83629800 -2.18866900
C -2.71465500 3.70623100 -1.00080500
H -3.14209000 2.18059000 0.44190400
C -1.17479600 3.10338500 -2.73713900
H -0.37470000 1.12212600 -2.64547300
C -2.00646900 4.04261600 -2.14449700
H -3.36707400 4.43206300 -0.53041100
H -0.61720100 3.35879700 -3.63052500
H -2.10271100 5.03278400 -2.57377700

***anti-Z*-P2**

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.69420612
Gibbs Free Energy (T = 213K) = -1635.217547
C 2.08084200 0.94532900 1.01449300
N 2.24624200 2.21339400 1.00908500
C 0.83380600 0.12937800 0.78452900
B -1.80479100 -0.55386600 -0.79497100
H 2.99626500 0.38523600 1.21463300
S 0.94768600 3.25121500 0.66936000
O 0.70735000 3.21909600 -0.77272100
O -0.17081800 3.02832300 1.58286900
H -0.02289800 0.72839200 1.10636900
C 4.05180300 -1.79631100 -2.70612600
C 3.03124400 -2.63565200 -2.26598800
C 1.90344400 -2.10459500 -1.64642200
C 1.78801400 -0.72677900 -1.46175600
C 2.80436000 0.11318900 -1.92284000
C 3.93465600 -0.41888100 -2.53599700
H 4.93058900 -2.21291600 -3.18933700
H 3.11189100 -3.70965000 -2.40594800
H 1.10576900 -2.75353500 -1.30252100
H 2.70367100 1.19026500 -1.81002100
H 4.71764100 0.24406300 -2.89183200
C 0.59916600 -0.12278200 -0.74998300
H 0.38356700 0.85313200 -1.19578500
O -0.51257400 -0.98285900 -0.87712500
C -2.97660700 -1.60172700 -0.85777200
H -2.60764400 -2.62657900 -0.98980600
C -2.32303800 0.92588300 -0.61904600
H -1.53945500 1.69044500 -0.57272300
C -3.09609000 0.98812700 0.72395900
H -3.58443600 1.96732200 0.82043800
H -2.35637400 0.95317300 1.53608600
C -3.18937200 1.23641000 -1.86804800
H -2.51834600 1.28387200 -2.73771900
H -3.62878000 2.23854500 -1.77016600
C -3.86804300 -1.25112200 -2.07455900
H -4.75892300 -1.89484900 -2.08731900
H -3.30070200 -1.49912800 -2.98275300
C -3.69759700 -1.53140700 0.51302600
H -3.01076900 -1.93812500 1.26887000
H -4.57279600 -2.19633300 0.51078200
C -4.30811100 0.22203700 -2.16338900
H -4.69873400 0.41290400 -3.17070500
H -5.14878600 0.39870200 -1.48738400
C -4.14156700 -0.12221200 0.94939100
H -5.06925100 0.14045700 0.43441100
H -4.39968500 -0.14880700 2.01557600
C 1.71607700 4.79640300 1.08907700
H 2.59880100 4.93237800 0.46403000
H 0.97926900 5.57744200 0.89278200
H 1.98469800 4.77973000 2.14582600
C 0.84814500 -1.14809800 1.60022600
C -0.26931300 -1.45950500 2.37755500
C 1.92544100 -2.03839800 1.58956500
C -0.32298400 -2.63768300 3.11472700
H -1.10857600 -0.76938700 2.40695200
C 1.87662900 -3.21614000 2.33023100
H 2.80567300 -1.83072300 0.98872800
C 0.75242700 -3.52137800 3.09206400
H -1.20377700 -2.86159500 3.70901600
H 2.72143800 -3.89794100 2.30772500
H 0.71629700 -4.44135500 3.66759600

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.07026279
Gibbs Free Energy (T = 213K) = -1635.598092
C 2.03711000 1.05494200 0.96292300
N 2.12908000 2.32213800 0.94930900
C 0.83312900 0.17462300 0.76193300
B -1.78102200 -0.63459500 -0.77813000
H 2.98186600 0.54261700 1.14645600
S 0.78795000 3.28517100 0.63827600
O 0.50597000 3.21759400 -0.77588200

O -0.27263300 3.02680300 1.58082500
H -0.04691400 0.73559800 1.07915700
C 4.09545000 -1.70298600 -2.69076800
C 3.10566000 -2.56592400 -2.24249900
C 1.96498800 -2.06572500 -1.63157200
C 1.80529400 -0.69560500 -1.46405300
C 2.79123000 0.16740400 -1.93356000
C 3.93452000 -0.33301300 -2.53761700
H 4.98547000 -2.09594900 -3.16775600
H 3.22096100 -3.63594800 -2.36933900
H 1.19089000 -2.73459400 -1.27924300
H 2.65710800 1.23964100 -1.83221400
H 4.69448400 0.34871500 -2.90050700
C 0.60078600 -0.12094900 -0.76040300
H 0.35046100 0.83374100 -1.22723200
O -0.48100100 -1.02043100 -0.86702700
C -2.91619200 -1.71658700 -0.82995800
H -2.51408000 -2.72656400 -0.95623900
C -2.34407800 0.82431000 -0.60838500
H -1.58386800 1.60784100 -0.56742800
C -3.11751200 0.87046400 0.73177100
H -3.63286400 1.83299800 0.82221100
H -2.37916200 0.86190800 1.54195400
C -3.21795100 1.10071200 -1.85677800
H -2.55004600 1.16401800 -2.72447800
H -3.68580600 2.08714700 -1.76401900
C -3.81809100 -1.40325800 -2.04601200
H -4.68582500 -2.07315200 -2.05188900
H -3.24586400 -1.64056600 -2.95072300
C -3.63690600 -1.66136100 0.53842600
H -2.93785800 -2.03737100 1.29501100
H -4.48597300 -2.35463100 0.54095200
C -4.30229000 0.05216300 -2.14475800
H -4.69728400 0.22335300 -3.15070900
H -5.14590300 0.20687600 -1.47180200
C -4.12672600 -0.26735100 0.96203400
H -5.05786800 -0.03875600 0.44333500
H -4.38644700 -0.29394600 2.02480300
C 1.49049500 4.86676000 1.00328200
H 2.33717500 5.02983000 0.34122100
H 0.70575900 5.59957700 0.82298700
H 1.79619800 4.87546900 2.04683400
C 0.91711900 -1.08130900 1.60151000
C -0.17760500 -1.43860200 2.38227500
C 2.03748300 -1.90861100 1.60596500
C -0.16603000 -2.59982200 3.13856100
H -1.05245800 -0.79789600 2.39790700
C 2.05364900 -3.06944700 2.36492100
H 2.90305100 -1.66470700 1.00176400
C 0.95203000 -3.42057200 3.13070200
H -1.03138500 -2.86122300 3.73590000
H 2.93222900 -3.70340200 2.35378000
H 0.96624400 -4.32863200 3.72140900

R-2a

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.05384735
Gibbs Free Energy (T = 213K) = -1635.585729
C 0.24438100 0.12788000 0.83880500
N -1.11039800 -0.30121400 0.84033400
C 0.58644100 1.41152400 0.81582300
B -2.12244300 0.20271800 -0.05117400
H 0.97431100 -0.66728400 0.86344100
S -1.43883400 -1.49517800 1.98672500
O -2.50473500 -2.32413800 1.50412300
O -0.17973300 -2.09340600 2.34388600
H -0.20475200 2.15532600 0.84010600
C 4.73439500 -2.00136400 -0.54781100
C 3.70279900 -2.69100400 0.08440100
C 2.40673900 -2.57428900 -0.38233800
C 2.13888200 -1.75508900 -1.47905700
C 3.16915900 -1.05948900 -2.10110800
C 4.47040700 -1.18739900 -1.63926900
H 5.74941000 -2.09792500 -0.18063800
H 3.91540700 -3.31774400 0.94159600
H 1.58561000 -3.09229900 0.09912400
H 2.94858100 -0.41446700 -2.94513600
H 5.27416900 -0.64530200 -2.12161000
C 0.75593400 -1.60296100 -1.97620700
H 0.63188700 -0.88054200 -2.80890400
O -0.19591800 -2.19599500 -1.53287700
C -3.67697500 0.07986100 0.15940500
H -3.96540200 -0.49018000 1.04235800
C -1.78653300 1.02554700 -1.35250600
H -0.71264200 1.12344500 -1.53116300
C -2.36625700 2.45168600 -1.21858900
H -2.26715800 2.98091500 -2.17303700
H -1.74406200 3.00426200 -0.50460900
C -2.37626500 0.21521600 -2.53533700
H -1.82508400 -0.72828900 -2.59774500
H -2.18700600 0.75535800 -3.47022700
C -4.29553300 -0.64386700 -1.05580200
H -5.38866100 -0.62483500 -0.97974400
H -3.99897300 -1.69518700 -0.98322700
C -4.16961200 1.53522800 0.37443600
H -3.73400200 1.90437900 1.31314300
H -5.25400100 1.52923600 0.53021300
C -3.87187600 -0.10639900 -2.43038600
H -4.12274100 -0.85245700 -3.19013100

H -4.45874500 0.77684500 -2.68433200
C -3.82634400 2.52368000 -0.74612700
H -4.49727900 2.36087700 -1.58903100
H -4.03566300 3.53963800 -0.39799000
C -2.01916800 -0.55472200 3.37474200
H -2.93196500 -0.03860800 3.08403800
H -2.21272400 -1.25945000 4.18182700
H -1.23815500 0.14918800 3.65562100
C 1.95403200 1.93740400 0.73113800
C 2.13591000 3.32043800 0.68509100
C 3.08653400 1.11925100 0.69394600
C 3.40488900 3.87351900 0.60803500
H 1.26717800 3.96994200 0.70892400
C 4.35252300 1.67133400 0.61818600
H 2.98702900 0.04089100 0.71896700
C 4.51959200 3.04996600 0.57519500
H 3.52166200 4.95020100 0.57294200
H 5.21567500 1.01677300 0.58756900
H 5.51319000 3.47766200 0.51453200

R-2b

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.05378905
Gibbs Free Energy (T = 213K) = -1635.586764
C -1.61679300 -1.02204000 0.65644800
N -0.20972100 -1.26102500 0.72240200
C -2.13986800 -0.02560900 -0.04496100
B 0.65178400 -1.40831800 -0.41900100
H -2.22973600 -1.70297500 1.23317900
S 0.36101700 -1.45406100 2.30643600
O 1.56343400 -0.68590900 2.47326500
O -0.75724900 -1.21392800 3.17778300
H -1.47222500 0.66633000 -0.54491000
C 4.06611900 2.83971500 0.62049200
C 3.47611300 3.27159000 -0.56470700
C 2.10045300 3.26739000 -0.68972400
C 1.31058200 2.83254600 0.37454400
C 1.90259400 2.40186900 1.55692500
C 3.28357600 2.40402200 1.67930200
H 5.14580800 2.83837200 0.71298200
H 4.09600900 3.60529900 -1.38786900
H 1.61549400 3.59091500 -1.60280300
H 1.28381200 2.04168500 2.37038600
H 3.74640700 2.05467600 2.59341500
C -0.15715700 2.80114600 0.25140600
H -0.69830300 2.45877200 1.15545700
O -0.76333400 3.09706100 -0.75233500
C 2.20750500 -1.66574400 -0.37405500
H 2.62409300 -1.75570900 0.62897400
C 0.13882600 -1.30349500 -1.90415100
H -0.94078900 -1.16832900 -1.98069600
C 0.47722000 -2.62204100 -2.63666800
H 0.19059900 -2.53541500 -3.69058500
H -0.16118100 -3.40844300 -2.21503400
C 0.80291900 -0.04108900 -2.50827800
H 0.36539800 0.83590400 -2.01681700
H 0.53209600 0.04322800 -3.56647600
C 2.85407900 -0.39679800 -0.98718600
H 3.93979100 -0.53549300 -1.03956900
H 2.68813900 0.42349300 -0.28299600
C 2.52245600 -2.97561900 -1.13069200
H 2.13443200 -3.81403300 -0.53693200
H 3.60792000 -3.11750500 -1.17503300
C 2.33024000 0.02292000 -2.36689900
H 2.65783200 1.04807300 -2.56216700
H 2.79587800 -0.58648700 -3.14174600
C 1.93771900 -3.07662700 -2.54360200
H 2.54932600 -2.49902400 -3.23635000
H 2.00918000 -4.11381100 -2.88441700
C 0.76455900 -3.17983500 2.39594300
H 1.55076500 -3.40326600 1.67917100
H 1.10838200 -3.36405600 3.41250200
H -0.13829800 -3.74907600 2.18560200
C -3.57265200 0.25445700 -0.19574600
C -3.95886100 1.54560700 -0.56094700
C -4.56283700 -0.70641600 0.01703100
C -5.29979100 1.87292600 -0.68573900
H -3.19245400 2.29377400 -0.73709000
C -5.90205200 -0.37679400 -0.10701100
H -4.28530400 -1.72500300 0.26274200
C -6.27604300 0.91440800 -0.45584600
H -5.58284500 2.88090500 -0.96520800
H -6.65910200 -1.13412500 0.05945200
H -7.32451500 1.16831400 -0.55691800

R-2c

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.05283980
Gibbs Free Energy (T = 213K) = -1635.584481
C 0.50733600 -1.01517900 -0.59306500
N -0.69848000 -0.28605900 -0.84794000
C 1.71234400 -0.47462000 -0.48301700
B -1.85303100 -0.54821700 -0.02418900
H 0.35791800 -2.08307500 -0.47999300
S -0.80065700 0.61742500 -2.26683300
O -1.74278500 1.67730400 -2.02973800
O 0.52789200 0.94528500 -2.70378100

H 1.82700700 0.58967100 -0.64186400
C 3.27817400 2.21736900 1.19280100
C 2.83187100 2.97957900 0.12247500
C 1.47326800 3.20930500 -0.03929100
C 0.56555400 2.68418200 0.87400300
C 1.01820200 1.91238800 1.94296100
C 2.37134900 1.67753000 2.09945100
H 4.33777100 2.02793200 1.31595800
H 3.54014500 3.38848300 -0.58756500
H 1.11142300 3.79204700 -0.87934800
H 0.29414000 1.50621100 2.63889500
H 2.72691900 1.06999800 2.92240000
C -0.87539800 2.97092600 0.71026500
H -1.14009600 3.55584300 -0.18876600
O -1.72732200 2.61433600 1.48833300
C -3.36576400 -0.34715900 -0.39927300
H -3.53068100 0.22255300 -1.31405100
C -1.69027500 -1.32745100 1.33405700
H -0.64550300 -1.43171000 1.64175200
C -2.24821300 -2.75042500 1.08791000
H -2.22921400 -3.32248600 2.02212400
H -1.56623300 -3.27052900 0.40219000
C -2.41415500 -0.53695000 2.44697300
H -1.84912500 0.38385600 2.61750600
H -2.37556900 -1.10796000 3.38192600
C -4.09824400 0.40044900 0.73390400
H -5.17386200 0.41613200 0.52383700
H -3.75750500 1.43861200 0.70897400
C -3.88454400 -1.79190500 -0.65235800
H -3.38825700 -2.18412600 -1.55006800
H -4.95206200 -1.75013700 -0.89421800
C -3.86916900 -0.15127800 2.14856100
H -4.18013500 0.60845100 2.87131400
H -4.52206700 -1.00691300 2.32568400
C -3.66216900 -2.79096700 0.49118100
H -4.39734300 -2.61715400 1.27591600
H -3.86151000 -3.80071600 0.12001900
C -1.49136000 -0.51553600 -3.44549500
H -2.48844000 -0.79962900 -3.11776900
H -1.53266500 0.00694300 -4.39982000
H -0.83151000 -1.37870100 -3.50983200
C 2.93931900 -1.22714800 -0.19146400
C 2.93223500 -2.43764400 0.50429900
C 4.16555300 -0.70221500 -0.60053700
C 4.11444800 -3.11217800 0.75990400
H 1.99611400 -2.84448500 0.86971400
C 5.34884000 -1.37780300 -0.34699000
H 4.18282600 0.24466500 -1.12865100
C 5.32695000 -2.58720000 0.33238500
H 4.09147400 -4.04821000 1.30548100
H 6.29101000 -0.95779800 -0.67896400
H 6.25085200 -3.11488700 0.53673700

R-2d

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.0491325
Gibbs Free Energy (T = 213K) = -1635.581543
C 0.05205400 -1.26108000 -0.00415900
N 1.19555900 -0.69413200 0.63360900
C -1.21342900 -1.03687000 0.33722400
B 2.17219300 0.01256900 -0.17618900
H 0.30203800 -1.91320600 -0.83225000
S 1.21195600 -0.78686200 2.31399300
O 2.54438800 -0.51569400 2.77504100
O 0.12081800 -0.02022300 2.85849100
H -1.41778800 -0.35106300 1.15024400
C -4.45482400 2.63377000 0.72063700
C -3.38440900 2.61075000 1.61113100
C -2.10020100 2.40539000 1.14230300
C -1.88814000 2.20876500 -0.22162900
C -2.96008400 2.21593800 -1.10682400
C -4.24529600 2.43855200 -0.63676600
H -5.45928800 2.79908300 1.09216400
H -3.55822100 2.75292000 2.67060400
H -1.25106600 2.36953100 1.81420900
H -2.78568500 2.04286900 -2.16351700
H -5.08195000 2.44815600 -1.32417600
C -0.52754100 1.96432000 -0.73507500
H -0.47222300 1.66997500 -1.80223200
O 0.47881500 2.06601800 -0.07468400
C 3.52378900 0.65508900 0.30128000
H 3.55149200 0.88673500 1.36215700
C 2.15485600 -0.17666900 -1.74542800
H 1.19517600 -0.51037900 -2.14881400
C 3.16361600 -1.34265300 -1.94320400
H 3.25730400 -1.57060300 -3.01073900
H 2.73972800 -2.24177400 -1.47686500
C 2.52358300 1.11190800 -2.50390300
H 1.66639800 1.78817800 -2.43971600
H 2.65576100 0.88239000 -3.56793100
C 3.81590600 1.96043300 -0.46256100
H 4.80110700 2.33836100 -0.16569500
H 3.08446500 2.70320700 -0.13066600
C 4.56013400 -0.47853200 0.05939500
H 4.35418200 -1.26742200 0.79086800
H 5.56508000 -0.10678500 0.28829100
C 3.75665300 1.86217600 -1.98881000
H 3.75460400 2.87166300 -2.41124400
H 4.66548300 1.39148700 -2.36572500

C 4.56053300 -1.09157000 -1.35233800
H 5.12527200 -0.45235700 -2.03063100
H 5.10511700 -2.04025800 -1.32416500
C 0.88908800 -2.51082500 2.61234000
H 1.66276200 -3.09273000 2.11647800
H 0.95330200 -2.62892000 3.69281900
H -0.10210400 -2.77589600 2.25705600
C -2.38742800 -1.62573500 -0.31788900
C -3.63294300 -1.04327400 -0.07866900
C -2.32217700 -2.72419300 -1.17864100
C -4.77527800 -1.52332900 -0.69899700
H -3.69892600 -0.19393900 0.59273300
C -3.46358900 -3.20452600 -1.79755700
H -1.37545000 -3.22088500 -1.35719800
C -4.69455300 -2.60430100 -1.56390800
H -5.73087100 -1.05089100 -0.50404500
H -3.39490000 -4.05862500 -2.46094400
H -5.58605200 -2.98495300 -2.04778900

R-2e

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.04946751
Gibbs Free Energy (T = 213K) = -1635.581146
C 0.07842800 -1.10331800 0.45041100
N 1.23628200 -0.38942600 0.85153600
C -1.17820300 -0.92120400 0.85074000
B 2.34185500 -0.22933200 -0.08226700
H 0.29896600 -1.83416100 -0.31403400
S 1.21875500 0.36690700 2.36027200
O 2.56408000 0.76076600 2.66845600
O 0.17244200 1.35809900 2.39850900
H -1.42302900 -0.12336800 1.54157700
C -4.76179000 2.37457200 -0.25451400
C -4.35699900 1.84886300 -1.47730500
C -3.01294300 1.64319800 -1.72836800
C -2.07050900 1.96392700 -0.75465200
C -2.47677100 2.48321600 0.47090500
C -3.82491900 2.69043200 0.72047900
H -5.81585700 2.53505400 -0.06035200
H -5.09469400 1.59682000 -2.22918500
H -2.67145000 1.22920500 -2.66912600
H -1.73226100 2.70710900 1.22741800
H -4.14589300 3.09460600 1.67270400
C -0.63083500 1.74317600 -0.99891500
H 0.02993300 2.01070600 -0.15233200
O -0.17221600 1.30323100 -2.02633600
C 3.37898400 0.94983200 -0.11333200
H 3.18574100 1.72206000 0.62919300
C 2.64845500 -1.29220700 -1.20330800
H 1.95701400 -2.13793000 -1.23664200
C 4.02511800 -1.88440700 -0.79096700
H 4.31463000 -2.64996000 -1.51910000
H 3.89487500 -2.41029100 0.16379500
C 2.62065300 -0.62979000 -2.59647100
H 1.57367000 -0.42582000 -2.83713200
H 2.98581800 -1.33962500 -3.34752000
C 3.23189900 1.61561700 -1.50638800
H 3.94964400 2.44026400 -1.57938000
H 2.23525500 2.06477900 -1.56259700
C 4.78333200 0.37440200 0.17768800
H 4.81325700 0.11959500 1.24213200
H 5.53835100 1.15397800 0.02713800
C 3.40386900 0.68524500 -2.71140100
H 3.06927500 1.21188400 -3.60978800
H 4.46311600 0.47925900 -2.86916100
C 5.16248200 -0.86756100 -0.64219600
H 5.51341400 -0.57112100 -1.63047000
H 6.01389700 -1.36136500 -0.16432300
C 0.79857700 -0.96135700 3.46283600
H 1.56793500 -1.72454200 3.37331100
H 0.81373500 -0.51477900 4.45590900
H -0.18579800 -1.35700800 3.23463300
C -2.31187800 -1.70480100 0.34009600
C -3.58663600 -1.13852700 0.38182000
C -2.17332100 -2.98631200 -0.19727800
C -4.68382500 -1.81574800 -0.12459600
H -3.71173200 -0.14507000 0.79823000
C -3.27010300 -3.66298200 -0.70484000
H -1.20294200 -3.46970100 -0.20253200
C -4.52991800 -3.08001000 -0.67432500
H -5.66224500 -1.35082600 -0.09153300
H -3.14257700 -4.65687800 -1.11753400
H -5.38669800 -3.61305100 -1.06881200

TS1-2a

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.66655369
Gibbs Free Energy (T = 213K) = -1635.192645
Imaginary Frequency = 93.2298*i*
C -0.32032400 -0.70980400 0.86849800
N 1.04444400 -0.31355300 0.98338300
C -0.72729900 -1.89263900 0.39778000
B 1.83090800 -0.00188000 -0.27072000
H -1.04200900 0.04289300 1.18420400
S 1.28448700 0.48357600 2.45184700
O 2.68417400 0.84788500 2.59863200
O 0.26549000 1.51959300 2.62569700
H 0.01584600 -2.65178100 0.16722600

C -3.91271300 3.57767500 -0.26817500
C -2.73069600 3.79006000 0.44395200
C -1.58684500 3.07617800 0.11805400
C -1.63321400 2.14283900 -0.92570100
C -2.82239600 1.92095600 -1.62957800
C -3.96232400 2.64489400 -1.30325800
H -4.80513500 4.13877900 -0.00770000
H -2.70819600 4.50724200 1.25785800
H -0.66489800 3.19813500 0.67699200
H -2.85018500 1.17952900 -2.42416700
H -4.88658200 2.48161000 -1.84780600
C -0.45410700 1.34248800 -1.24836900
H -0.60401800 0.49950600 -1.94372900
O 0.65525500 1.54716100 -0.76557100
C 3.28718700 0.63360400 -0.24888800
H 3.42094000 1.38765500 0.52824600
C 1.71429700 -1.01885500 -1.49582700
H 0.71140100 -1.44359000 -1.62949700
C 2.64563300 -2.19555400 -1.09930000
H 2.64416700 -2.95508500 -1.89375500
H 2.22254000 -2.68079100 -0.20836100
C 2.09402900 -0.35764200 -2.83866300
H 1.27871700 0.31760500 -3.12979000
H 2.13973300 -1.12524700 -3.62451600
C 3.59692500 1.31888800 -1.59605900
H 4.62934100 1.69638200 -1.58393900
H 2.94966600 2.20159000 -1.67627600
C 4.24058000 -0.54116500 0.09738600
H 4.05102400 -0.81892200 1.14150400
H 5.28296400 -0.19481700 0.05861200
C 3.40197200 0.44934500 -2.84558700
H 3.41685900 1.09077000 -3.73608700
H 4.25399500 -0.22612000 -2.96108100
C 4.09956000 -1.79636800 -0.78585800
H 4.64461700 -1.65467800 -1.72272300
H 4.59509500 -2.63855700 -0.28620200
C 0.94186200 -0.82147800 3.62296100
H 1.66142900 -1.62476200 3.46061900
H 1.06674700 -0.38824200 4.61697600
H -0.07822200 -1.18296300 3.49082600
C -2.13126100 -2.25703900 0.15360100
C -2.46120000 -3.60620100 -0.02754000
C -3.15938900 -1.30572700 0.07839400
C -3.77648900 -3.99767500 -0.25347600
H -1.67485900 -4.35578700 0.01376600
C -4.47364400 -1.69665800 -0.14518900
H -2.93393100 -0.24822900 0.17722900
C -4.78929300 -3.04399700 -0.31044800
H -4.00970500 -5.04970900 -0.38782700
H -5.25307700 -0.94230200 -0.20143300
H -5.81616600 -3.34691900 -0.49113600

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.04368839
Gibbs Free Energy (T = 213K) = -1635.574039
Imaginary Frequency = 108.6331*i*
C 0.31614300 0.71626500 0.86678800
N -1.05052700 0.33698100 0.98206900
C 0.74280700 1.86900800 0.35914300
B -1.81703500 -0.01672100 -0.27452600
H 1.02355500 -0.02879100 1.22138500
S -1.30044000 -0.41173800 2.45750700
O -2.68689400 -0.75688300 2.60287300
O -0.30389400 -1.43842100 2.66095700
H 0.01439600 2.62358000 0.08246900
C 3.89176200 -3.54420900 -0.25294900
C 2.71645900 -3.76168700 0.46025900
C 1.57344800 -3.05555800 0.13879300
C 1.61326200 -2.12427300 -0.90073700
C 2.79503000 -1.89697100 -1.60441100
C 3.93468400 -2.61463900 -1.28381900
H 4.78528300 -4.10043100 0.00466300
H 2.70015800 -4.47760400 1.27227100
H 0.65401000 -3.18167600 0.69688400
H 2.81691600 -1.15389400 -2.39420200
H 4.85509300 -2.44719600 -1.82879600
C 0.43667700 -1.32298300 -1.21454700
H 0.58534300 -0.47692900 -1.90323500
O -0.66497300 -1.52856500 -0.72867600
C -3.27267700 -0.64617700 -0.24515700
H -3.40239300 -1.38831700 0.54020700
C -1.70859700 0.98804200 -1.50765300
H -0.70900600 1.41039900 -1.64815800
C -2.63583600 2.16704600 -1.12213900
H -2.63180300 2.91829600 -1.92047400
H -2.21372600 2.65655000 -0.23656600
C -2.09049500 0.31614000 -2.84153100
H -1.27502400 -0.35437500 -3.13286400
H -2.14369600 1.07651000 -3.62996300
C -3.58017900 -1.35001200 -1.57987300
H -4.60796100 -1.73127300 -1.56044800
H -2.93108400 -2.22903800 -1.64926500
C -4.22970800 0.52662400 0.08286200
H -4.04685200 0.81342400 1.12244000
H -5.26789500 0.17701100 0.04171600
C -3.39206100 -0.49581400 -2.83704800
H -3.40557100 -1.14534200 -3.71801800
H -4.24528300 0.17250600 -2.95726700
C -4.08730900 1.77090600 -0.81023400

H -4.62714500 1.62033900 -1.74540200
H -4.58384500 2.61491500 -0.32119800
C -0.95425000 0.91034100 3.59567500
H -1.65831600 1.71674100 3.40409900
H -1.10007800 0.49467700 4.59125800
H 0.07201800 1.24622900 3.46810700
C 2.15250900 2.20941900 0.12682700
C 2.48783000 3.53364600 -0.15974400
C 3.17967400 1.26103800 0.16645100
C 3.80469700 3.90592200 -0.38054200
H 1.70236100 4.28030300 -0.20660000
C 4.49461800 1.63307200 -0.05270300
H 2.95461400 0.21800300 0.35443100
C 4.81445300 2.95698300 -0.32561400
H 4.04168200 4.94042500 -0.59887100
H 5.27457200 0.88134000 -0.01867900
H 5.84403300 3.24434600 -0.50170400

TS1-2b

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.66817560
Gibbs Free Energy (T = 213K) = -1635.195431
Imaginary Frequency = 45.1016*i*
C -1.72601700 -0.00314200 0.78528600
N -0.58135800 -0.84422200 0.91920900
C -1.82338100 0.96626300 -0.12697600
B 0.02615700 -1.58799000 -0.20184900
H -2.53742900 -0.20598700 1.47976300
S 0.06339400 -0.84093800 2.48275800
O 1.51528400 -0.92504300 2.40291900
O -0.54743200 0.28530300 3.17847700
H -0.95990400 1.18458800 -0.75057500
C 4.98887500 3.68858400 -0.36756800
C 4.93088500 2.58043100 -1.21558800
C 3.88262000 1.67906900 -1.10451400
C 2.88846300 1.88834100 -0.14181900
C 2.94944400 2.99722200 0.70615800
C 4.00179900 3.89866200 0.59277400
H 5.81171400 4.39161500 -0.45677800
H 5.70599700 2.42483800 -1.95921200
H 3.81628400 0.80906300 -1.75010500
H 2.17554800 3.14587200 1.45502200
H 4.05457400 4.76017500 1.25046000
C 1.76889000 0.94955500 -0.00435400
H 1.02273400 1.19804700 0.77006200
O 1.62746800 -0.04720300 -0.69409400
C 0.92355100 -2.88321700 0.01267400
H 1.47353300 -2.89319900 0.95925100
C -0.68262900 -1.65023800 -1.62307200
H -1.26796300 -0.75894600 -1.86519000
C -1.69484200 -2.81912500 -1.51127100
H -2.23705500 -2.93145700 -2.46018100
H -2.45016300 -2.54520300 -0.75921200
C 0.35541500 -1.82270200 -2.75385800
H 0.86783300 -0.86184400 -2.87277700
H -0.16745000 -2.01464700 -3.70188500
C 1.97277900 -3.01123400 -1.11148300
H 2.51163100 -3.96324700 -1.00218900
H 2.71203700 -2.21698700 -0.96368800
C -0.08235800 -4.07205600 0.05396200
H -0.67893400 -3.99316400 0.97273900
H 0.47564000 -5.01503600 0.13643200
C 1.41828900 -2.91757800 -2.54341300
H 2.25217600 -2.73291800 -3.23248600
H 1.01116200 -3.88867900 -2.83948700
C -1.06870900 -4.16675400 -1.12291700
H -0.57185400 -4.60259100 -1.99290200
H -1.86692800 -4.87129700 -0.85704300
C -0.53643800 -2.33375600 3.25218200
H -0.06457500 -3.19533900 2.78187400
H -0.25746700 -2.27746300 4.30620500
H -1.62199500 -2.37478700 3.14936900
C -3.02173200 1.78518400 -0.36185300
C -2.87862700 3.04299000 -0.96147400
C -4.30960300 1.35732400 -0.01281700
C -3.98138900 3.86136300 -1.17883100
H -1.88784200 3.38412500 -1.25132900
C -5.41208100 2.17665100 -0.22599200
H -4.45364600 0.36621400 0.40745800
C -5.25315800 3.43287900 -0.80715400
H -3.84720500 4.83499100 -1.64084000
H -6.40233800 1.82666600 0.05047700
H -6.11653200 4.06835200 -0.97949100

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.04627770
Gibbs Free Energy (T = 213K) = -1635.578086
Imaginary Frequency = 68.9711*i*
C -1.71319500 0.00478800 0.74882800
N -0.55016100 -0.80156300 0.90494700
C -1.80406900 1.00173400 -0.12273900
B 0.08222900 -1.54526200 -0.20346200
H -2.54792000 -0.24716800 1.39528600
S 0.00841100 -0.84816200 2.48137800
O 1.43762600 -1.00844000 2.46136000
O -0.56471400 0.29067100 3.15212700
H -0.92515300 1.27283400 -0.69856600
C 4.98931300 3.67813800 -0.37113300

C 4.96375800 2.55106500 -1.18782600
C 3.94323000 1.62915800 -1.05780700
C 2.94324300 1.83667400 -0.10756800
C 2.97196300 2.96412700 0.70860600
C 3.99732700 3.88652000 0.57644800
H 5.79212200 4.39833600 -0.47595700
H 5.74400200 2.39801000 -1.92305600
H 3.90212300 0.74356400 -1.68004600
H 2.19182300 3.11033600 1.44797700
H 4.02516700 4.76396800 1.21017700
C 1.84544300 0.87992900 0.05309900
H 1.09123900 1.13710300 0.81484900
O 1.73016200 -0.13640900 -0.60021400
C 0.87763300 -2.89727900 0.03010000
H 1.38372700 -2.94473000 0.99620700
C -0.57247800 -1.55096400 -1.64810800
H -1.07851600 -0.61869400 -1.90170800
C -1.66705200 -2.64230400 -1.58766900
H -2.17528200 -2.71000900 -2.55600900
H -2.42976400 -2.32075000 -0.86637300
C 0.48883500 -1.79229800 -2.74071400
H 1.06787000 -0.87105700 -2.84053000
H -0.01261600 -1.94623100 -3.70377900
C 1.95494200 -3.09716600 -1.05109600
H 2.41555000 -4.08468800 -0.92912500
H 2.74432600 -2.36404200 -0.86985200
C -0.20931200 -4.00986400 0.02548200
H -0.83058100 -3.89289900 0.91973800
H 0.27645700 -4.98747800 0.12228000
C 1.46362200 -2.95660800 -2.49910200
H 2.33104600 -2.82694700 -3.15381000
H 1.00260400 -3.89286300 -2.81670500
C -1.15202400 -4.02927800 -1.18652100
H -0.65421900 -4.49223700 -2.03817300
H -2.00446200 -4.67649100 -0.95771300
C -0.69850900 -2.30165800 3.21385400
H -0.23925900 -3.18008700 2.76959200
H -0.47411100 -2.24789100 4.27800100
H -1.77451000 -2.28914900 3.05080000
C -3.01540000 1.79254400 -0.37268700
C -2.88865300 3.07618300 -0.90593100
C -4.29786900 1.31250200 -0.09857500
C -4.00327300 3.86785300 -1.13083800
H -1.90034100 3.45857400 -1.13794400
C -5.41203800 2.10470000 -0.32003600
H -4.42744400 0.30152300 0.26974000
C -5.27009600 3.38662300 -0.83381500
H -3.88228100 4.86348300 -1.54108000
H -6.39926700 1.71417700 -0.10273200
H -6.14357100 4.00207100 -1.01256100

TS1-2d

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.67064555
Gibbs Free Energy (T = 213K) = -1635.195203
Imaginary Frequency = 53.5439*i*
C -0.01497100 -1.33804200 0.07001100
N 1.15250500 -0.77670200 0.65965200
C -1.27898200 -1.07364600 0.42562000
B 2.03132000 0.04124600 -0.22588400
H 0.20645300 -2.00423500 -0.75875700
S 1.15870000 -0.66188600 2.34334000
O 2.52046200 -0.40545600 2.78529000
O 0.09934800 0.22981900 2.81304400
H -1.45831100 -0.36246100 1.22655800
C -4.12905300 3.02060800 0.59785700
C -3.04416400 2.96553600 1.47653900
C -1.80554700 2.53400100 1.02399200
C -1.65916600 2.14363200 -0.31253200
C -2.74875400 2.18345500 -1.18601500
C -3.98372600 2.63298700 -0.73244100
H -5.09537600 3.36185700 0.95707400
H -3.17052200 3.25720000 2.51418300
H -0.95377600 2.45596600 1.69214500
H -2.62878800 1.85609400 -2.21557300
H -4.83201900 2.66908300 -1.40818800
C -0.37233800 1.63102500 -0.79552100
H -0.38036000 1.16692200 -1.79777100
O 0.66872900 1.68772800 -0.15517000
C 3.40012200 0.69819300 0.21842600
H 3.40454000 1.04270100 1.25362600
C 2.07724200 -0.33864300 -1.77366400
H 1.12825500 -0.70791800 -2.18358600
C 3.07595800 -1.52793200 -1.81610000
H 3.20250100 -1.87049400 -2.85248500
H 2.62724800 -2.36987200 -1.26840200
C 2.49076300 0.85946600 -2.65494800
H 1.63960900 1.55074300 -2.70446500
H 2.65882500 0.51455500 -3.68524500
C 3.74084800 1.91199500 -0.66915100
H 4.72974100 2.30245500 -0.39009200
H 3.01920600 2.70497700 -0.43645600
C 4.42712800 -0.46567700 0.12934200
H 4.18934600 -1.17098300 0.93506300
H 5.43466400 -0.08354700 0.34487600
C 3.71837200 1.65336300 -2.18169000
H 3.74064900 2.61462500 -2.71074100
H 4.63398900 1.13638900 -2.48191200
C 4.46045700 -1.22849200 -1.21067000

H 5.05612600 -0.67184200 -1.93876400
H 4.99209800 -2.17715500 -1.06395700
C 0.74775100 -2.32892200 2.84204800
H 1.50323100 -3.00307100 2.43699600
H 0.78369500 -2.32761500 3.93298700
H -0.24823800 -2.59950300 2.49547500
C -2.47584000 -1.63827500 -0.21264200
C -3.69239100 -0.96421000 -0.04218000
C -2.45946800 -2.79835400 -0.99855700
C -4.85220900 -1.41684900 -0.66095900
H -3.72039500 -0.06837400 0.57328000
C -3.61926100 -3.25113800 -1.61650000
H -1.53869900 -3.36312100 -1.11477300
C -4.81929600 -2.56090100 -1.45391100
H -5.78306500 -0.87511700 -0.52121500
H -3.58881000 -4.15340000 -2.22022000
H -5.72431700 -2.91981300 -1.93469500

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.04760477
Gibbs Free Energy (T = 213K) = -1635.577074
Imaginary Frequency = 84.5286*i*
C -0.02335700 -1.34327700 0.05501600
N 1.14912300 -0.80506400 0.64648200
C -1.27940800 -1.10168000 0.43118000
B 1.98954200 0.06932400 -0.22874100
H 0.18438700 -1.96764600 -0.80616100
S 1.17367100 -0.74261100 2.31681600
O 2.52406800 -0.49681800 2.74286500
O 0.13225000 0.12222400 2.82006200
H -1.45457100 -0.42936300 1.26273200
C -4.06791800 3.06335300 0.65978900
C -2.98297300 2.99249400 1.52982200
C -1.76111000 2.53495500 1.07479000
C -1.63120100 2.13554800 -0.25586400
C -2.72089600 2.19118900 -1.12012200
C -3.93942700 2.66679300 -0.66386600
H -5.02307100 3.42479500 1.02208400
H -3.09794400 3.29167900 2.56413400
H -0.90768700 2.44560800 1.73576500
H -2.61291400 1.85412000 -2.14530600
H -4.78941300 2.71560000 -1.33275500
C -0.36455200 1.58830600 -0.74202200
H -0.39050500 1.10960800 -1.73459700
O 0.67713300 1.63117900 -0.11118300
C 3.36094000 0.71529300 0.21648000
H 3.36473500 1.04381600 1.25421100
C 2.04019800 -0.29413500 -1.77903500
H 1.09414500 -0.66108900 -2.19026300
C 3.03933500 -1.47734400 -1.84045000
H 3.16014600 -1.80716300 -2.87859500
H 2.59691000 -2.32378300 -1.30041100
C 2.44735200 0.91303000 -2.64597400
H 1.59479700 1.59859500 -2.69313600
H 2.61909800 0.57954200 -3.67640200
C 3.69239600 1.94292100 -0.65048700
H 4.67739900 2.33255200 -0.36797400
H 2.97030500 2.72764100 -0.40349900
C 4.39413900 -0.43604100 0.10575000
H 4.16703900 -1.15112300 0.90157900
H 5.39752200 -0.04992200 0.31909500
C 3.66809000 1.70684700 -2.16365100
H 3.68381100 2.67304300 -2.67768200
H 4.58379400 1.20076200 -2.47128200
C 4.42321400 -1.17972100 -1.24139300
H 5.01009400 -0.61288600 -1.96448000
H 4.95864400 -2.12514200 -1.10991500
C 0.77372300 -2.41551700 2.77333100
H 1.51605400 -3.07451400 2.32915700
H 0.84129000 -2.43660900 3.85975600
H -0.23098500 -2.66805600 2.44826100
C -2.47621500 -1.63659100 -0.22725200
C -3.68846300 -0.97316900 -0.02608200
C -2.46171400 -2.75568100 -1.06287900
C -4.84525600 -1.39547100 -0.66122000
H -3.71492500 -0.10706600 0.62707200
C -3.61827600 -3.17810600 -1.69658000
H -1.54359900 -3.31397700 -1.20572900
C -4.81379800 -2.49808500 -1.50235000
H -5.77421500 -0.86242000 -0.49610200
H -3.58971700 -4.05016000 -2.33922800
H -5.71748000 -2.83397000 -1.99660200

TS1-2e

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.66748514
Gibbs Free Energy (T = 213K) = -1635.194675
Imaginary Frequency = 17.7032*i*
C 0.03454200 -1.52859600 0.06489500
N 1.05355600 -0.72438800 0.67588400
C -1.27790500 -1.35500900 0.23651800
B 1.95271400 0.04629000 -0.19315400
H 0.42109700 -2.32567800 -0.56493700
S 1.08276800 -0.78974400 2.35926800
O 2.30289100 -0.16338100 2.84207000
O -0.19411400 -0.31893100 2.89410000
H -1.62162600 -0.57679600 0.91222700
C -4.13457200 4.11502500 -0.04743500

C -3.23988100 4.08674100 -1.11952600
C -2.04298200 3.39520300 -1.00355300
C -1.73918100 2.73263500 0.19055000
C -2.63601100 2.76180200 1.26174600
C -3.83621300 3.45391600 1.14193800
H -5.07109200 4.65648000 -0.14249800
H -3.48263300 4.60413600 -2.04230200
H -1.33291000 3.35468900 -1.82353200
H -2.38844900 2.23978800 2.18319900
H -4.53627500 3.47925200 1.97082800
C -0.48759600 1.97475700 0.33813800
H -0.34164500 1.48668200 1.31739000
O 0.34698800 1.84831600 -0.54175500
C 3.23862600 0.84456400 0.25525200
H 3.19289100 1.22581500 1.27628700
C 2.04205600 -0.36992300 -1.72110900
H 1.12709900 -0.83154400 -2.11151100
C 3.14213200 -1.47025200 -1.70295800
H 3.31645700 -1.83737600 -2.72375800
H 2.76029300 -2.33106500 -1.13240000
C 2.35863700 0.82601400 -2.64104200
H 1.44664200 1.42831500 -2.71111600
H 2.57282100 0.46154000 -3.65619200
C 3.49946100 2.04580400 -0.67737300
H 4.45559000 2.51501600 -0.40467200
H 2.72094700 2.79182700 -0.47880700
C 4.35909800 -0.23589700 0.22789200
H 4.16266300 -0.93466900 1.05183900
H 5.32611700 0.23453100 0.45352100
C 3.50933100 1.73633700 -2.18186200
H 3.45434400 2.68054400 -2.73843900
H 4.46974100 1.29240900 -2.45982700
C 4.48449000 -1.03183800 -1.08684800
H 5.04084200 -0.44395100 -1.82098200
H 5.09635900 -1.92403000 -0.90287600
C 1.19605000 -2.54388300 2.67319700
H 2.12235500 -2.91255500 2.23042600
H 1.21409200 -2.66563500 3.75769000
H 0.32784900 -3.04848200 2.24919800
C -2.32380700 -2.18182600 -0.38810800
C -3.59563600 -2.21702800 0.19575000
C -2.10330200 -2.92645100 -1.55479500
C -4.61210500 -2.99242800 -0.35226000
H -3.78446700 -1.63332900 1.09313700
C -3.11820500 -3.70125900 -2.10265800
H -1.13870400 -2.88247700 -2.05253400
C -4.37535300 -3.74079100 -1.50181500
H -5.59057400 -3.00962500 0.11830900
H -2.93083800 -4.26855900 -3.00950200
H -5.16790500 -4.34382100 -1.93440200

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.045403
Gibbs Free Energy (T = 213K) = -1635.578091
Imaginary Frequency = 45.1108*i*
C -0.32888500 -1.59764500 0.13448900
N 0.75120400 -0.85966200 0.71952000
C -1.61311500 -1.27801600 0.23580300
B 1.76229500 -0.28419000 -0.17755900
H -0.01621200 -2.47707900 -0.41817000
S 0.74862600 -0.84238600 2.38652000
O 1.95083000 -0.21010400 2.85271300
O -0.51600400 -0.33211300 2.85915300
H -1.89460800 -0.42018700 0.83565400
C -2.65855600 5.46105200 -0.19327400
C -1.75899500 5.13967300 -1.20587600
C -0.95346300 4.02399600 -1.08338700
C -1.04817100 3.22635400 0.05670400
C -1.94865800 3.55010600 1.06788500
C -2.75537300 4.66988200 0.94248500
H -3.28839000 6.33712600 -0.29327600
H -1.69187300 5.76449700 -2.08789600
H -0.24588000 3.75274700 -1.85728900
H -2.01034000 2.92195000 1.95043900
H -3.45665700 4.92638100 1.72661100
C -0.21097600 2.03144700 0.21483300
H -0.36353900 1.46059800 1.14673400
O 0.60109800 1.65706700 -0.60471900
C 3.16059000 0.30671600 0.24970100
H 3.15641700 0.77662900 1.23031300
C 1.81851800 -0.83554900 -1.66168300
H 0.84776100 -1.16402800 -2.04371600
C 2.71175000 -2.09862500 -1.52685600
H 2.84635700 -2.56282200 -2.51031500
H 2.17529800 -2.83687600 -0.91613100
C 2.35294000 0.20797400 -2.65785600
H 1.56480600 0.95103900 -2.80207100
H 2.51488300 -0.26674200 -3.63318400
C 3.66017500 1.35604300 -0.76123000
H 4.68040100 1.65619700 -0.49403700
H 3.03729600 2.24738400 -0.64425400
C 4.06849100 -0.94864400 0.35392700
H 3.72660400 -1.53347100 1.21522800
H 5.09351100 -0.63994700 0.58814400
C 3.63709700 0.93309900 -2.23496500
H 3.76024300 1.82293100 -2.86033500
H 4.50386100 0.30685500 -2.45120500
C 4.08986100 -1.85201300 -0.89097800
H 4.75928800 -1.42702200 -1.63866300

H 4.53016100 -2.81676900 -0.62026100
C 0.82670400 -2.56901000 2.79620400
H 1.75921800 -2.96878900 2.40341300
H 0.80399900 -2.63062300 3.88268900
H -0.03595100 -3.07505900 2.36841300
C -2.71364700 -2.04452900 -0.36681700
C -3.99263100 -1.93311900 0.17858200
C -2.53321100 -2.87463900 -1.47560000
C -5.05646800 -2.64840000 -0.34904800
H -4.14968100 -1.28234200 1.03194800
C -3.59546700 -3.58837600 -2.00337500
H -1.55867200 -2.94652000 -1.94477500
C -4.86060800 -3.48173100 -1.44001700
H -6.04147000 -2.55207900 0.09202800
H -3.43854100 -4.22387600 -2.86691700
H -5.69103600 -4.03841800 -1.85738300

Int-2a

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.66769642
Gibbs Free Energy (T = 213K) = -1635.192685
C 0.33405800 0.90216400 0.87425300
N -1.04237000 0.55747800 0.97960500
C 0.79344800 1.98430600 0.23489000
B -1.70342000 -0.03964200 -0.31042300
H 1.03180400 0.19956900 1.33370900
S -1.33444900 -0.10883700 2.49488600
O -2.75348500 -0.38947000 2.65186700
O -0.37774400 -1.18501400 2.77276600
H 0.08197800 2.71525500 -0.14047700
C 3.55628300 -4.00324700 -0.08725000
C 2.35295000 -4.08801300 0.61667800
C 1.31706400 -3.21486000 0.32453500
C 1.49421800 -2.25255800 -0.68115100
C 2.70807900 -2.15907600 -1.37595800
C 3.73812300 -3.04108600 -1.08021400
H 4.36401700 -4.68967400 0.14785600
H 2.23166200 -4.83108000 1.39760600
H 0.38413400 -3.23828700 0.87753800
H 2.83811000 -1.39621200 -2.13908700
H 4.67962300 -2.97962000 -1.61553900
C 0.44279300 -1.30249900 -0.97910000
H 0.67501400 -0.46715800 -1.65121700
O -0.69004300 -1.39067800 -0.48624900
C -3.19515300 -0.62161500 -0.24976600
H -3.34943100 -1.29614400 0.59671100
C -1.59864700 0.90012400 -1.61681200
H -0.59724400 1.32305400 -1.78126500
C -2.53706200 2.10213700 -1.35837300
H -2.51397700 2.78892200 -2.21686500
H -2.13974500 2.66386100 -0.50162400
C -1.94598200 0.10939000 -2.89931400
H -1.11927900 -0.58336700 -3.11423900
H -1.98268100 0.79557100 -3.75774700
C -3.46653500 -1.44894900 -1.52522100
H -4.49495500 -1.83694700 -1.50192800
H -2.81106100 -2.33071700 -1.50180000
C -4.16368700 0.56816000 -0.05606200
H -4.00998800 0.94981500 0.95969000
H -5.20418200 0.21434500 -0.09522100
C -3.24801400 -0.70810200 -2.85241400
H -3.24027800 -1.43471300 -3.67529900
H -4.10142700 -0.05427900 -3.05097000
C -3.99885900 1.73175500 -1.05232000
H -4.51604000 1.50048500 -1.98773900
H -4.50908000 2.61715200 -0.65127100
C -0.93914800 1.26069000 3.57378000
H -1.60590800 2.08951600 3.33371000
H -1.11129100 0.91164200 4.59356900
H 0.10305500 1.55360700 3.44412300
C 2.21567000 2.26593900 -0.01005200
C 2.60534200 3.57104500 -0.33834600
C 3.20580300 1.27402700 0.05337000
C 3.94050800 3.88299300 -0.56960300
H 1.84953500 4.34941500 -0.40622500
C 4.54070700 1.58603700 -0.17447500
H 2.93308400 0.24446400 0.26638300
C 4.91499400 2.89177400 -0.48523000
H 4.22001300 4.90240500 -0.81833800
H 5.29034800 0.80194000 -0.11992800
H 5.95753600 3.13251600 -0.66957000

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.04458114
Gibbs Free Energy (T = 213K) = -1635.574409
C -0.30765400 -1.00097500 0.81225300
N 1.06521600 -0.64921600 0.91898900
C -0.77322700 -1.99930700 0.06451400
B 1.67924100 0.10669300 -0.29926300
H -0.99295200 -0.37363300 1.37897200
S 1.41086600 -0.24753600 2.49802400
O 2.79567800 0.11619900 2.62239700
O 0.41280800 0.66372000 3.01495600
H -0.06818200 -2.66342200 -0.42359100
C -3.59032900 4.05000100 0.19100200
C -2.36459200 4.16767700 0.84099600
C -1.33040600 3.31185800 0.52081800
C -1.52860900 2.33406800 -0.45833800

C -2.76097200 2.21325500 -1.10316800
C -3.79238600 3.07603100 -0.77806900
H -4.39860600 4.72385800 0.44890800
H -2.22553700 4.92544500 1.60132500
H -0.37357600 3.37097000 1.02362100
H -2.90449300 1.44008800 -1.85006200
H -4.75086100 2.99069000 -1.27370400
C -0.47977400 1.39662700 -0.79396600
H -0.72052700 0.59359800 -1.49917600
O 0.64925200 1.45731300 -0.30605100
C 3.16253000 0.69731500 -0.21670700
H 3.33041400 1.26845200 0.69643000
C 1.54977100 -0.67370100 -1.70178400
H 0.55187900 -1.08773300 -1.88644300
C 2.50498800 -1.88321300 -1.60913100
H 2.46126100 -2.46649600 -2.53682800
H 2.14038100 -2.54194200 -0.81262800
C 1.85194200 0.25948300 -2.89304700
H 1.01169600 0.95473700 -3.01056100
H 1.87637800 -0.32537000 -3.82044700
C 3.38799700 1.66987800 -1.39132700
H 4.41011500 2.06455000 -1.34922900
H 2.72749700 2.53254100 -1.24673400
C 4.15023400 -0.48862600 -0.19165000
H 4.03563100 -0.98558200 0.77513900
H 5.18107600 -0.11516200 -0.22101500
C 3.14069100 1.08685100 -2.78683300
H 3.09852500 1.90233500 -3.51610100
H 3.99454900 0.47724600 -3.08352800
C 3.96841300 -1.52956900 -1.30832900
H 4.45034600 -1.18392700 -2.22364300
H 4.50054000 -2.44465600 -1.02905200
C 1.19092900 -1.80785500 3.32442800
H 1.90392800 -2.51561700 2.90819300
H 1.39317400 -1.62465900 4.37831300
H 0.16915700 -2.15400200 3.18627900
C -2.19712900 -2.27093400 -0.16911600
C -2.57588600 -3.51405900 -0.67912900
C -3.19825900 -1.32687300 0.08091800
C -3.90879800 -3.81590200 -0.90920000
H -1.81157800 -4.25344700 -0.89286900
C -4.53002500 -1.62922600 -0.14631500
H -2.93720000 -0.33965500 0.44420800
C -4.89237000 -2.87546900 -0.64062900
H -4.17971900 -4.78873200 -1.30197700
H -5.28967700 -0.88289400 0.05499800
H -5.93458600 -3.10780300 -0.82334800

Int-2b
ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.67288026
Gibbs Free Energy (T = 213K) = -1635.198923
C -1.74682200 -0.02527700 0.77106800
N -0.46317600 -0.60075100 0.95259900
C -2.00496900 0.96587600 -0.08709000
B 0.40364600 -1.18934500 -0.19311700
H -2.54911400 -0.45173500 1.37228000
S 0.04529200 -0.60539500 2.53792000
O 1.50642000 -0.57677700 2.54491400
O -0.68712800 0.44698800 3.23692700
H -1.17742000 1.43801500 -0.61174500
C 5.15244600 3.42124600 -0.57196900
C 5.08592000 2.16624000 -1.18268900
C 3.98890500 1.34941100 -0.96343900
C 2.95245100 1.79474500 -0.12929800
C 3.02232800 3.05269300 0.48164900
C 4.12591300 3.86578800 0.25895300
H 6.01520100 4.05696900 -0.74603500
H 5.89302100 1.83199800 -1.82600100
H 3.91646300 0.37002100 -1.42529500
H 2.21658700 3.38300200 1.13137300
H 4.18852200 4.84045700 0.73085600
C 1.78937600 0.96781400 0.11675600
H 0.98857900 1.36343600 0.75137400
O 1.66729600 -0.15434100 -0.38525500
C 1.06417900 -2.64151300 0.07064000
H 1.56417200 -2.70312100 1.04676600
C -0.28328100 -1.25406400 -1.65639100
H -0.75042300 -0.30279100 -1.94157100
C -1.40736600 -2.30915200 -1.63999300
H -1.86416900 -2.38637500 -2.63710600
H -2.20204300 -1.95032500 -0.97086300
C 0.80612400 -1.53264200 -2.71868700
H 1.43681900 -0.63767200 -2.79648900
H 0.33486500 -1.65566500 -3.70459900
C 2.15420300 -2.92135000 -0.98614600
H 2.55060800 -3.93882300 -0.85563900
H 2.99241800 -2.24219300 -0.78639400
C -0.07603500 -3.68835200 0.07180900
H -0.72955100 -3.48946500 0.93114200
H 0.33879300 -4.69405100 0.23227900
C 1.71353800 -2.74938100 -2.45213100
H 2.60731000 -2.66865400 -3.08462400
H 1.20787700 -3.65915300 -2.78728000
C -0.96903900 -3.70755700 -1.17907600
H -0.45655500 -4.22305700 -1.99554000
H -1.86090100 -4.31165100 -0.96744500
C -0.46419000 -2.15321300 3.26900200
H 0.10352400 -2.96813800 2.82222200

H -0.25144300 -2.08066600 4.33738000
H -1.53527000 -2.28820800 3.10788500
C -3.34798100 1.48583900 -0.38244300
C -3.49015500 2.80167600 -0.84211500
C -4.50409200 0.70928900 -0.22598600
C -4.74602000 3.33585900 -1.10693000
H -2.60282100 3.41414900 -0.98244100
C -5.76096100 1.24470100 -0.48452600
H -4.41683900 -0.33014900 0.07702800
C -5.88848000 2.56045600 -0.92362400
H -4.83292100 4.36015900 -1.45752200
H -6.64438000 0.62576900 -0.35719200
H -6.87022100 2.97447300 -1.13286900

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.05017824
Gibbs Free Energy (T = 213K) = -1635.579921
C -1.73906600 -0.01023200 0.76470000
N -0.45474000 -0.57629600 0.95027500
C -2.00091800 0.96979100 -0.09395200
B 0.40345600 -1.17944000 -0.18923100
H -2.53799800 -0.43189500 1.36954900
S 0.03561500 -0.59171700 2.52585100
O 1.47920400 -0.59699100 2.54094800
O -0.66837600 0.46525000 3.21050300
H -1.17779400 1.43702500 -0.62506400
C 5.16886500 3.38537700 -0.56731500
C 5.09088300 2.14223100 -1.19058300
C 3.99545900 1.33213200 -0.97343500
C 2.97159400 1.77195000 -0.12912400
C 3.05313000 3.01690800 0.49422400
C 4.15557100 3.82408900 0.27362800
H 6.03213700 4.01679700 -0.74032600
H 5.88973800 1.81271800 -1.84262600
H 3.91305300 0.36060500 -1.44485200
H 2.25509100 3.34117600 1.15249800
H 4.22765600 4.79048400 0.75566900
C 1.80680200 0.95150100 0.11899000
H 1.01879000 1.34826000 0.76651900
O 1.67396800 -0.16033500 -0.38685100
C 1.04657500 -2.63367000 0.08017000
H 1.54011600 -2.69060900 1.05602800
C -0.28180800 -1.24470600 -1.64896400
H -0.73823300 -0.29212100 -1.93534900
C -1.41309400 -2.28787600 -1.63149300
H -1.86685800 -2.36251800 -2.62697400
H -2.20462700 -1.92169300 -0.96725200
C 0.80294400 -1.53690400 -2.70844400
H 1.43753000 -0.64893000 -2.79355700
H 0.32989400 -1.66274600 -3.68983000
C 2.13437800 -2.92862900 -0.97067700
H 2.51585800 -3.94804500 -0.83570400
H 2.97909600 -2.26218300 -0.77109800
C -0.09916900 -3.66996700 0.08282900
H -0.74994000 -3.46614600 0.93912000
H 0.30876700 -4.67489200 0.24605200
C 1.69957400 -2.75676400 -2.43552600
H 2.59323500 -2.68421800 -3.06399800
H 1.18953200 -3.66128400 -2.76858900
C -0.98759600 -3.68581100 -1.16756400
H -0.47835800 -4.20541600 -1.97948800
H -1.88238500 -4.28057000 -0.95714500
C -0.51225400 -2.11714500 3.25371900
H 0.05183400 -2.93953700 2.82349100
H -0.31939500 -2.03335500 4.32203900
H -1.57944500 -2.23018100 3.07033200
C -3.34238200 1.48769800 -0.38720600
C -3.48246600 2.79096100 -0.86808000
C -4.49695400 0.72221400 -0.20804000
C -4.73367900 3.32392300 -1.13192500
H -2.59548800 3.39502700 -1.02723600
C -5.74869500 1.25636500 -0.46663200
H -4.41321600 -0.30916000 0.11420800
C -5.87374600 2.55993900 -0.92677300
H -4.81921400 4.33964000 -1.49998800
H -6.63220700 0.64558200 -0.32209200
H -6.85314600 2.97330300 -1.13567800

Int-2d

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.67317521
Gibbs Free Energy (T = 213K) = -1635.196814
C -0.04320300 -1.42636400 0.18314700
N 1.14835600 -0.88432500 0.71598300
C -1.30504600 -1.14211800 0.55145500
B 1.84899500 0.11160200 -0.27705900
H 0.14353600 -2.07723800 -0.66692300
S 1.16626700 -0.60618300 2.37010800
O 2.53669500 -0.33442900 2.77960500
O 0.13232600 0.35129300 2.77773400
H -1.47102500 -0.43826100 1.36224800
C -3.78203500 3.40685000 0.49642400
C -2.65268100 3.37655500 1.31858300
C -1.51148200 2.70755200 0.90472600
C -1.50942300 2.06144500 -0.34016500
C -2.64750900 2.07854600 -1.15571900
C -3.78270700 2.76082300 -0.73863200
H -4.67230500 3.93306000 0.82741000

H -2.67069400 3.87070700 2.28423100
H -0.63332900 2.64075400 1.53802100
H -2.64124600 1.55132500 -2.10565700
H -4.66740100 2.78091500 -1.36616000
C -0.35192000 1.30588500 -0.77480600
H -0.44596800 0.69321700 -1.67829800
O 0.73441300 1.34666400 -0.17373200
C 3.27284900 0.73667400 0.10210800
H 3.28602500 1.16174200 1.11006400
C 1.94437700 -0.45054500 -1.79090600
H 1.00564200 -0.86704200 -2.18660500
C 2.94926600 -1.62506400 -1.75305100
H 3.06993800 -2.05028800 -2.75979600
H 2.51406400 -2.42208400 -1.13312900
C 2.33747900 0.68384600 -2.76457300
H 1.47881000 1.36435100 -2.86327800
H 2.50096000 0.26866600 -3.76949300
C 3.59557100 1.89088800 -0.87056600
H 4.58240500 2.31321200 -0.63293800
H 2.87057500 2.69712100 -0.69073200
C 4.30952400 -0.41038300 0.08777500
H 4.08747000 -1.05687400 0.94421700
H 5.31769800 -0.00709000 0.26182100
C 3.56158700 1.52243700 -2.36099400
H 3.57436700 2.44124300 -2.96157000
H 4.47775200 0.98844700 -2.62722000
C 4.33709500 -1.27256600 -1.18926600
H 4.92292500 -0.77198100 -1.96541500
H 4.87645100 -2.20454900 -0.97603900
C 0.72784000 -2.20843100 3.03277700
H 1.46944400 -2.93257000 2.69431100
H 0.76689700 -2.10127400 4.11831400
H -0.27386200 -2.49539600 2.71639500
C -2.50926200 -1.67272100 -0.10151100
C -3.70965900 -0.96522600 0.05264300
C -2.51314600 -2.82534500 -0.89926400
C -4.87063700 -1.37761500 -0.59211900
H -3.72399900 -0.07539100 0.67714500
C -3.67390000 -3.23749500 -1.54310500
H -1.60767800 -3.41636900 -1.00360500
C -4.85630500 -2.51399000 -1.39642600
H -5.78827200 -0.81116300 -0.46311500
H -3.65828500 -4.13457400 -2.15504200
H -5.76215100 -2.84148200 -1.89754200

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.04950167
Gibbs Free Energy (T = 213K) = -1635.577792
C -0.04519700 -1.42012300 0.17916000
N 1.14504800 -0.88274700 0.71323600
C -1.30140200 -1.15386100 0.55450500
B 1.83844700 0.11950700 -0.27012700
H 0.13715500 -2.05567400 -0.68035100
S 1.16814000 -0.63142100 2.35733100
O 2.52341800 -0.35953000 2.75542500
O 0.14573200 0.30407400 2.77817900
H -1.46991500 -0.46505200 1.37430400
C -3.77057100 3.40784600 0.51655000
C -2.64760100 3.37140200 1.33939400
C -1.50977700 2.70833700 0.92521300
C -1.50359400 2.07485600 -0.32052800
C -2.63467200 2.09819900 -1.13617700
C -3.76752000 2.77446500 -0.71888600
H -4.66007400 3.93004200 0.84850400
H -2.66941900 3.85653000 2.30691900
H -0.63408100 2.63695500 1.55784900
H -2.62381100 1.57924600 -2.08796600
H -4.64862800 2.79950700 -1.34719000
C -0.34785200 1.32120500 -0.75666800
H -0.44597900 0.71146000 -1.66019300
O 0.73055200 1.35543000 -0.15588200
C 3.26205600 0.73764100 0.10339800
H 3.27719600 1.15415200 1.11161300
C 1.92614800 -0.43005500 -1.78476000
H 0.98612600 -0.84021400 -2.17455800
C 2.92589500 -1.60569700 -1.75974900
H 3.03882500 -2.02348400 -2.76731300
H 2.49280700 -2.40337200 -1.14412900
C 2.31732000 0.70569700 -2.75292200
H 1.46175600 1.38583200 -2.84848200
H 2.47738600 0.29421100 -3.75678100
C 3.58242600 1.89608800 -0.86038200
H 4.56839900 2.31290800 -0.62307300
H 2.86219900 2.70066800 -0.67119700
C 4.29581400 -0.40794700 0.07712700
H 4.07826500 -1.05717300 0.92908400
H 5.30218500 -0.00678200 0.24796400
C 3.54182100 1.53858300 -2.34999100
H 3.55303700 2.45896400 -2.94270100
H 4.45367900 1.00652000 -2.62277000
C 4.31491700 -1.26008800 -1.20309400
H 4.89502100 -0.75603100 -1.97714800
H 4.85254800 -2.19164700 -0.99923500
C 0.74370300 -2.23582700 3.00224700
H 1.47630800 -2.95154400 2.63715700
H 0.80967400 -2.13426100 4.08420000
H -0.26433300 -2.51061600 2.70625100
C -2.50055100 -1.67902200 -0.10738000
C -3.70070800 -0.98264900 0.05491000

C -2.49803600 -2.81557800 -0.91987200
C -4.85490400 -1.38977200 -0.59511800
H -3.71968600 -0.10353900 0.69056400
C -3.65187400 -3.22235300 -1.56856600
H -1.59169500 -3.39936400 -1.03215800
C -4.83400600 -2.50967600 -1.41334900
H -5.77391100 -0.83180400 -0.45901400
H -3.63187100 -4.10816400 -2.19245700
H -5.73559600 -2.83366900 -1.91914600

Int-2e

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.67210146
Gibbs Free Energy (T = 213K) = -1635.198210
C -1.37296500 -0.71256700 0.02954400
N -0.15772600 -1.05411900 0.67888600
C -2.37377100 0.07571800 0.44843400
B 1.13492500 -1.05761400 -0.19815100
H -1.46105500 -1.20076600 -0.93310100
S -0.20224000 -1.10741800 2.34435400
O 1.06705100 -1.60618200 2.85091500
O -0.67597500 0.17478900 2.88162300
H -2.32458600 0.55456000 1.42114400
C 2.45391300 5.44767800 -0.13542300
C 3.01063100 4.44103500 -0.92897300
C 2.58989100 3.13028200 -0.77647200
C 1.60563000 2.82816400 0.17690400
C 1.05038500 3.83922700 0.97153800
C 1.47692300 5.15124200 0.81292700
H 2.78776700 6.47337500 -0.25912300
H 3.77136200 4.68642200 -1.66248300
H 3.00898800 2.33211400 -1.38069700
H 0.29142700 3.59005100 1.70814100
H 1.05235700 5.94000600 1.42458800
C 1.13890700 1.47123800 0.36741700
H 0.37373200 1.28381600 1.13014600
O 1.58375000 0.52624100 -0.29809700
C 2.44077400 -1.85929900 0.30075300
H 2.71888900 -1.60216600 1.32550800
C 0.87577300 -1.50016900 -1.73655100
H 0.03919900 -0.96463700 -2.20774100
C 0.51045000 -3.00173100 -1.72378000
H 0.34961800 -3.36015800 -2.75066800
H -0.45365700 -3.12023900 -1.20798200
C 2.10388700 -1.16217200 -2.61054200
H 2.15943400 -0.06886900 -2.69469400
H 1.94253200 -1.53700400 -3.63178000
C 3.65589100 -1.50341500 -0.58372100
H 4.52555400 -2.09795100 -0.26852700
H 3.91983900 -0.45547100 -0.38692000
C 2.08671300 -3.36321100 0.29828700
H 1.34040400 -3.52927000 1.08563600
H 2.96660300 -3.95507500 0.58932500
C 3.45608400 -1.68157200 -2.09660700
H 4.26286700 -1.16237900 -2.63053000
H 3.56850100 -2.73707300 -2.35979000
C 1.53884800 -3.91424200 -1.03113000
H 2.36753500 -4.11118900 -1.71677600
H 1.07602900 -4.89261400 -0.84771400
C -1.44836200 -2.34202300 2.68063700
H -1.09096200 -3.29446700 2.28732200
H -1.55795200 -2.38967700 3.76535700
H -2.39061800 -2.05599100 2.21383200
C -3.60349900 0.31093600 -0.33014400
C -4.75672900 0.73791000 0.34082600
C -3.67260300 0.14768000 -1.72129600
C -5.94423400 0.97072300 -0.34552300
H -4.71970000 0.88214500 1.41792200
C -4.85890300 0.37686400 -2.40782100
H -2.78601900 -0.14138700 -2.27898300
C -6.00213700 0.78656800 -1.72394500
H -6.82567100 1.29690700 0.19893800
H -4.88808400 0.24553700 -3.48565100
H -6.92662800 0.96908800 -2.26339500

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.04865848
Gibbs Free Energy (T = 213K) = -1635.579338
C -1.44544200 -0.49248900 0.05772900
N -0.27010200 -0.94083100 0.70210600
C -2.42747800 0.30065700 0.49435200
B 0.99677900 -1.14369700 -0.18590700
H -1.52250200 -0.89748800 -0.93963000
S -0.29385700 -0.94512800 2.35799900
O 0.93786200 -1.49428700 2.85282900
O -0.67559500 0.36327400 2.85005600
H -2.39563900 0.71894300 1.49176300
C 3.22858200 5.08230500 -0.22783200
C 3.66407500 3.98768800 -0.97116700
C 3.05544400 2.76055600 -0.80822200
C 2.00413800 2.63009200 0.10464500
C 1.57116000 3.72826400 0.84846000
C 2.18629300 4.95652800 0.68000500
H 3.71061800 6.04360000 -0.35981800
H 4.47910000 4.10103200 -1.67459200
H 3.37740300 1.89479400 -1.37363100
H 0.75743000 3.61048000 1.55520400
H 1.85699900 5.81327200 1.25359000

C 1.33938700 1.36235500 0.30469200
H 0.52298100 1.31296400 1.03354500
O 1.66804500 0.34961800 -0.31494800
C 2.17370800 -2.11779400 0.31637500
H 2.50146800 -1.87881200 1.32674600
C 0.66376800 -1.57641000 -1.70928100
H -0.08635700 -0.93415100 -2.18536600
C 0.08302300 -3.00503700 -1.66435600
H -0.12698000 -3.35673000 -2.68149000
H -0.88670600 -2.96875700 -1.15323000
C 1.91579500 -1.44063400 -2.59884600
H 2.13553000 -0.37263400 -2.70212100
H 1.68627400 -1.80103500 -3.60894900
C 3.41569000 -1.97452500 -0.58564200
H 4.18400400 -2.68726000 -0.26257400
H 3.83942000 -0.97861900 -0.41493500
C 1.59648200 -3.54668800 0.36006300
H 0.84143900 -3.57478300 1.15270200
H 2.37596700 -4.25520400 0.66497800
C 3.17439500 -2.15209800 -2.08892900
H 4.04304400 -1.77676600 -2.63990400
H 3.11735600 -3.21458500 -2.32880400
C 0.96295000 -4.04244900 -0.94922600
H 1.74636700 -4.38130600 -1.62782700
H 0.35880200 -4.93065200 -0.73820100
C -1.59713600 -2.08726000 2.74991700
H -1.29402900 -3.06938800 2.39398300
H -1.69591100 -2.07885800 3.83382100
H -2.52153200 -1.76395200 2.27794100
C -3.61742500 0.63659500 -0.30465400
C -4.73533600 1.15775600 0.34979000
C -3.68699300 0.47853900 -1.69226400
C -5.88700000 1.49048400 -0.34699800
H -4.69841600 1.29907000 1.42486100
C -4.83667000 0.80858000 -2.38873900
H -2.82915500 0.10921700 -2.24258100
C -5.94502500 1.31373700 -1.72072700
H -6.74144800 1.88993400 0.18687200
H -4.86563400 0.67882700 -3.46441400
H -6.84217200 1.57384100 -2.26948500

TS2-2a

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.66432644
Gibbs Free Energy (T = 213K) = -1635.186406
Imaginary Frequency = 275.4945*i*
C -0.19587600 1.28108900 0.36264700
N 1.08586200 1.05267500 0.00746500
C -0.96556700 0.45724800 1.16092600
B 1.67266100 -0.49234900 0.03219100
H -0.67081700 2.13507600 -0.11479900
S 1.74173900 2.33445200 -0.93719400
O 2.50097000 1.79110100 -2.04749200
O 0.67616800 3.29046800 -1.21903800
H -0.46792300 -0.11037200 1.93401300
C -4.22348100 -1.36427400 -2.43658200
C -3.05309300 -0.82660300 -2.97507000
C -1.88072800 -0.82812400 -2.23252100
C -1.87589900 -1.37259100 -0.94352300
C -3.04920500 -1.90872100 -0.40706200
C -4.22123600 -1.90613800 -1.15423900
H -5.13938200 -1.35751200 -3.01979800
H -3.05865700 -0.40465400 -3.97515600
H -0.96359600 -0.40960500 -2.63462800
H -3.04634500 -2.31074800 0.60233800
H -5.13258800 -2.31768000 -0.73277500
C -0.66313300 -1.32978800 -0.12356000
H -0.67468600 -1.89071000 0.81318500
O 0.46676800 -1.11949200 -0.69473400
C 2.98070800 -0.85476800 -0.84197100
H 2.88366400 -0.50878800 -1.87538100
C 1.96438600 -1.02787000 1.53545000
H 1.15754300 -0.85570700 2.25927700
C 3.16883500 -0.23269100 2.08395700
H 3.38907300 -0.54591900 3.11445500
H 2.86364600 0.82153200 2.15407700
C 2.17559500 -2.56057900 1.51029700
H 1.20285000 -3.03237600 1.30938500
H 2.47618500 -2.91253100 2.50794400
C 3.05493900 -2.39901700 -0.90000100
H 3.90716500 -2.70148800 -1.52523400
H 2.15524500 -2.77088800 -1.40635500
C 4.27348600 -0.23447600 -0.27263700
H 4.30359000 0.81774400 -0.57395700
H 5.14650100 -0.69035400 -0.76171900
C 3.17731900 -3.08446200 0.46744900
H 3.03141000 -4.16561900 0.34692300
H 4.19852400 -2.96888200 0.84235100
C 4.46112900 -0.33936000 1.25640300
H 4.95381800 -1.28447900 1.50134100
H 5.16036900 0.44049600 1.58764700
C 2.84684300 3.10171900 0.23186100
H 3.58516200 2.37674200 0.57130500
H 3.33243800 3.92814500 -0.29110300
H 2.25321800 3.47246600 1.06827500
C -2.39949800 0.70744400 1.37014700
C -3.00936000 0.26261500 2.54980100
C -3.20389800 1.30331000 0.38926100
C -4.37479400 0.42785100 2.75490400

H -2.40268700 -0.21453400 3.31604800
C -4.56685300 1.47606400 0.59727400
H -2.77192500 1.59938500 -0.56261900
C -5.15902400 1.03952800 1.77997200
H -4.82669100 0.07880700 3.67875900
H -5.17224100 1.93637000 -0.17777000
H -6.22584000 1.16682200 1.93685900

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.04044108
Gibbs Free Energy (T = 213K) = -1635.566355
Imaginary Frequency = 308.8063*i*
C -0.18299500 1.28721300 0.33724600
N 1.08710000 1.05157600 -0.02200500
C -0.95886400 0.46877200 1.13165700
B 1.66412100 -0.49632500 0.02527400
H -0.65009200 2.14578800 -0.13410500
S 1.75405500 2.32052900 -0.95256900
O 2.50817900 1.77274400 -2.03961500
O 0.71024100 3.27165900 -1.23977900
H -0.46735400 -0.08626800 1.91379900
C -4.23937200 -1.42293300 -2.36713400
C -3.08501400 -0.88423000 -2.92554700
C -1.90814900 -0.86212000 -2.19963500
C -1.88224400 -1.38329300 -0.90711700
C -3.03927400 -1.92169700 -0.35152600
C -4.21597900 -1.94317500 -1.08160700
H -5.16007100 -1.43462000 -2.93816800
H -3.10687600 -0.47949900 -3.92999400
H -1.00212900 -0.44192500 -2.61873500
H -3.01926800 -2.30953200 0.66071300
H -5.11584500 -2.35775400 -0.64472000
C -0.66317500 -1.31577100 -0.09972200
H -0.66672300 -1.86773900 0.83984100
O 0.45870400 -1.12278100 -0.68683000
C 2.96864000 -0.87227600 -0.83984600
H 2.87057200 -0.53717100 -1.87388800
C 1.95352000 -1.01059800 1.53191200
H 1.14659800 -0.82674000 2.24738600
C 3.15687600 -0.21492500 2.07322200
H 3.37377900 -0.51857500 3.10419000
H 2.85570000 0.83801200 2.13392600
C 2.16071100 -2.54142800 1.52740900
H 1.18978700 -3.01323700 1.33463400
H 2.46031700 -2.87805400 2.52750300
C 3.04037700 -2.41429300 -0.87967100
H 3.89097100 -2.72346400 -1.49860600
H 2.14327300 -2.78958400 -1.38201900
C 4.25991100 -0.24839200 -0.27841200
H 4.29251100 0.79650500 -0.59243100
H 5.12931900 -0.71231500 -0.75979200
C 3.16004800 -3.08016400 0.49426000
H 3.01237000 -4.15961000 0.38851600
H 4.17845800 -2.96141200 0.86733900
C 4.44654200 -0.33418500 1.24900100
H 4.93628300 -1.27432500 1.50546400
H 5.14517000 0.44688500 1.56887300
C 2.85059000 3.07861500 0.21601500
H 3.58113400 2.35001400 0.55559200
H 3.33807700 3.89699200 -0.31202800
H 2.25304300 3.45359300 1.04381200
C -2.38783900 0.73816400 1.33757000
C -3.00422500 0.30829100 2.51331400
C -3.17954200 1.33581200 0.35440000
C -4.36422500 0.48680200 2.71105800
H -2.40663000 -0.17049200 3.28230100
C -4.53664300 1.52179100 0.55497700
H -2.74114800 1.62540200 -0.59384100
C -5.13588700 1.09758800 1.73294000
H -4.82278600 0.14801400 3.63262700
H -5.13359100 1.98367900 -0.22234400
H -6.19975700 1.23518300 1.88412400

TS2-2b

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.66209476
Gibbs Free Energy (T = 213K) = -1635.185155
Imaginary Frequency = 336.4168*i*
C -0.01682500 -1.47762300 0.31451900
N -1.26152400 -1.08710500 -0.02977600
C 1.01059400 -0.65053800 0.74531200
B -1.61798800 0.49373500 -0.04009000
H 0.22349300 -2.50986400 0.07579700
S -2.15821800 -2.32602300 -0.81759400
O -2.82860000 -1.75084100 -1.96813000
O -1.27003900 -3.46696100 -1.01494800
H 0.77564000 0.26047200 1.28010300
C 4.48497900 2.50610000 -1.01918700
C 3.39073600 3.10213500 -0.39178700
C 2.15441400 2.47044100 -0.39955400
C 2.00638100 1.23935700 -1.04517400
C 3.10247900 0.64814800 -1.67846200
C 4.34022600 1.27990500 -1.66305300
H 5.45187900 2.99995700 -1.00548500
H 3.50494200 4.06042700 0.10538700
H 1.29529600 2.92101100 0.08677300
H 2.98767500 -0.31518300 -2.16736100
H 5.19128500 0.81391500 -2.14907700

C 0.72688600 0.51550400 -1.00139600
H 0.62270800 -0.31624700 -1.70581500
O -0.33177400 1.13907200 -0.62417400
C -2.87713900 1.05211000 -0.88693900
H -2.85366200 0.71006200 -1.92779500
C -1.80864400 1.03624900 1.48184200
H -1.01415000 0.69605200 2.16131200
C -3.11824700 0.45627400 2.05183400
H -3.27460200 0.81926700 3.07796600
H -2.98649000 -0.63074400 2.14487300
C -1.75480300 2.57814800 1.47731700
H -0.72091700 2.87145100 1.25464100
H -1.97238000 2.96722900 2.48296400
C -2.72821900 2.59342400 -0.91904300
H -3.55859500 3.02715700 -1.49480800
H -1.81094100 2.84167600 -1.46533300
C -4.23734400 0.62351500 -0.29802200
H -4.42829700 -0.41084400 -0.60124900
H -5.03998200 1.20525500 -0.77404200
C -2.68421600 3.26901800 0.46203300
H -2.36451000 4.31209600 0.34066700
H -3.69799300 3.32331600 0.87026700
C -4.38715000 0.75627800 1.23349700
H -4.72724700 1.76632200 1.47820400
H -5.19580600 0.09464600 1.57401300
C -3.35627200 -2.80973400 0.40840300
H -3.99551900 -1.96609100 0.66064500
H -3.94315200 -3.61417200 -0.03963300
H -2.82058100 -3.17119000 1.28702200
C 2.38546300 -1.14729500 0.92877500
C 3.25980600 -0.40861600 1.73485100
C 2.89339000 -2.25860600 0.24240400
C 4.59377300 -0.77544300 1.86776300
H 2.88835200 0.47199900 2.25236200
C 4.22528900 -2.63156900 0.38277700
H 2.25696100 -2.83053700 -0.42776000
C 5.08206400 -1.89190500 1.19454600
H 5.25377700 -0.18491000 2.49607300
H 4.59838500 -3.49715100 -0.15663000
H 6.12409100 -2.17977400 1.29478400

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.03825261
Gibbs Free Energy (T = 213K) = -1635.565023
Imaginary Frequency = 355.1899*i*
C -0.02057700 -1.47142800 0.29872900
N -1.25781100 -1.08507000 -0.04852400
C 1.00355100 -0.64587400 0.73041900
B -1.60984000 0.49461600 -0.04669000
H 0.21987200 -2.50185000 0.06323400
S -2.15306700 -2.31500400 -0.82233800
O -2.82476700 -1.74062700 -1.94894100
O -1.27705200 -3.44121100 -1.02800200
H 0.76646400 0.26021900 1.26689200
C 4.47364300 2.49845500 -1.02196100
C 3.38396000 3.09211600 -0.39529400
C 2.15229800 2.46207600 -0.40077900
C 2.00424600 1.23483500 -1.04263600
C 3.09527700 0.64696500 -1.67589800
C 4.32848400 1.27702100 -1.66372500
H 5.43822600 2.99165700 -1.01011400
H 3.49874900 4.04859700 0.10006000
H 1.29481900 2.91061000 0.08530200
H 2.97915300 -0.31380000 -2.16439800
H 5.17710500 0.81298500 -2.15063600
C 0.72652600 0.51076100 -0.99676500
H 0.62556800 -0.31487100 -1.70551200
O -0.32910300 1.13832100 -0.62722100
C -2.86885200 1.05781300 -0.88183700
H -2.84564700 0.72333400 -1.92221700
C -1.79698400 1.02404800 1.47642900
H -1.00294800 0.67661100 2.14741400
C -3.10405300 0.44715600 2.04752600
H -3.25487400 0.80789600 3.07216200
H -2.97533600 -0.63732100 2.13872800
C -1.73736000 2.56290100 1.48280800
H -0.70615800 2.85423700 1.25891200
H -1.94945800 2.94323100 2.48978000
C -2.72343200 2.59696100 -0.90396800
H -3.55781600 3.03078700 -1.46803800
H -1.81425200 2.84978800 -1.45601900
C -4.22400600 0.62257000 -0.29406500
H -4.40970500 -0.40896900 -0.59827400
H -5.02687000 1.20123500 -0.76675400
C -2.66880300 3.26144800 0.47905200
H -2.34792400 4.30165900 0.36298000
H -3.67705200 3.31516100 0.89316400
C -4.37161100 0.75126000 1.23465900
H -4.70965800 1.75801700 1.48232700
H -5.17797100 0.09042600 1.57275500
C -3.33496900 -2.79985300 0.40498500
H -3.97549300 -1.95961900 0.65359100
H -3.91354600 -3.60589200 -0.04427600
H -2.79090000 -3.15586100 1.27695300
C 2.37339800 -1.14571700 0.92364700
C 3.24378400 -0.40638000 1.72479900
C 2.87805400 -2.26174100 0.25284000
C 4.57144700 -0.77513300 1.86534800
H 2.87356100 0.47735500 2.23295500

C 4.20363300 -2.63567300 0.39974700
H 2.24293700 -2.83711800 -0.41159300
C 5.05705700 -1.89394800 1.20484000
H 5.23007300 -0.18304900 2.48948400
H 4.57554100 -3.50533900 -0.12899500
H 6.09559000 -2.18332300 1.31055400

TS2-2c

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.63515696
Gibbs Free Energy (T = 213K) = -1635.157500
Imaginary Frequency = 245.6214*i*
C 0.17843500 -1.20890000 0.65447400
N -1.13959100 -1.32223400 0.40069700
C 1.20510500 -1.42227400 -0.26527900
B -1.62965600 0.25157000 -0.06242700
H 0.39664200 -0.65416900 1.56431100
S -1.63623300 -2.63607700 -0.58571600
O -3.08298300 -2.71043000 -0.49119800
O -1.01345300 -2.62324400 -1.90763000
H 0.97306300 -2.03723300 -1.13107300
C 2.74464100 3.83737100 -0.06546500
C 2.26357200 3.63799700 -1.35588200
C 1.60957500 2.45340100 -1.67651700
C 1.40874600 1.46138300 -0.71068000
C 1.90659700 1.66556400 0.57375000
C 2.56986400 2.84522900 0.89415800
H 3.25920800 4.75857200 0.18968400
H 2.39789300 4.40148500 -2.11571800
H 1.23270300 2.30342500 -2.68495600
H 1.79964600 0.90593800 1.33693700
H 2.95211700 2.98531900 1.90034500
C 0.61959200 0.27778100 -1.22051200
H 1.02176600 -0.09112700 -2.16840600
O -0.68300300 0.30879900 -1.25287100
C -3.14276200 0.37885700 -0.57375100
H -3.36817000 -0.33111700 -1.37847000
C -1.42398700 1.30390500 1.14252800
H -0.41912200 1.31151800 1.58141400
C -2.39001000 0.92911200 2.28707000
H -2.27848700 1.63911100 3.11961900
H -2.08457300 -0.05286900 2.67713800
C -1.62968800 2.72686700 0.57168100
H -0.77499000 2.94723400 -0.08104500
H -1.58492300 3.46379700 1.38680400
C -3.27690600 1.79373300 -1.18503500
H -4.30013300 1.94286500 -1.55902400
H -2.61822300 1.84446900 -2.06241800
C -4.13263400 0.09576100 0.57573400
H -4.09189600 -0.97869100 0.78256900
H -5.15999700 0.30518100 0.24321100
C -2.92286900 2.94857600 -0.23403100
H -2.81991900 3.87336100 -0.81668200
H -3.75903200 3.12708800 0.44778900
C -3.87179100 0.85662400 1.88848300
H -4.27729500 1.87045600 1.82488200
H -4.43304400 0.37006300 2.69699400
C -0.96630400 -4.01334000 0.33884900
H -1.36455400 -3.97878300 1.35306400
H -1.31150600 -4.91246800 -0.17525100
H 0.12358800 -3.97861200 0.34115900
C 2.63890400 -1.38373000 0.11706400
C 3.05804000 -1.55733300 1.43962300
C 3.60360100 -1.16821200 -0.87232800
C 4.40742300 -1.48075600 1.76994000
H 2.32981100 -1.76889900 2.21816100
C 4.95124100 -1.09166700 -0.54315500
H 3.29555400 -1.04650800 -1.90748900
C 5.35694500 -1.24122200 0.78103000
H 4.71660100 -1.61775300 2.80157800
H 5.68618200 -0.91390300 -1.32199100
H 6.40977600 -1.18208800 1.03868300

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.01028800
Gibbs Free Energy (T = 213K) = -1635.537139
Imaginary Frequency = 254.9577*i*
C 0.16504700 -1.20554100 0.65335600
N -1.14675300 -1.32173800 0.40480400
C 1.18948100 -1.42439200 -0.26139000
B -1.62726300 0.25934800 -0.06968200
H 0.38753000 -0.64790600 1.55809300
S -1.64451800 -2.62427400 -0.57304500
O -3.07345400 -2.68690000 -0.47149200
O -1.04034100 -2.61250300 -1.88295100
H 0.95593100 -2.04179200 -1.12099600
C 2.78241900 3.79584500 -0.06672500
C 2.32469000 3.58563200 -1.35830500
C 1.65759100 2.41260800 -1.67240800
C 1.41957300 1.44348300 -0.69939100
C 1.89492200 1.65785700 0.58612100
C 2.57164400 2.82547100 0.90063000
H 3.30787300 4.70935800 0.18378200
H 2.48778400 4.33302500 -2.12514700
H 1.30037600 2.25264500 -2.68389900
H 1.75695100 0.91675000 1.35878800
H 2.93637600 2.97434300 1.90953800
C 0.62135900 0.26517100 -1.20381000

H 1.02467200 -0.10294200 -2.14928200
O -0.67886300 0.31356900 -1.24642300
C -3.13392300 0.39406100 -0.58496200
H -3.35505200 -0.31623700 -1.38649300
C -1.42448500 1.30497400 1.13610600
H -0.42559500 1.30230700 1.57944000
C -2.39937200 0.94079000 2.27249800
H -2.28516400 1.64805400 3.10318100
H -2.10732200 -0.04185800 2.66354900
C -1.61375600 2.72753200 0.56545700
H -0.75205800 2.94359000 -0.07501500
H -1.57331300 3.46061700 1.38044000
C -3.25422100 1.80603600 -1.19941900
H -4.27253800 1.96085400 -1.57584700
H -2.59435900 1.84791000 -2.07277800
C -4.13252000 0.12215200 0.55555200
H -4.10155100 -0.94899900 0.76605600
H -5.15276400 0.33736100 0.21449200
C -2.89525500 2.95802100 -0.25123200
H -2.77824600 3.87696800 -0.83484200
H -3.73251900 3.14696600 0.42165300
C -3.87573400 0.88438700 1.86437200
H -4.26779900 1.89982600 1.79271000
H -4.44745400 0.40842700 2.66778000
C -0.98059500 -4.00139600 0.33976700
H -1.37092100 -3.96160200 1.35352400
H -1.34210600 -4.88852800 -0.17790300
H 0.10651900 -3.97346900 0.32698900
C 2.62090000 -1.38866500 0.11998500
C 3.03895600 -1.53993100 1.44004800
C 3.58237600 -1.19565200 -0.87023900
C 4.38410400 -1.46238300 1.76675400
H 2.31271500 -1.73311500 2.22189900
C 4.92536100 -1.11665300 -0.54470900
H 3.27414300 -1.09175100 -1.90478400
C 5.33001000 -1.24299500 0.77695600
H 4.69373600 -1.58204400 2.79791900
H 5.65907100 -0.95505200 -1.32490900
H 6.38078300 -1.18169900 1.03243200

TS2-2d

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.65505256
Gibbs Free Energy (T = 213K) = -1635.177388
Imaginary Frequency = 338.3881*i*
C -0.12199300 -1.43135000 0.51645400
N -1.27353900 -1.35504600 -0.15912000
C 1.14019000 -1.01492200 0.05855700
B -1.77164800 0.35161200 0.23651700
H -0.26134100 -1.55590600 1.58917400
S -1.26757000 -1.77033600 -1.81849100
O -2.64927300 -1.72070600 -2.26286900
O -0.25037600 -1.06706500 -2.59912800
H 1.31008700 -1.06322200 -1.01368900
C 3.78745100 2.69462500 -2.04776400
C 2.64430500 2.26011900 -2.71862900
C 1.60619300 1.66019400 -2.01671900
C 1.70996200 1.49719000 -0.63289100
C 2.85468700 1.92957300 0.03809100
C 3.89214100 2.52866000 -0.66956900
H 4.59610100 3.16312800 -2.60086100
H 2.56274500 2.38912200 -3.79353900
H 0.71657100 1.30543600 -2.52599200
H 2.93639300 1.79270900 1.11307700
H 4.78005200 2.86558000 -0.14369500
C 0.60969600 0.84694400 0.13077500
H 0.67729700 0.98388500 1.21458900
O -0.59073800 0.97138700 -0.39998000
C -3.14575400 0.76306000 -0.45953400
H -3.11125300 0.64154600 -1.54788500
C -1.92413500 0.51134000 1.83154400
H -1.02907100 0.24482000 2.41524100
C -3.05770800 -0.40967700 2.32631500
H -3.21411500 -0.27204700 3.40594000
H -2.72605300 -1.44977100 2.19381100
C -2.14836700 2.02090400 2.09733600
H -1.21283800 2.54430900 1.85137600
H -2.31677800 2.18934100 3.17054500
C -3.33085600 2.27489800 -0.18383600
H -4.27954700 2.62010800 -0.61898000
H -2.53421400 2.81120600 -0.71678500
C -4.29122400 -0.12523000 0.06755200
H -4.14040400 -1.12886400 -0.34517200
H -5.25306600 0.22902200 -0.33059200
C -3.28849600 2.67822000 1.29967400
H -3.18382400 3.76837300 1.37145500
H -4.24722300 2.44611200 1.77116600
C -4.40216500 -0.23368900 1.59978500
H -4.91582500 0.64492400 2.00029400
H -5.04884000 -1.08520700 1.84790500
C -0.77917400 -3.48624200 -1.70311100
H -1.49168500 -4.01150600 -1.06701500
H -0.80818200 -3.88189000 -2.72018700
H 0.23269400 -3.55481200 -1.30051000
C 2.35805800 -1.17440300 0.89455500
C 3.58444200 -1.39220000 0.26179200
C 2.33341500 -1.03308100 2.28675600
C 4.75846200 -1.48744900 1.00136900
H 3.61808200 -1.47440400 -0.82115000

C 3.50668700 -1.12803000 3.02710500
H 1.39889800 -0.83222300 2.80528100
C 4.72255000 -1.35726100 2.38672000
H 5.70268500 -1.65651800 0.49307900
H 3.47150700 -1.01552100 4.10634100
H 5.63817700 -1.42717100 2.96574700

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.02985733
Gibbs Free Energy (T = 213K) = -1635.557061
Imaginary Frequency = 356.0573*i*
C -0.12137100 -1.38422000 0.60954000
N -1.26796200 -1.37021900 -0.06625800
C 1.13789900 -1.01077600 0.12497300
B -1.76742500 0.37530500 0.20437900
H -0.25673700 -1.42692900 1.68736100
S -1.26403200 -1.89696200 -1.67794800
O -2.63286800 -1.88622300 -2.10757900
O -0.27385800 -1.24760200 -2.50413800
H 1.30772700 -1.13505300 -0.93784600
C 3.78581700 2.52467200 -2.21975300
C 2.64823400 2.04657200 -2.85986000
C 1.60897600 1.50567700 -2.12286100
C 1.70554300 1.44486900 -0.73526000
C 2.84373200 1.92242600 -0.09529000
C 3.88275500 2.46260000 -0.83772900
H 4.59680900 2.94727300 -2.80097300
H 2.57251700 2.09602300 -3.93938900
H 0.72130300 1.11849600 -2.60666000
H 2.91942100 1.86600800 0.98504700
H 4.76725600 2.83499900 -0.33552600
C 0.60315700 0.85547000 0.06736000
H 0.67180400 1.06503700 1.13677300
O -0.59187900 0.94290000 -0.47128900
C -3.13939500 0.73111300 -0.51416600
H -3.10186200 0.53246800 -1.58797900
C -1.91808400 0.64047100 1.78046100
H -1.02307200 0.41401800 2.37422700
C -3.04829900 -0.24234200 2.33939100
H -3.20215300 -0.02934900 3.40410400
H -2.71670600 -1.28626200 2.28040900
C -2.14249100 2.16221200 1.94209100
H -1.20986800 2.66725300 1.66147700
H -2.30988600 2.40212600 2.99876800
C -3.32666800 2.25579400 -0.34508400
H -4.27442300 2.56579800 -0.80080100
H -2.53427400 2.75359800 -0.91472700
C -4.28229100 -0.11696500 0.07268300
H -4.13163200 -1.14381600 -0.26903400
H -5.24142800 0.20829500 -0.34801000
C -3.28242600 2.76002300 1.10396400
H -3.17919400 3.84969000 1.09949100
H -4.23752000 2.56026300 1.59064400
C -4.39128100 -0.11812000 1.60579600
H -4.90367900 0.78355900 1.94374300
H -5.03519400 -0.94865900 1.91214100
C -0.76496400 -3.59050000 -1.45509900
H -1.46472200 -4.07077500 -0.77605800
H -0.81017100 -4.04354000 -2.44419200
H 0.25209400 -3.62193900 -1.06916000
C 2.35182800 -1.10549500 0.97046100
C 3.57443700 -1.37168000 0.36053900
C 2.32629100 -0.85710000 2.34267400
C 4.74395200 -1.40661700 1.10363300
H 3.60857600 -1.53902100 -0.71025100
C 3.49451600 -0.89177600 3.08628000
H 1.39324100 -0.61752600 2.84170500
C 4.70706700 -1.16786600 2.46910300
H 5.68699500 -1.61352700 0.61249100
H 3.45912700 -0.69498900 4.15097800
H 5.62026500 -1.19037200 3.05128200

TS2-2e

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.63638723
Gibbs Free Energy (T = 213K) = -1635.160952
Imaginary Frequency = 393.1267*i*
C 0.07168300 1.21858400 0.88551600
N 1.32697300 1.36904800 0.46704600
C -1.13040900 1.25861700 0.15816400
B 1.72706400 -0.58128600 0.23696000
H 0.02582400 0.71160500 1.85009100
S 1.60407700 2.47407200 -0.79332500
O 3.04308700 2.59812300 -0.94635200
O 0.79906400 2.18300500 -1.98440200
H -1.17764100 1.88571300 -0.72830100
C -4.17411700 -2.35441500 -1.69118600
C -3.34437600 -2.86486900 -0.69534000
C -2.13734100 -2.24026200 -0.40475000
C -1.75483300 -1.10104700 -1.11556100
C -2.58750100 -0.59348000 -2.11682600
C -3.79329600 -1.21906100 -2.40464800
H -5.11766600 -2.84315600 -1.91433100
H -3.63970700 -3.75176500 -0.14336700
H -1.48030700 -2.63099000 0.36483300
H -2.28687700 0.29481400 -2.66710400
H -4.43638500 -0.82351800 -3.18447900
C -0.49739300 -0.39811100 -0.80630800

H -0.06937700 0.20518500 -1.61066800
O 0.36529100 -1.05671600 -0.05598900
C 2.81783600 -0.79936400 -0.90344300
H 2.55665800 -0.33483600 -1.86434600
C 2.24267000 -1.14062100 1.62912600
H 1.53394200 -0.95653300 2.45091700
C 3.58587200 -0.49309300 2.00632400
H 3.95667800 -0.90969100 2.95391700
H 3.40341400 0.57491200 2.18363600
C 2.29687400 -2.68096000 1.42854300
H 1.26066400 -3.04014900 1.38251400
H 2.74966000 -3.15806000 2.30926800
C 2.77322900 -2.34010100 -1.11208900
H 3.51087100 -2.62476500 -1.87507000
H 1.78905700 -2.60779500 -1.51648500
C 4.21714100 -0.29106600 -0.49250900
H 4.21704900 0.79527700 -0.59791100
H 4.96244300 -0.67246500 -1.20559800
C 3.03622900 -3.16762700 0.16214100
H 2.74872200 -4.20914500 -0.02966800
H 4.11191600 -3.19456900 0.35322900
C 4.67927900 -0.63570800 0.93683200
H 5.08916700 -1.64926900 0.97297700
H 5.51603400 0.02474200 1.19763100
C 1.00611200 3.99778900 -0.07362100
H 1.56029200 4.18554800 0.84621800
H 1.20883400 4.78054800 -0.80706600
H -0.06473500 3.93040800 0.12079800
C -2.42442400 1.06108200 0.85365000
C -3.54679800 1.77233800 0.42109300
C -2.57648100 0.13567400 1.89317900
C -4.78513700 1.58704700 1.02712900
H -3.44753300 2.47877200 -0.39935200
C -3.81260300 -0.04888300 2.50064200
H -1.73251600 -0.47007300 2.21265300
C -4.92092700 0.67819500 2.07232700
H -5.64499900 2.15158400 0.67936800
H -3.91329700 -0.77334900 3.30312300
H -5.88681800 0.52973100 2.54530800

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.01006442
Gibbs Free Energy (T = 213K) = -1635.538617
Imaginary Frequency = 399.2358*i*
Single point calculation at the ωB97XD/6-31G structure.

TS3-*syn*-P2
ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.66620726
Gibbs Free Energy (T = 213K) = -1635.190586
Imaginary Frequency = 208.0923*i*
C 0.22702000 -2.73528900 -0.59178900
N -1.00894300 -2.54724200 -0.66669700
C 1.25846800 -1.63809700 -0.73936000
B -1.00236500 0.94345200 0.56867000
H 0.62982400 -3.74443100 -0.42441300
S -2.57540400 -2.30892000 -0.76159800
O -2.97501400 -1.55957500 0.42042500
O -2.85915600 -1.79239100 -2.09236900
H 1.74095000 -1.82525200 -1.71067800
C 3.38834700 2.82813700 -1.95451100
C 3.25439300 2.46420700 -0.61614000
C 2.35478300 1.46936100 -0.24797000
C 1.57651700 0.83122600 -1.21597200
C 1.71362800 1.20008900 -2.55331900
C 2.61712300 2.19272600 -2.92385800
H 4.08732500 3.60869800 -2.23988400
H 3.85168400 2.95792900 0.14465900
H 2.24401700 1.18878500 0.79466800
H 1.09760200 0.71839400 -3.30952400
H 2.70844300 2.47800500 -3.96766100
C 0.59159300 -0.25023000 -0.82865300
H -0.18403200 -0.31879700 -1.60059800
O -0.00239700 0.02187300 0.42600900
C -1.46068300 1.36494000 2.01156300
H -1.06597300 0.69361200 2.78519400
C -1.62583600 1.85469100 -0.55786000
H -1.36005500 1.56042100 -1.58124300
C -1.00569600 3.26134300 -0.31766300
H -1.46575100 3.98628600 -1.00385800
H 0.05646200 3.21047500 -0.59278100
C -3.16747300 1.80858400 -0.44456300
H -3.49209000 0.81098900 -0.76302700
H -3.61083300 2.52160700 -1.15447500
C -3.00204200 1.36394100 2.10565600
H -3.32194000 1.79907400 3.06383200
H -3.32521200 0.31664000 2.11306400
C -0.79716100 2.75573400 2.21634900
H 0.29210000 2.60657400 2.25104300
H -1.08071300 3.16566400 3.19608800
C -3.73501200 2.08692700 0.95926500
H -4.78956800 1.78407600 0.97416500
H -3.74026700 3.16498700 1.14442800
C -1.11417200 3.79476900 1.12457300
H -2.11322300 4.20483800 1.29252200
H -0.42665100 4.64282200 1.23581100
C -3.32297300 -3.92466200 -0.64289200

H -3.04777200 -4.36587800 0.31608000
H -4.40556700 -3.79793000 -0.70537900
H -2.96538600 -4.53742000 -1.47167200
C 2.31852800 -1.74926000 0.33767800
C 3.67211500 -1.68661800 0.00271600
C 1.95746700 -1.88116900 1.68154700
C 4.65035200 -1.74895100 0.99017600
H 3.96146500 -1.57167400 -1.03866900
C 2.93505500 -1.94656400 2.66974900
H 0.90721700 -1.90789100 1.95529400
C 4.28322700 -1.88010900 2.32682800
H 5.69918100 -1.69321900 0.71469100
H 2.64167300 -2.04563800 3.71054200
H 5.04511300 -1.92921200 3.09904200

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.04399077
Gibbs Free Energy (T = 213K) = -1635.573101
Imaginary Frequency = -213.6649
C 0.22387800 -2.72770600 -0.60372600
N -1.00605100 -2.54842100 -0.68474400
C 1.25301600 -1.63139700 -0.73619000
B -0.99824900 0.94284100 0.57506900
H 0.63176200 -3.73415000 -0.44288400
S -2.56482800 -2.30711100 -0.76598000
O -2.94338900 -1.56264400 0.40368700
O -2.85149800 -1.79899600 -2.07928200
H 1.73824400 -1.81331400 -1.70412500
C 3.37459600 2.82694300 -1.95517100
C 3.24968800 2.46202400 -0.62138600
C 2.35605200 1.46974300 -0.25082400
C 1.57679500 0.83309300 -1.21136400
C 1.70449900 1.20324400 -2.54381500
C 2.60086300 2.19453200 -2.91708200
H 4.06889500 3.60741700 -2.24298300
H 3.84941700 2.95481300 0.13466300
H 2.25004300 1.18949800 0.79009100
H 1.08422900 0.72428100 -3.29485600
H 2.68466300 2.48213700 -3.95838600
C 0.59358900 -0.24473100 -0.82041800
H -0.18275100 -0.30732300 -1.58842000
O 0.00436100 0.03142900 0.43468800
C -1.44975400 1.37271400 2.01309700
H -1.04906700 0.70902900 2.78617600
C -1.63207600 1.83829900 -0.55184400
H -1.37371800 1.53164900 -1.57004200
C -1.01172400 3.24536500 -0.33113800
H -1.47666200 3.96032100 -1.01969600
H 0.04577000 3.19256000 -0.61358300
C -3.16993900 1.79291300 -0.42808500
H -3.49431800 0.79416000 -0.73291400
H -3.61648300 2.49650000 -1.14084300
C -2.98731200 1.37207700 2.11890600
H -3.29796500 1.81442800 3.07341700
H -3.31034000 0.32748500 2.13887200
C -0.78696300 2.76382400 2.20153000
H 0.29967300 2.61541100 2.23195600
H -1.06534600 3.17965400 3.17685500
C -3.72643900 2.08431400 0.97395600
H -4.77828000 1.78326600 0.99883500
H -3.72899300 3.16098300 1.14945200
C -1.11064700 3.79044400 1.10414000
H -2.10610200 4.20060900 1.27413300
H -0.42428600 4.63719200 1.20291400
C -3.31556500 -3.91157400 -0.63728000
H -3.03256800 -4.34543100 0.31938400
H -4.39437100 -3.77403800 -0.69138700
H -2.96579300 -4.52233100 -1.46693400
C 2.30950800 -1.75044100 0.33913100
C 3.65863600 -1.68070900 0.00853900
C 1.94865200 -1.89132900 1.67685100
C 4.63202100 -1.74324200 0.99387700
H 3.94881100 -1.55947400 -1.02948400
C 2.92093000 -1.95749900 2.66309000
H 0.90016300 -1.92488300 1.94778500
C 4.26450300 -1.88178100 2.32430400
H 5.67883200 -1.68098200 0.72161900
H 2.62721900 -2.06345000 3.70062400
H 5.02352400 -1.93053900 3.09598500

TS3-*anti*-P2

ωB97XD/6-31G*
Solvent = Toluene
Potential Energy = -1635.65699933
Gibbs Free Energy (T = 213K) = -1635.181356
Imaginary Frequency = 242.1384*i*
C 1.32367200 -0.76000600 -1.13778800
N 1.55246600 -1.85792000 -0.58195100
C 1.04310700 0.52400100 -0.37581100
B -1.91869200 -0.31814100 -0.71192500
H 1.35010200 -0.67685100 -2.23283800
S 1.94680200 -3.23549700 0.10993600
O 0.78146400 -4.10182700 0.02093700
O 3.23177800 -3.67085400 -0.41264700
H 0.70158300 0.23746700 0.62348100
C -1.96624200 4.59256100 0.95999900
C -0.78379700 4.06297500 1.46439600
C -0.15456200 3.00100100 0.81763000
C -0.70301100 2.45333700 -0.34148200

C -1.88668800 2.99973600 -0.84859500
C -2.51572200 4.05787600 -0.20342400
H -2.45685400 5.41729500 1.46783600
H -0.34491700 4.47270600 2.36915800
H 0.76754100 2.60760700 1.23081100
H -2.32359500 2.58124700 -1.75070000
H -3.43679900 4.46501400 -0.60961800
C -0.07674800 1.29321600 -1.09978100
H 0.33318400 1.69140000 -2.03531400
O -1.06222100 0.35757700 -1.53889200
C -2.90494000 -1.36896200 -1.34000100
H -2.81659900 -1.41280600 -2.43290100
C -2.04960800 -0.23866800 0.85985000
H -1.39142900 0.49517900 1.33743700
C -1.66024600 -1.63904100 1.40084300
H -1.80224400 -1.66937400 2.49038600
H -0.58256000 -1.76900400 1.22701300
C -3.50328900 0.19743500 1.17406900
H -3.60486400 1.24644100 0.86170000
H -3.66420200 0.18651000 2.26097900
C -4.34942500 -0.93056500 -0.99475400
H -5.06574600 -1.68957000 -1.33897800
H -4.56869500 -0.02146200 -1.57345200
C -2.49001900 -2.75309600 -0.77550700
H -1.50831600 -3.01130500 -1.19546500
H -3.18688100 -3.52543700 -1.12958300
C -4.60582600 -0.63342400 0.49378800
H -5.55771300 -0.09592700 0.58759100
H -4.74630400 -1.57128300 1.03699900
C -2.38477800 -2.83395300 0.75742800
H -3.38038800 -2.94051100 1.19625300
H -1.83925600 -3.74771400 1.01768300
C 2.20646300 -2.82298600 1.82765700
H 1.27566500 -2.43692900 2.24551300
H 2.50824800 -3.73309700 2.34983800
H 2.99979800 -2.07551900 1.88474900
C 2.37147500 1.25372700 -0.24817400
C 3.07086500 1.18580100 0.96044900
C 2.95190500 1.92804700 -1.32483700
C 4.31309400 1.79489600 1.09885100
H 2.62965100 0.65896700 1.80343300
C 4.19568700 2.53825700 -1.18726700
H 2.44178600 1.98277500 -2.28209900
C 4.87871000 2.47541400 0.02343300
H 4.83884300 1.73854600 2.04706000
H 4.63170300 3.06245300 -2.03203600
H 5.84799800 2.95265600 0.12836900

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1636.03490680
Gibbs Free Energy (T = 213K) = -1635.563608
Imaginary Frequency = 251.5885*i*
C 1.32494400 -0.78616000 -1.13383300
N 1.51243900 -1.88762000 -0.58501800
C 1.06196100 0.49730200 -0.37186300
B -1.91514300 -0.28562000 -0.70703200
H 1.36794000 -0.69491400 -2.22629900
S 1.87034500 -3.27369000 0.09126500
O 0.69961200 -4.09929300 -0.01440300
O 3.13186900 -3.72231600 -0.42607300
H 0.71864000 0.21412500 0.62440100
C -1.87056900 4.60777100 0.94792700
C -0.74340100 4.01562800 1.49327100
C -0.13266900 2.94571900 0.85216700
C -0.64397100 2.45378700 -0.34178800
C -1.77186000 3.06289700 -0.88901700
C -2.38315300 4.12805700 -0.24997300
H -2.34800900 5.43956400 1.45164800
H -0.33394600 4.38269400 2.42680500
H 0.74531000 2.50052800 1.30126000
H -2.18068300 2.68510700 -1.81911800
H -3.26261700 4.58506600 -0.68769800
C -0.04181900 1.28134800 -1.09434400
H 0.37311300 1.66921500 -2.02891600
O -1.04837500 0.36734600 -1.53183600
C -2.93073000 -1.30429100 -1.33053200
H -2.84858600 -1.34388400 -2.42126500
C -2.03523700 -0.20833800 0.86115100
H -1.35360200 0.50104500 1.33458100
C -1.68538600 -1.61846900 1.39604200
H -1.82394400 -1.64632800 2.48310400
H -0.61602000 -1.77787800 1.21723700
C -3.47021900 0.27200900 1.18216100
H -3.54151900 1.32054800 0.86803000
H -3.62389600 0.26905200 2.26722800
C -4.35897000 -0.83131700 -0.97583900
H -5.09346000 -1.57111300 -1.31426800
H -4.55940600 0.08001500 -1.55262000
C -2.54866300 -2.69873700 -0.77638800
H -1.57594300 -2.97697200 -1.19787200
H -3.26231400 -3.44984400 -1.13345600
C -4.59684600 -0.52739900 0.51135000
H -5.53102800 0.03358100 0.61093000
H -4.75736300 -1.45839300 1.05498600
C -2.44401900 -2.78792200 0.75275000
H -3.43893800 -2.86820600 1.19141700
H -1.92491100 -3.71527100 1.00810400
C 2.12999200 -2.89446200 1.80818700
H 1.20628700 -2.49666700 2.22305000

H 2.40867100 -3.81991500 2.30993100
H 2.93831700 -2.16850900 1.87396000
C 2.39357800 1.21355000 -0.23953800
C 3.09857300 1.11179800 0.95749000
C 2.96727400 1.91160300 -1.29776400
C 4.34035500 1.70840600 1.10244100
H 2.66126300 0.56634900 1.78750200
C 4.21093400 2.50929900 -1.15399900
H 2.45061500 1.99595600 -2.24634300
C 4.89988200 2.41143900 0.04490700
H 4.87170000 1.62530400 2.04283800
H 4.64264500 3.05303100 -1.98551100
H 5.87006800 2.88018000 0.15508700

7···PhCHO

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1866.447502
Gibbs Free Energy (T = 323K) = -1865.940752

C	0.639139	-1.390793	0.217353
N	0.191433	-0.196491	-0.434179
C	0.097104	-1.811443	1.347852
B	0.086952	1.050679	0.283483
C	0.525977	-3.004935	2.159025
C	1.011388	-2.494023	3.525018
H	1.883194	-1.846042	3.40684
H	1.287867	-3.333228	4.169167
H	0.229317	-1.920959	4.030037
H	1.448997	-1.902326	-0.283907
S	-0.585471	-0.431469	-1.888255
O	-0.427017	0.753604	-2.684421
O	-0.126817	-1.699344	-2.393893
C	-4.394041	0.407969	-0.933931
C	-3.091023	0.532784	-1.383709
C	-2.280925	-0.592385	-1.420479
C	-2.755912	-1.831351	-1.012946
C	-4.061131	-1.936583	-0.563712
C	-4.897938	-0.823027	-0.517623
H	-5.031403	1.284511	-0.903236
H	-2.694356	1.49122	-1.689757
H	-2.109837	-2.698479	-1.049705
H	-4.43664	-2.90169	-0.24285
O	0.576404	1.189852	1.548187
O	-0.529198	2.161756	-0.204258
C	0.441198	2.589503	1.89685
C	-0.67791	3.073507	0.910017
C	0.07187	2.68737	3.365484
H	-0.128379	3.726511	3.636305
H	-0.807148	2.088666	3.600552
H	0.903069	2.330958	3.9761
C	-0.500824	4.491511	0.40255
H	0.433745	4.600866	-0.145383
H	-1.323512	4.746853	-0.267376
H	-0.508121	5.196971	1.236653
C	-2.089157	2.870815	1.451647
H	-2.304624	3.561312	2.26872
H	-2.80386	3.05288	0.64765
H	-2.23503	1.849022	1.808467
C	1.793587	3.244907	1.64602
H	2.081323	3.175405	0.595772
H	1.782739	4.295623	1.941414
H	2.546526	2.729702	2.24563
C	-6.322341	-0.952453	-0.054939
H	-6.680712	-0.022204	0.387659
H	-6.976253	-1.190989	-0.898263
H	-6.428486	-1.750782	0.680715
H	-0.722933	-1.234566	1.77069
C	4.339185	-1.898055	-0.431185
C	3.844299	-1.949289	-1.726589
C	3.284907	-0.813447	-2.29326
C	3.22833	0.37163	-1.567685
C	3.715338	0.41529	-0.262583
C	4.266426	-0.718752	0.304605
H	4.777456	-2.783904	0.013214
H	3.891035	-2.872006	-2.29134
H	2.88564	-0.84446	-3.301005
H	3.651976	1.342893	0.292373
H	4.642154	-0.690444	1.320072
C	2.647477	1.574296	-2.200258
H	2.257111	1.421129	-3.222854
O	2.590618	2.66219	-1.677429
C	1.643107	-3.801208	1.484727
H	1.333762	-4.16919	0.503099
H	2.540359	-3.192427	1.353272
H	1.907977	-4.664029	2.100694
C	-0.701795	-3.906773	2.358911
H	-0.448711	-4.759161	2.994978
H	-1.518221	-3.358027	2.836159
H	-1.063207	-4.288912	1.400917

TS1-7a

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1866.420487
Gibbs Free Energy (T = 323K) = -1865.903468
Imaginary Frequency = 320.3*i*

C	0.994016	-0.926561	1.00651
N	-0.119869	-0.593437	0.334065

C	1.858501	0.009047	1.524107
B	-0.217549	0.888219	-0.257464
C	3.032651	-0.398962	2.406033
C	3.969591	0.801288	2.583189
H	4.461294	1.068786	1.648217
H	4.749683	0.566552	3.311438
H	3.421135	1.674898	2.946338
H	1.242671	-1.982177	1.024038
S	-0.856334	-1.870868	-0.507933
O	-0.596746	-1.729858	-1.914393
O	-0.442814	-3.084344	0.154947
C	-4.794744	-1.381732	-1.031927
C	-3.434481	-1.485324	-1.274908
C	-2.572634	-1.628264	-0.203084
C	-3.04273	-1.667337	1.101729
C	-4.399909	-1.544845	1.327254
C	-5.295419	-1.400435	0.266362
H	-5.476328	-1.273853	-1.867715
H	-3.042015	-1.449434	-2.2818
H	-2.355996	-1.786288	1.930506
H	-4.774912	-1.566011	2.344045
O	-0.215815	1.884229	0.761973
O	-1.303175	1.117913	-1.123983
C	-0.960025	2.988162	0.237019
C	-2.026223	2.2587	-0.641424
C	-1.527602	3.792402	1.394141
H	-2.20435	4.568267	1.027502
H	-2.069905	3.155888	2.092191
H	-0.715289	4.280921	1.936497
C	-2.520165	3.061225	-1.833699
H	-1.707069	3.294108	-2.520532
H	-3.270815	2.484169	-2.377792
H	-2.982626	3.995553	-1.505065
C	-3.214514	1.776652	0.185818
H	-3.832786	2.614398	0.515539
H	-3.829589	1.114625	-0.423277
H	-2.881455	1.220251	1.062626
C	-0.01751	3.868161	-0.586704
H	0.377854	3.329644	-1.449024
H	-0.521067	4.770579	-0.939304
H	0.821311	4.16892	0.044652
C	-6.766125	-1.240765	0.530324
H	-6.991329	-0.206432	0.804358
H	-7.357804	-1.488563	-0.351248
H	-7.089399	-1.876415	1.356115
H	1.422803	0.968433	1.775625
C	5.504551	-1.138584	-2.212627
C	4.216317	-1.650062	-2.33356
C	3.1476	-0.978455	-1.768955
C	3.364337	0.204153	-1.063879
C	4.649505	0.725075	-0.96387
C	5.719116	0.054401	-1.538116
H	6.340253	-1.66879	-2.653233
H	4.049098	-2.575982	-2.870061
H	2.138397	-1.363026	-1.862356
H	4.813284	1.662134	-0.443731
H	6.718793	0.463415	-1.458904
C	2.229847	0.901414	-0.433303
H	2.447785	1.811398	0.124085
O	1.098499	0.827944	-1.047632
C	3.823089	-1.591349	1.856371
H	3.208483	-2.491679	1.783018
H	4.24024	-1.381197	0.870788
H	4.650515	-1.821967	2.532095
C	2.457022	-0.769806	3.784734
H	3.264569	-1.014834	4.480473
H	1.884204	0.060377	4.206201
H	1.794567	-1.636088	3.71098

TS1-7b

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1866.414230
Gibbs Free Energy (T = 323K) = -1865.899624
Imaginary Frequency = 358.4*i*

C	-0.235747	-0.182777	1.830294
N	0.964417	0.063498	1.265418
C	-1.125702	-1.149745	1.42165
B	1.279572	-0.677991	-0.103763
C	-2.368088	-1.441927	2.259156
C	-3.155398	-0.173173	2.605328
H	-2.576244	0.522466	3.217075
H	-4.047282	-0.438391	3.178142
H	-3.480203	0.349532	1.704081
H	-0.533379	0.514281	2.606494
S	1.645505	1.558246	1.662147
O	1.17126	1.893132	2.981726
O	3.051876	1.476819	1.412619
C	-0.903739	4.158037	-0.017381
C	-0.228392	3.388002	0.914727
C	0.877742	2.655198	0.5088
C	1.318954	2.686833	-0.80682
C	0.629587	3.460509	-1.722815
C	-0.489802	4.202328	-1.347028
H	-1.768458	4.732586	0.294366
H	-0.554478	3.352628	1.945862
H	2.162794	2.080217	-1.107519
H	0.961482	3.48141	-2.754552
O	1.42984	-2.074911	0.132491

O	2.374621	-0.219002	-0.861399
C	2.409013	-2.54872	-0.793882
C	3.318929	-1.28979	-0.9721
C	3.109099	-3.755497	-0.191585
H	3.945423	-4.069831	-0.82121
H	3.484888	-3.53715	0.807341
H	2.40797	-4.589652	-0.118267
C	4.00711	-1.194754	-2.323922
H	3.282968	-1.135086	-3.135917
H	4.63244	-0.30007	-2.356679
H	4.649938	-2.063116	-2.48976
C	4.350217	-1.15137	0.145274
H	5.136304	-1.904328	0.054386
H	4.802964	-0.161269	0.086026
H	3.881093	-1.244442	1.125481
C	1.70307	-2.954588	-2.089477
H	1.218561	-2.098275	-2.560192
H	2.399224	-3.40226	-2.802029
H	0.935117	-3.69371	-1.850923
C	-1.216336	5.049285	-2.353545
H	-1.244691	4.56233	-3.32942
H	-2.239532	5.253692	-2.036935
H	-0.708073	6.009074	-2.479743
H	-0.742143	-1.984467	0.846174
C	-4.674999	-1.558949	-2.27947
C	-4.701083	-0.331116	-1.632717
C	-3.547288	0.161751	-1.043735
C	-2.369429	-0.576123	-1.098719
C	-2.338844	-1.79654	-1.770031
C	-3.491781	-2.287257	-2.353892
H	-5.577545	-1.948087	-2.735021
H	-5.619076	0.241491	-1.58814
H	-3.558137	1.122775	-0.540955
H	-1.408804	-2.350207	-1.814511
H	-3.474476	-3.240209	-2.86821
C	-1.155095	-0.049175	-0.459898
H	-1.242076	0.960222	-0.051915
O	-0.019465	-0.426501	-0.928538
C	-3.288056	-2.422685	1.520894
H	-3.754292	-1.970436	0.645962
H	-2.734337	-3.306671	1.193603
H	-4.084903	-2.754066	2.19141
C	-1.894223	-2.116324	3.559909
H	-1.252752	-1.448126	4.139992
H	-2.753088	-2.388946	4.179587
H	-1.327417	-3.025277	3.343169

TS1-7c

ωB97XD/6-311G(2d,p)

Solvent = THF

Potential Energy = -1866.400086

Gibbs Free Energy (T = 323K) = -1865.881768

Imaginary Frequency = 251.2*i*

C	0.968492	-1.074478	0.785217
N	-0.27377	-0.735169	0.408763
C	1.839526	-1.815673	-0.001546
B	-0.138466	0.788162	-0.268295
C	3.072033	-2.531274	0.539902
C	2.51897	-3.829259	1.162842
H	1.867292	-3.608104	2.011323
H	3.346562	-4.450446	1.513957
H	1.941436	-4.404746	0.436055
H	1.359203	-0.493595	1.617165
S	-1.152206	-1.9074	-0.457363
O	-0.877861	-1.868961	-1.870979
O	-0.945693	-3.147584	0.25187
C	-4.888939	-0.582395	-1.045288
C	-3.55883	-0.910134	-1.250255
C	-2.813836	-1.38562	-0.186152
C	-3.373212	-1.537392	1.074051
C	-4.698173	-1.194115	1.265194
C	-5.474858	-0.711948	0.211107
H	-5.479181	-0.213603	-1.876245
H	-3.097555	-0.794973	-2.220898
H	-2.779465	-1.922936	1.892878
H	-5.14155	-1.30758	2.24782
O	0.214998	1.681069	0.779059
O	-1.293185	1.262492	-0.911409
C	-0.459034	2.913298	0.505015
C	-1.765401	2.402634	-0.181503
C	-0.671694	3.659171	1.81059
H	-1.295213	4.54248	1.651252
H	-1.147725	3.024373	2.557047
H	0.290467	3.991634	2.206332
C	-2.393112	3.378997	-1.161249
H	-1.714194	3.611124	-1.981231
H	-3.300836	2.941688	-1.582661
H	-2.666302	4.309048	-0.6562
C	-2.80577	1.945518	0.837615
H	-3.23131	2.79531	1.375724
H	-3.612422	1.42912	0.317662
H	-2.368236	1.255035	1.559874
C	0.413983	3.746154	-0.434759
H	0.556062	3.241163	-1.39153
H	-0.023114	4.729802	-0.618721
H	1.394671	3.885028	0.024306
C	-6.905824	-0.313489	0.439267
H	-7.478184	-0.338376	-0.488481
H	-7.388414	-0.971236	1.163649

H	-6.956331	0.704785	0.834893
H	1.372768	-2.379189	-0.804432
C	5.53114	2.006779	0.23378
C	4.342402	2.15067	0.938126
C	3.201306	1.474761	0.539452
C	3.237628	0.634095	-0.570824
C	4.425911	0.517026	-1.287794
C	5.568374	1.194403	-0.888648
H	6.421606	2.534286	0.553942
H	4.303513	2.795307	1.80816
H	2.274116	1.609327	1.078289
H	4.459114	-0.106045	-2.174856
H	6.48385	1.088411	-1.457695
C	2.066835	-0.145933	-1.087397
H	2.353088	-0.749285	-1.95022
O	0.902816	0.436783	-1.291189
C	4.006567	-2.91263	-0.612745
H	4.486979	-2.03905	-1.051236
H	4.79492	-3.573162	-0.244964
H	3.46384	-3.443063	-1.399827
C	3.846496	-1.765378	1.615488
H	3.206475	-1.475238	2.452294
H	4.627135	-2.416108	2.016457
H	4.326491	-0.870548	1.222343

TS1-7d

ωB97XD/6-311G(2d,p)
Solvent = THF
Potential Energy = -1866.408980
Gibbs Free Energy (T = 323K) = -1865.892064
Imaginary Frequency = 309.5*i*

C	0.834696	-0.549115	1.437522
N	-0.320223	-0.502325	0.756093
C	2.040831	-1.006002	0.925939
B	-0.303392	1.057585	0.065177
C	3.230212	-1.299217	1.842026
C	2.76219	-2.405737	2.806282
H	1.961547	-2.046967	3.457896
H	3.595267	-2.732152	3.43388
H	2.387236	-3.271295	2.255252
H	0.84298	0.081196	2.323564
S	-0.679756	-1.816124	-0.248783
O	-0.114529	-1.687104	-1.568717
O	-0.367009	-2.99873	0.518473
C	-4.383587	-1.181015	-1.655743
C	-3.003066	-1.250562	-1.56058
C	-2.433098	-1.66977	-0.372137
C	-3.217126	-2.020635	0.717424
C	-4.592256	-1.938711	0.609247
C	-5.195713	-1.515884	-0.575885
H	-4.835839	-0.855945	-2.585631
H	-2.372014	-0.976596	-2.394158
H	-2.754492	-2.356597	1.636558
H	-5.210998	-2.210829	1.456757
O	-0.230821	1.978558	1.143103
O	-1.407033	1.342586	-0.747789
C	-1.147289	3.036211	0.833381
C	-2.211939	2.295524	-0.039805
C	-1.684012	3.62139	2.12797
H	-2.470273	4.352198	1.922469
H	-2.088688	2.845066	2.776374
H	-0.880231	4.130589	2.663886
C	-2.925272	3.173212	-1.053179
H	-2.224927	3.604868	-1.767392
H	-3.652744	2.575149	-1.606151
H	-3.460962	3.982974	-0.551346
C	-3.235448	1.544178	0.809018
H	-3.910355	2.235417	1.31828
H	-3.828041	0.898052	0.160801
H	-2.743766	0.918147	1.554848
C	-0.389735	4.107432	0.049298
H	-0.02317	3.712857	-0.900027
H	-1.017859	4.977607	-0.152583
H	0.468952	4.433085	0.639668
C	-6.691404	-1.401599	-0.669121
H	-7.182883	-2.221677	-0.143244
H	-7.029589	-0.468248	-0.210597
H	-7.026693	-1.404021	-1.706609
H	1.977211	-1.658584	0.060193
C	5.450848	0.170968	-2.618524
C	4.272922	-0.526437	-2.864481
C	3.172429	-0.343017	-2.046292
C	3.251034	0.532393	-0.966944
C	4.421407	1.242805	-0.732229
C	5.521402	1.062516	-1.558681
H	6.311394	0.022698	-3.25968
H	4.215505	-1.215647	-3.69814
H	2.247303	-0.877962	-2.227827
H	4.473879	1.941493	0.095214
H	6.43233	1.618254	-1.373208
C	2.078259	0.742123	-0.079017
H	2.248449	1.424603	0.753847
O	0.94073	0.888691	-0.718003
C	3.67686	-0.080396	2.655389
H	4.452382	-0.381619	3.363042
H	4.099185	0.697771	2.018559
H	2.85861	0.353768	3.234875
C	4.409151	-1.847924	1.028927
H	4.82247	-1.10814	0.344585

H	5.205726	-2.161755	1.70775
H	4.103242	-2.719837	0.444942

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ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -702.956234
Gibbs Free Energy (T = 213K) = -702.614191

C	-0.457681	-1.739971	0.309582
C	-1.247576	-0.852137	0.90542
B	1.567724	-0.769776	0.304382
H	-0.648587	-2.222904	-0.636408
H	-0.914477	-0.410022	1.841653
C	2.058258	-0.678053	-1.156082
H	1.800693	-1.53814	-1.78154
C	1.870934	0.447024	1.204651
H	1.478499	0.366734	2.223286
C	1.269185	1.711841	0.545217
H	1.621111	2.59946	1.07829
H	0.184217	1.674673	0.693419
C	3.428707	0.443108	1.300924
H	3.735234	-0.426918	1.894757
H	3.743846	1.321534	1.870363
C	3.612132	-0.629047	-1.038034
H	4.034332	-0.451883	-2.030855
H	3.960578	-1.623692	-0.735577
C	1.41508	0.586005	-1.782687
H	0.349911	0.375985	-1.931088
H	1.83873	0.74763	-2.777698
C	4.159721	0.409246	-0.048156
H	5.214632	0.192003	0.134665
H	4.139828	1.39839	-0.501385
C	1.554532	1.872802	-0.956005
H	2.547395	2.29616	-1.099395
H	0.861903	2.615991	-1.357913
C	-2.535974	-0.374271	0.40995
C	-3.14716	0.684818	1.081726
C	-3.160996	-0.917199	-0.715899
C	-4.350865	1.202529	0.631365
H	-2.671989	1.108176	1.959888
C	-4.36317	-0.402183	-1.160232
H	-2.718042	-1.751635	-1.246068
C	-4.95876	0.660704	-0.49011
H	-4.813483	2.02821	1.156929
H	-4.842261	-0.82965	-2.031917
H	-5.899368	1.063823	-0.8443
N	0.882083	-2.032531	0.856442
H	1.233972	-2.911241	0.480497
H	0.87192	-2.097382	1.873616

PhCHO

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -345.546874499
Gibbs Free Energy (T = 213K) = -345.456717

C	-0.457681	-1.739971	0.309582
C	2.204032	-0.243301	-0.000017
C	1.722014	1.057896	-0.000004
C	0.35415	1.282318	0.00002
C	-0.528547	0.207461	0.000032
C	-0.04011	-1.097847	0.000018
C	1.323961	-1.321236	-0.000006
H	3.272963	-0.421338	-0.000036
H	2.411942	1.892764	-0.000012
H	-0.035334	2.29541	0.000031
H	-0.747415	-1.918467	0.000028
H	1.709499	-2.333539	-0.000016
C	-1.984839	0.464064	0.000065
H	-2.266712	1.537247	-0.000075
O	-2.831114	-0.393525	-0.000071

R-8c

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1048.52132477
Gibbs Free Energy (T = 213K) = -1048.072356

C	0.424122	0.248982	2.280158
C	-0.660235	0.85706	1.826803
B	2.046092	-0.138064	0.600357
H	0.40842	-0.653346	2.873351
H	-1.608494	0.414331	2.110675
C	-3.800763	-0.666983	-1.847677
C	-2.606835	-1.3816	-1.89007
C	-2.073784	-1.902894	-0.725916
C	-2.738699	-1.72143	0.485511
C	-3.940184	-1.018694	0.521517
C	-4.466359	-0.48246	-0.643845
H	-4.216542	-0.257728	-2.760428
H	-2.096986	-1.529649	-2.834252
H	-1.147896	-2.463476	-0.740164
H	-4.459009	-0.887865	1.465634
H	-5.397129	0.069707	-0.615943
C	-2.172679	-2.240557	1.746315
H	-2.856639	-2.198861	2.617289
O	-1.047241	-2.660585	1.874027
C	1.956314	0.523065	-0.786087

H	1.502586	1.517855	-0.792387
C	2.587107	-1.576715	0.655829
H	2.568264	-2.039557	1.646795
C	4.08733	-1.374015	0.256794
H	4.558874	-2.357448	0.182488
H	4.598247	-0.856986	1.078635
C	1.774573	-2.466287	-0.312734
H	0.814098	-2.658984	0.173206
H	2.269396	-3.436709	-0.410986
C	1.157752	-0.388602	-1.741894
H	1.252521	-0.00997	-2.764023
H	0.101478	-0.283716	-1.475698
C	3.469303	0.693167	-1.149999
H	3.898564	1.458216	-0.490601
H	3.535676	1.100818	-2.162304
C	1.539117	-1.876795	-1.712634
H	0.740192	-2.445863	-2.197041
H	2.418921	-2.041633	-2.333102
C	4.30976	-0.587102	-1.042651
H	4.11394	-1.228458	-1.899785
H	5.366511	-0.318242	-1.111032
C	-0.693727	2.027212	0.930515
C	-1.380193	1.922064	-0.277265
C	-0.022852	3.209658	1.23809
C	-1.347179	2.965162	-1.187175
H	-1.920915	1.011785	-0.510669
C	-0.000111	4.255947	0.327635
H	0.447119	3.333123	2.209163
C	-0.649605	4.12884	-0.891257
H	-1.869041	2.86915	-2.131232
H	0.516591	5.174725	0.575474
H	-0.626769	4.942739	-1.605028
N	1.782961	0.674864	1.886382
H	2.43999	0.465583	2.636887
H	1.801726	1.679261	1.70663

R-8d

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1048.52335541
Gibbs Free Energy (T = 213K) = -1048.075030

C	-0.43223	-2.071655	0.016201
C	0.466329	-1.901772	-0.942302
B	-2.444697	-0.79602	-0.162454
H	-0.229503	-2.030301	1.076176
H	0.14179	-1.866037	-1.979816
C	2.723654	2.877885	-1.015623
C	1.41851	2.394306	-0.979121
C	1.027291	1.557506	0.046231
C	1.933762	1.200074	1.042546
C	3.236659	1.682629	1.000002
C	3.631875	2.522469	-0.030182
H	3.030914	3.537944	-1.817948
H	0.713941	2.679624	-1.751436
H	0.02142	1.161651	0.094869
H	3.941818	1.395373	1.772434
H	4.645714	2.901037	-0.064738
C	1.531092	0.298083	2.133975
H	2.326304	0.063056	2.866654
O	0.425469	-0.179635	2.260147
C	-2.883143	-0.013671	-1.411749
H	-2.467184	-0.376269	-2.356137
C	-2.889919	-0.251139	1.203151
H	-2.46171	-0.765502	2.067117
C	-4.419811	-0.60202	1.145419
H	-4.890779	-0.2057	2.048435
H	-4.537741	-1.691821	1.202138
C	-2.593392	1.256877	1.328557
H	-1.532147	1.350962	1.569089
H	-3.132747	1.658885	2.190962
C	-2.567696	1.487304	-1.26626
H	-3.07511	2.043437	-2.059787
H	-1.496749	1.612201	-1.451937
C	-4.416526	-0.357349	-1.420309
H	-4.537048	-1.416735	-1.679649
H	-4.884522	0.202255	-2.234321
C	-2.923697	2.112285	0.092971
H	-2.390949	3.062148	0.182506
H	-3.980948	2.375217	0.101216
C	-5.15018	-0.079773	-0.100054
H	-5.330743	0.98827	0.003273
H	-6.137775	-0.544249	-0.14783
C	1.901923	-1.7356	-0.697731
C	2.666236	-1.014498	-1.613937
C	2.518535	-2.263745	0.437013
C	4.013217	-0.795188	-1.382911
H	2.196631	-0.604297	-2.50068
C	3.867861	-2.051301	0.660734
H	1.947951	-2.86202	1.137435
C	4.615831	-1.312052	-0.245069
H	4.594536	-0.219213	-2.091683
H	4.339507	-2.473269	1.53961
H	5.671662	-1.14721	-0.068991
N	-1.864899	-2.222903	-0.294869
H	-2.28368	-2.875644	0.367958
H	-1.98591	-2.614232	-1.229062

Int1-8c

ωB97XD/6-311G(2d,p)
Solvent = Toluene

Potential Energy = -1048.55863578
Gibbs Free Energy (T = 213K) = -1048.106843

C	0.644517	-1.983872	-1.457491
C	-0.662444	-2.098667	-1.652625
B	1.786769	-0.211809	0.084665
H	1.344779	-1.998529	-2.280831
H	-0.9671	-2.195103	-2.689848
C	-4.105142	2.562093	0.211142
C	-3.417049	1.940566	1.251726
C	-2.149018	1.449562	1.037063
C	-1.564632	1.591625	-0.229553
C	-2.258014	2.2219	-1.269848
C	-3.532447	2.703539	-1.04718
H	-5.103367	2.944652	0.386723
H	-3.88282	1.838437	2.222932
H	-1.602092	0.949176	1.82559
H	-1.792928	2.326354	-2.243432
H	-4.078717	3.191354	-1.843493
C	-0.268594	1.067009	-0.508346
H	0.154471	1.204638	-1.506644
O	0.395056	0.44996	0.347499
C	2.642805	-0.134046	1.424512
H	2.103944	-0.564424	2.278956
C	2.623289	0.413407	-1.12016
H	2.103278	0.393696	-2.08717
C	3.895987	-0.446551	-1.296715
H	4.521969	-0.021002	-2.086866
H	3.601593	-1.437763	-1.668668
C	2.922012	1.894996	-0.793829
H	1.990385	2.467211	-0.883446
H	3.590886	2.310144	-1.554415
C	2.875862	1.357983	1.738403
H	3.492156	1.460241	2.637208
H	1.906657	1.805674	1.985654
C	3.944293	-0.945733	1.241678
H	3.69834	-2.017484	1.240766
H	4.5912	-0.812557	2.114164
C	3.517129	2.164505	0.599052
H	3.411011	3.229929	0.819936
H	4.590761	1.98096	0.580233
C	4.745688	-0.623424	-0.02968
H	5.337105	0.276237	0.131721
H	5.473594	-1.420732	-0.2019
C	-1.753551	-2.056292	-0.661277
C	-2.925293	-1.37553	-0.996164
C	-1.674293	-2.675959	0.586637
C	-3.968266	-1.27528	-0.091548
H	-3.014572	-0.913721	-1.973085
C	-2.71808	-2.572924	1.493557
H	-0.824234	-3.301526	0.839078
C	-3.862516	-1.864066	1.160472
H	-4.866324	-0.735442	-0.365154
H	-2.643405	-3.066392	2.454599
H	-4.678159	-1.788727	1.868907
N	1.283056	-1.743325	-0.178914
H	2.094914	-2.352034	-0.081263
H	0.65753	-1.979663	0.589875

Int1-8d

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1048.5579526
Gibbs Free Energy (T = 213K) = -1048.105951

C	-0.099966	-1.797206	-0.722084
C	1.080047	-1.373698	-1.157013
B	-2.049244	-0.107425	-0.364829
H	-0.244227	-2.451406	0.126613
H	1.096114	-0.686104	-2.000496
C	3.608527	3.061712	-0.024724
C	2.607204	3.217084	-0.98419
C	1.411612	2.549512	-0.841591
C	1.218334	1.720246	0.273759
C	2.225788	1.570742	1.233501
C	3.422583	2.243542	1.080869
H	4.547604	3.587521	-0.147567
H	2.772507	3.862186	-1.837199
H	0.621779	2.653505	-1.57473
H	2.068618	0.91654	2.083105
H	4.209033	2.129381	1.814656
C	0.032352	0.943018	0.435311
H	-0.049796	0.307427	1.320013
O	-0.905561	0.95205	-0.390641
C	-3.325269	0.484082	-1.103886
H	-3.082519	0.855114	-2.108688
C	-2.466713	-0.634903	1.083805
H	-1.644069	-1.07793	1.661322
C	-3.509922	-1.760714	0.896084
H	-3.86885	-2.095135	1.874253
H	-3.006263	-2.639456	0.467818
C	-2.994173	0.567825	1.89864
H	-2.1494	1.224478	2.140949
H	-3.377704	0.218768	2.862676
C	-3.809021	1.697561	-0.281787
H	-4.714826	2.117079	-0.730976
H	-3.045008	2.479309	-0.357478
C	-4.381072	-0.629116	-1.265885
H	-4.027136	-1.341384	-2.024199
H	-5.302322	-0.211805	-1.68371
C	-4.07608	1.410467	1.203451
H	-4.170771	2.36231	1.732739

H	-5.044118	0.923109	1.313545
C	-4.720843	-1.400868	0.019769
H	-5.429768	-0.824233	0.611784
H	-5.24695	-2.321418	-0.246443
C	2.388637	-1.666659	-0.565596
C	3.466313	-0.860285	-0.930063
C	2.587998	-2.67159	0.383382
C	4.712072	-1.038627	-0.349884
H	3.322216	-0.075644	-1.665472
C	3.832277	-2.849708	0.960124
H	1.775118	-3.330982	0.664767
C	4.896751	-2.031658	0.599007
H	5.537809	-0.401275	-0.641144
H	3.976962	-3.634142	1.69269
H	5.868993	-2.176417	1.053521
N	-1.335033	-1.285229	-1.27366
H	-2.017109	-2.036649	-1.369983
H	-1.184605	-0.919974	-2.213463

TS2-8c

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1048.53130347
Gibbs Free Energy (T = 213K) = -1048.080155
Imaginary Frequency = 257.46*i*

C	0.145924	-1.241533	-2.03541
C	-1.131416	-0.88342	-1.687311
B	1.866962	0.071903	0.096055
H	0.568682	-0.822378	-2.941731
H	-1.656435	-0.343474	-2.466624
C	-3.959134	2.611478	0.456358
C	-3.26424	1.835311	1.374915
C	-2.043859	1.284393	1.032405
C	-1.515922	1.515267	-0.239904
C	-2.21687	2.300126	-1.159663
C	-3.434748	2.847588	-0.810072
H	-4.915058	3.041369	0.729099
H	-3.678115	1.659932	2.359442
H	-1.494414	0.677255	1.738735
H	-1.799854	2.476782	-2.145346
H	-3.978135	3.461084	-1.516993
C	-0.253198	0.939196	-0.643613
H	0.229215	1.338717	-1.53023
O	0.49448	0.380154	0.26722
C	2.608977	-0.580556	1.294031
H	1.943363	-1.129872	1.966582
C	2.800089	0.764817	-0.945196
H	2.312484	1.148791	-1.847133
C	3.941882	-0.17013	-1.391923
H	4.68816	0.407644	-1.945666
H	3.532756	-0.879507	-2.121672
C	3.279703	2.008034	-0.127851
H	2.41744	2.666868	0.030417
H	3.988377	2.57869	-0.734815
C	3.132368	0.662851	2.077837
H	3.755217	0.326168	2.911788
H	2.265721	1.162197	2.524515
C	3.713195	-1.533584	0.80069
H	3.229463	-2.434521	0.404897
H	4.316068	-1.872949	1.648419
C	3.914029	1.684017	1.234096
H	4.000982	2.612864	1.803151
H	4.935515	1.337624	1.085493
C	4.646513	-0.95365	-0.272217
H	5.391449	-0.316971	0.202537
H	5.213504	-1.771408	-0.724467
C	-1.992917	-1.447001	-0.640964
C	-3.373364	-1.355001	-0.836784
C	-1.530443	-1.987872	0.563269
C	-4.262251	-1.810177	0.119975
H	-3.751379	-0.915747	-1.753132
C	-2.422829	-2.447162	1.5193
H	-0.477083	-1.998597	0.808956
C	-3.78892	-2.363647	1.301264
H	-5.327753	-1.727425	-0.054252
H	-2.044329	-2.861579	2.445576
H	-4.482974	-2.721129	2.051611
N	1.006568	-1.962227	-1.302342
H	1.87186	-2.249134	-1.733378
H	0.653243	-2.59253	-0.596808

TS2-8d

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1048.53342493
Gibbs Free Energy (T = 213K) = -1048.083660
Imaginary Frequency = 5320.33*i*

C	-0.093511	-1.733795	-1.208954
C	1.073921	-1.01767	-1.196221
B	-2.092675	0.216409	-0.224317
H	-0.228441	-2.594685	-0.563122
H	1.212359	-0.285666	-1.985999
C	3.556085	3.171038	0.076842
C	2.532402	3.34337	-0.852126
C	1.440676	2.499703	-0.841984
C	1.371622	1.471575	0.103756
C	2.402441	1.299099	1.029162
C	3.490634	2.153922	1.01654
H	4.407971	3.839891	0.065103
H	2.590571	4.142357	-1.58014

H	0.635977	2.630422	-1.55478
H	2.351451	0.495286	1.754163
H	4.286981	2.023962	1.737683
C	0.246112	0.563018	0.154416
H	0.188067	-0.114144	1.001101
O	-0.866147	0.903183	-0.436085
C	-3.374902	0.802489	-0.881998
H	-3.166295	1.393607	-1.778759
C	-2.37122	-0.720784	0.995986
H	-1.496797	-1.219266	1.427532
C	-3.388671	-1.819605	0.628429
H	-3.708011	-2.337945	1.537512
H	-2.867037	-2.58091	0.034614
C	-2.887162	0.292893	2.063776
H	-2.049895	0.941483	2.349408
H	-3.168539	-0.254272	2.968143
C	-3.892208	1.787311	0.210481
H	-4.841457	2.221737	-0.116248
H	-3.180238	2.617786	0.272946
C	-4.368532	-0.318219	-1.247221
H	-3.984901	-0.835013	-2.135576
H	-5.321296	0.120407	-1.558446
C	-4.061606	1.173946	1.609562
H	-4.18467	1.98351	2.333225
H	-4.987165	0.601736	1.653436
C	-4.633969	-1.350096	-0.140489
H	-5.359711	-0.946322	0.563741
H	-5.119863	-2.223481	-0.582721
C	2.292208	-1.469526	-0.509541
C	3.525559	-1.015509	-0.970625
C	2.253238	-2.272688	0.631765
C	4.696647	-1.370346	-0.320098
H	3.565367	-0.37211	-1.842337
C	3.423381	-2.625673	1.281447
H	1.305472	-2.616214	1.033951
C	4.649188	-2.176105	0.806605
H	5.647321	-1.010149	-0.693296
H	3.379595	-3.248906	2.166157
H	5.563107	-2.451133	1.318179
N	-1.187835	-1.360809	-1.890113
H	-1.956164	-2.009855	-1.96838
H	-1.100361	-0.704048	-2.653101

syn-P8

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1048.56495748
Gibbs Free Energy (T = 213K) = -1048.113990

C	-1.343852	-2.283711	-1.794491
C	-1.67962	-0.901856	-1.375177
B	1.744087	-0.612756	-0.025597
H	-0.600875	-2.436062	-2.572764
H	-2.13727	-0.454165	-2.26829
C	-1.04834	3.917535	0.023616
C	-0.939003	2.924062	0.98587
C	-0.704069	1.61123	0.608597
C	-0.574981	1.285595	-0.736358
C	-0.677445	2.283927	-1.696203
C	-0.915544	3.596725	-1.319436
H	-1.228384	4.943566	0.319882
H	-1.037342	3.170766	2.035794
H	-0.615114	0.838966	1.362241
H	-0.551795	2.039837	-2.746417
H	-0.984739	4.370587	-2.073781
C	-0.339246	-0.137405	-1.177136
H	0.172267	-0.122563	-2.145801
O	0.418826	-0.894576	-0.251519
C	2.515379	-1.356832	1.111247
H	1.905423	-2.120789	1.604445
C	2.618212	0.457089	-0.766558
H	2.106445	0.980902	-1.579547
C	3.827957	-0.287839	-1.381515
H	4.503742	0.435839	-1.848977
H	3.455317	-0.921356	-2.196576
C	2.990489	1.525175	0.295009
H	2.082831	2.096706	0.517066
H	3.700714	2.236969	-0.138711
C	2.833121	-0.258782	2.161231
H	3.418076	-0.691268	2.979644
H	1.883861	0.064473	2.605971
C	3.758077	-2.048119	0.505
H	3.407064	-2.908292	-0.077937
H	4.381563	-2.461296	1.30496
C	3.563877	0.975933	1.611626
H	3.524154	1.767773	2.364616
H	4.622136	0.748495	1.487384
C	4.624671	-1.164233	-0.405562
H	5.275364	-0.535271	0.20049
H	5.296225	-1.80686	-0.981683
C	-2.66102	-0.821713	-0.230317
C	-3.873693	-0.168487	-0.41855
C	-2.369052	-1.369024	1.020203
C	-4.782503	-0.05837	0.621812
H	-4.10383	0.273358	-1.381732
C	-3.282764	-1.262614	2.057937
H	-1.412372	-1.849181	1.19006
C	-4.489992	-0.608529	1.860784
H	-5.720591	0.458617	0.463869
H	-3.046297	-1.686737	3.025925
H	-5.201262	-0.52482	2.672928

N	-1.890901	-3.327513	-1.307929
H	-1.648682	-4.256162	-1.629246
H	-2.585319	-3.237582	-0.567944

anti-P8

ωB97XD/6-311G(2d,p)
Solvent = Toluene
Potential Energy = -1048.55856213
Gibbs Free Energy (T = 213K) = -1048.106059

C	0.175652	-2.042612	-1.05299
C	1.099659	-0.902105	-0.914491
B	-2.058169	0.208875	-0.189473
H	0.136943	-2.811821	-0.28692
H	1.282507	-0.470113	-1.902576
C	2.977431	3.652367	-0.060857
C	2.07499	3.470656	-1.099688
C	1.229119	2.373066	-1.102313
C	1.275548	1.455098	-0.059307
C	2.17344	1.644363	0.984285
C	3.024755	2.738727	0.981381
H	3.639865	4.509343	-0.061025
H	2.027952	4.189557	-1.908522
H	0.514416	2.239063	-1.905099
H	2.213928	0.930981	1.799754
H	3.723757	2.878696	1.796631
C	0.389527	0.235027	-0.083216
H	0.235	-0.125453	0.934824
O	-0.834585	0.527421	-0.711578
C	-3.353815	0.72841	-0.891957
H	-3.134042	1.288793	-1.805681
C	-2.356251	-0.623654	1.109513
H	-1.476804	-1.047344	1.607615
C	-3.281524	-1.809369	0.739252
H	-3.612461	-2.312037	1.653644
H	-2.679117	-2.552487	0.200466
C	-2.989152	0.396697	2.093965
H	-2.212434	1.118035	2.374478
H	-3.275319	-0.116911	3.017256
C	-4.012896	1.708395	0.115125
H	-4.979903	2.041641	-0.275385
H	-3.381412	2.602686	0.163954
C	-4.222035	-0.491456	-1.271284
H	-3.70481	-1.033097	-2.075779
H	-5.170438	-0.156439	-1.703182
C	-4.200078	1.162145	1.53987
H	-4.416554	1.998958	2.208932
H	-5.082208	0.524215	1.579833
C	-4.507291	-1.464012	-0.11976
H	-5.29295	-1.055267	0.513603
H	-4.920184	-2.389893	-0.529748
C	2.400059	-1.338179	-0.273989
C	3.602669	-1.086957	-0.919284
C	2.407414	-1.932817	0.984784
C	4.803107	-1.41765	-0.309041
H	3.604427	-0.613263	-1.894201
C	3.606599	-2.267676	1.59161
H	1.477529	-2.119403	1.514469
C	4.806948	-2.008461	0.945242
H	5.737665	-1.210659	-0.814946
H	3.603896	-2.726767	2.57223
H	5.744923	-2.264657	1.421645
N	-0.633561	-2.174174	-2.034784
H	-1.273988	-2.956878	-2.096587
H	-0.671003	-1.484029	-2.777327