

## Supporting Information

# Metal-Free Borylative Ring-Opening of Vinyl Epoxides and Aziridines

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## 1. Instrumentation and chemicals

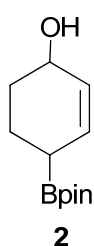
All reactions and manipulations were carried out under argon atmosphere using Schlenk-type techniques and oven-dried (120 °C) glassware, which was cooled in a stream of argon. Solvents were dried using a solvent purification system (Pure SOLV system-4). Substrates 3,4-epoxy-1-cyclohexene (**1**), 2-methyl-2-vinylloxirane (**7**), PCy<sub>3</sub> and Cu(acac)<sub>2</sub> were purchased from Sigma-Aldrich, and used as received. The substrates 3,4-aziridine-1-cyclohexene (**10**), 2-methyl-2-vinylaziridine (**11**) and 3-methyl-2-vinylaziridine (**12**), were prepared following the methodology established in the literature.<sup>[1]</sup>

Deuterated chloroform (CDCl<sub>3</sub>) was used as solvent for routine NMR measurements. NMR spectra were obtained using a Varian Mercury 400 spectrometer. <sup>1</sup>H NMR and <sup>13</sup>C{<sup>1</sup>H} NMR chemical shifts (δ) are reported in ppm relative to tetramethylsilane, referenced to the chemical shift of residual solvents resonances. <sup>11</sup>B{<sup>1</sup>H} NMR chemical shifts are reported in ppm (δ) relative to BF<sub>3</sub>·OEt<sub>2</sub> (δ <sup>11</sup>B{<sup>1</sup>H} = 0.00 ppm) as the external reference. Coupling constants (*J*) are given in Hz, and the multiplicity of the NMR signals is described as singlet (s), doublet (d), triplet (t), quartet (q) and multiplet (m).

GC-MS. Accurate mass determinations were carried out on a Kratos Concept IS spectrometer.

## 2. General procedures for the organocatalytic borylative ring-opening of vinyl epoxides and vinyl aziridines with B<sub>2</sub>pin<sub>2</sub>.

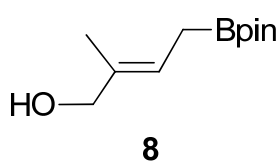
**Borylation of 3,4-epoxy-1-cyclohexene (1).** *Organocatalytic method:* The phosphine PCy<sub>3</sub> (9.54 mg, 10 mol%), sodium methoxide (33.4 mg, 0.6 mmol) and bis(pinacolato)diboron (114 mg, 0.45mmol) were transferred into an oven-dried Schlenk tube under argon. THF (3 mL) was added. The mixture was stirred for 10 minutes at room temperature to dissolve the phosphine and the borane reagent completely. The substrate (33 μL, 0.3 mmol) and MeOH (100 μl, 2.5 mmol) were added, and the reaction mixture was stirred at room temperature for 6 hours. An aliquot of 0.2 mL was taken from the solution and gently concentrated on a rotary evaporator at RT, and analyzed by <sup>1</sup>H-NMR showing that one single product was formed from the substrate. The obtained 4-cyclohexenyl hydroxyboronate (**2**) was purified by flash chromatography using a silica gel column previously deactivated with triethylamine, and a mixture of petroleum ether and ethyl acetate (10:3) as eluent (R.f.=0.35). The product could be isolated in 41.7 mg (62% yield).



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 5.88 (dd,  $J=10, 2.8$  Hz, 1H), 5.71 (dt,  $J=10, 2.6$  Hz, 1H), 4.18 (s, 1 H), 1.88-1.76 (m, 2 H), 1.73-1.52 (m, 3 H), 1.21 (s, 6 H), 1.19 (s, 6H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 131.72, 128.61, 83.66, 65.47, 32.06, 25.29, 25.04, 24.91, 20.50  
 $^{11}\text{B}$  NMR (128.52 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 33.26.

*Copper mediated borylation:* CuCl (1.5 mg, 0.015 mmol), 1,3-Bis(diphenylphosphino)propane (dppp) (13 mg, 0.03 mmol), cesium carbonate (2 eq.) and bis(pinacolato)diboron (114 mg, 0.45mmol) were transferred into an oven-dried Schlenk tube under argon. THF (3 mL) was added. The mixture was stirred for 10 minutes at room temperature to dissolve the borane reagent completely. The substrate (33  $\mu\text{L}$ , 0.3 mmol) and MeOH (100  $\mu\text{l}$ , 2.5 mmol) were added, and the reaction mixture was stirred at room temperature for 6 hours. An aliquot of 0.2 mL was taken from the solution and gently concentrated on a rotary evaporator at RT, and analyzed by  $^1\text{H}$ -NMR.

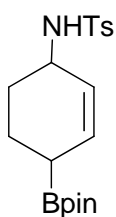
**Borylation of 2-methyl-2-vinyloxirane (7):** The phosphine  $\text{PCy}_3$  (9.54 mg, 10 mol%), sodium methoxide (33.4 mg, 0.6 mmol) and bis(pinacolato)diboron (114 mg, 0.45mmol) were transferred into an oven-dried Schlenk tube under argon. THF (3 mL) was added. The mixture was stirred for 10 minutes at room temperature to dissolve the phosphine and the borane reagent completely. The substrate (33  $\mu\text{L}$ , 0.3 mmol) and MeOH (100  $\mu\text{l}$ , 2.5 mmol) were added, and the reaction mixture was stirred at 50°C for 20 hours. The reaction mixture was cooled to room temperature. An aliquot of 0.2 mL was taken from the solution and gently concentrated on a rotary evaporator at RT, and analyzed by  $^1\text{H}$ -NMR to probe that one single product was formed from the substrate. The obtained 2-methyl-4-pinacolboryl-butenol (**8**) was purified by flash chromatography using a silica gel column previously treated with triethylamine, and a mixture of petroleum ether and ethyl acetate (1:1) as eluent (R.f.=0.42). The product could be isolated in 42.0 mg (66% yield).



$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 5.51 (t,  $J=8$  Hz, 1H), 4.40 (bs, 1H), 4.00 (s, 2H), 1.70 (s, 3H), 1.65 (d, 2H), 1.21 (s, 6H), 1.16 (s, 6H).  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 134.86, 121.34, 83.24, 69.20, 24.74, 18.61, 13.62

$^{11}\text{B}$  NMR (128.52 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 33.41

**Borylation of 3,4-aziridine-1-cyclohexene (10):** The phosphine  $\text{PCy}_3$  (9.54 mg, 10 mol%), sodium methoxide (33.4 mg, 0.6 mmol) and bis(pinacolato)diboron (114 mg, 0.45mmol) were transferred into an oven-dried Schlenk tube under argon. THF (3 mL) was added. The mixture was stirred for 10 minutes at room temperature to dissolve the phosphine and the borane reagent completely. The substrate (0.3 mmol) and MeOH (100  $\mu\text{l}$ , 2.5 mmol) were added, and the reaction mixture was stirred at 50°C for 20 hours. The reaction mixture was cooled to room temperature. An aliquot of 0.2 mL was taken from the solution and gently concentrated on a rotary evaporator at RT, and analyzed by  $^1\text{H-NMR}$  to probe that one single product was formed from the substrate. The obtained 1,4-cyclohexenyl tosylaminoboronate (**13**) was purified by flash chromatography using a silica gel column previously treated with triethylamine, and a mixture of petroleum ether and ethyl acetate (7:3) as eluent (R.f.=0.49). The product could be isolated in 80.3 mg (71% yield).



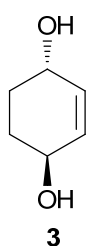
**13**

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 7.77 (d, 2H,  $J = 8.0$  Hz), 7.28 (d, 2H,  $J = 8.0$  Hz), 5.82-5.79 (m, 1H), 5.30-5.26 (dt, 1H,  $J = 9.8, 3.5$  Hz), 4.41 (d, 1H,  $J = 8.0$  Hz), 3.79 (br s, 1H), 2.43 (s, 3H), 1.52-1.90 (m, 5H), 1.20 (s, 12H).  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 143.2, 138.3, 132.4, 129.6, 127.0, 125.4, 83.4, 48.8, 30.1, 25.0, 24.7, 24.6, 21.6, 20.6.  $^{11}\text{B NMR}$  (128.52 MHz,  $\text{CDCl}_3$ )  $\delta$  (ppm) 33.44. Spectral data is in accordance with the literature.<sup>[2]</sup>

**Borylation of 2-methyl-2-vinylaziridine (11) and 3-methyl-2-vinylaziridine (12):** The phosphine  $\text{PCy}_3$  (9.54 mg, 10 mol%), sodium methoxide (33.4 mg, 0.6 mmol) and bis(pinacolato)diboron (114 mg, 0.45mmol) were transferred into an oven-dried Schlenk tube under argon. THF (3 mL) was added. The mixture was stirred for 10 minutes at room temperature to dissolve the phosphine and the borane reagent completely. The substrate mixture (0.3 mmol) and MeOH (100  $\mu\text{l}$ , 2.5 mmol) were added, and the reaction mixture was stirred at 50°C for 20 hours. The reaction mixture was cooled to room temperature. An aliquot of 0.2 mL was taken from the solution and gently concentrated on a rotary evaporator at RT, and analyzed by  $^1\text{H-NMR}$  to probe that one single product was formed from the substrate.

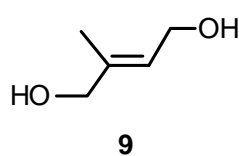
### 3. The oxidation protocol

The allyl boronates obtained in the above described procedure were converted into the corresponding alcohols in the following manner. To the crude organoboron product (cc. 0.3 mmol) in THF (3 mL), sodium perborate (90 mg, 0.9 mmol) and water (3 mL) were added. The reaction mixture was stirred vigorously overnight at room temperature. The reaction mixture was diluted with water and then extracted with dichloromethane (3 x 20mL). The combined organic phase was dried over MgSO<sub>4</sub> and concentrated.



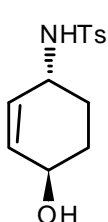
Product **3** was purified by flash chromatography using a silica gel column with ethyl acetate as eluent (R.f.=0.70). The product could be isolated in 32.5 mg (95% yield). Spectral data is in accordance with the literature<sup>[3]</sup>

Product **9** was purified by flash chromatography using a silica gel column with ethyl acetate as eluent (R.f.=0.52). The product could be isolated in 26.7 mg (87% yield).



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ (ppm) 5.70-5.65 (tq, 1H, J= 6.8, 1.6 Hz), 4.24-4.22 (d, 2 H, J= 6.8 Hz), 4.01 (s, 2 H), 1.71 (s, 3 H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ (ppm) 138.87, 124.14, 68.41, 59.47, 30.14.

Product **14** was purified by flash chromatography using a silica gel column with ethyl acetate as eluent (R.f.=0.75). The product could be isolated in 72.2 mg (90% yield).



<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ (ppm) 7.76 (d, 2H, J = 8.0 Hz), 7.31 (d, 2H, J = 8.0 Hz), 5.78-5.74 (d, 1H J = 10 Hz), 5.45-5.43 (d, 1H J = 10 Hz), 4.48 (d, 1H), 4.18 (m, 1H), 3.88-3.84 (m, 1H), 2.44 (s, 3H), 2.04-1.95 (m, 3H), 1.35-1.50 (m, 2H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ (ppm) 143.5, 138.1, 134.1, 129.9, 126.9, 65.6, 49.6, 30.7, 28.7, 21.6.

Spectral data is in accordance with the literature<sup>[2]</sup>

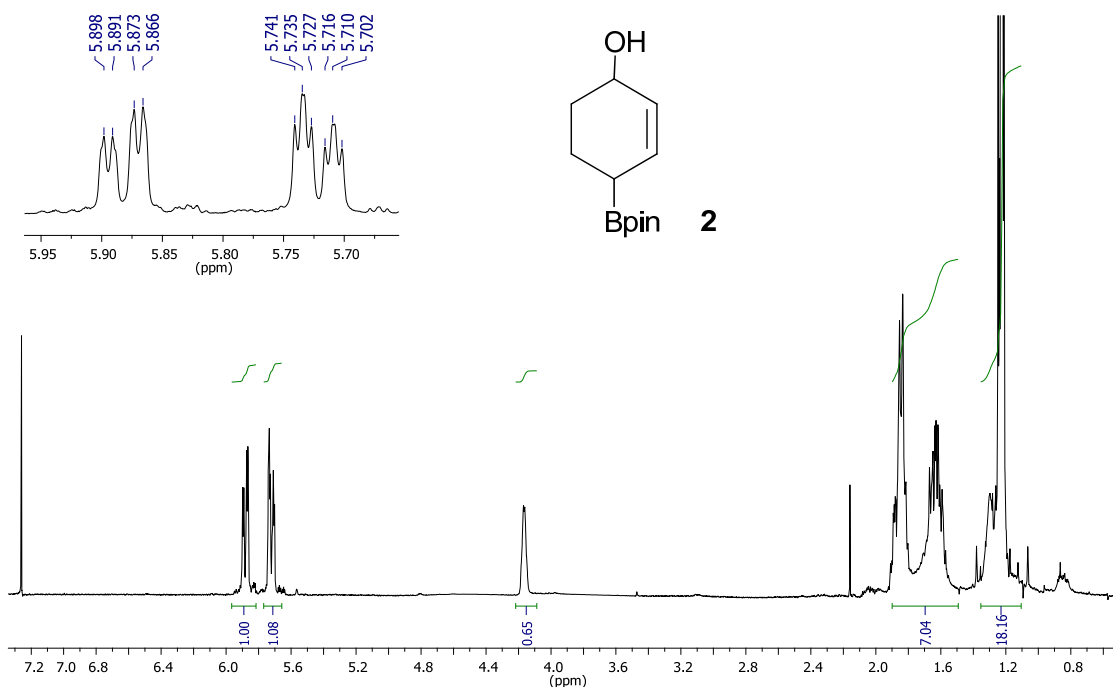
Products **15/16** were purified as a mixture of diols by flash chromatography using a silica gel column with ethyl acetate as eluent (R.f.=0.56). The product could be isolated in 30.6 mg (40% yield).

#### 4. Allylation reaction of allyl boronates with benzaldehyde

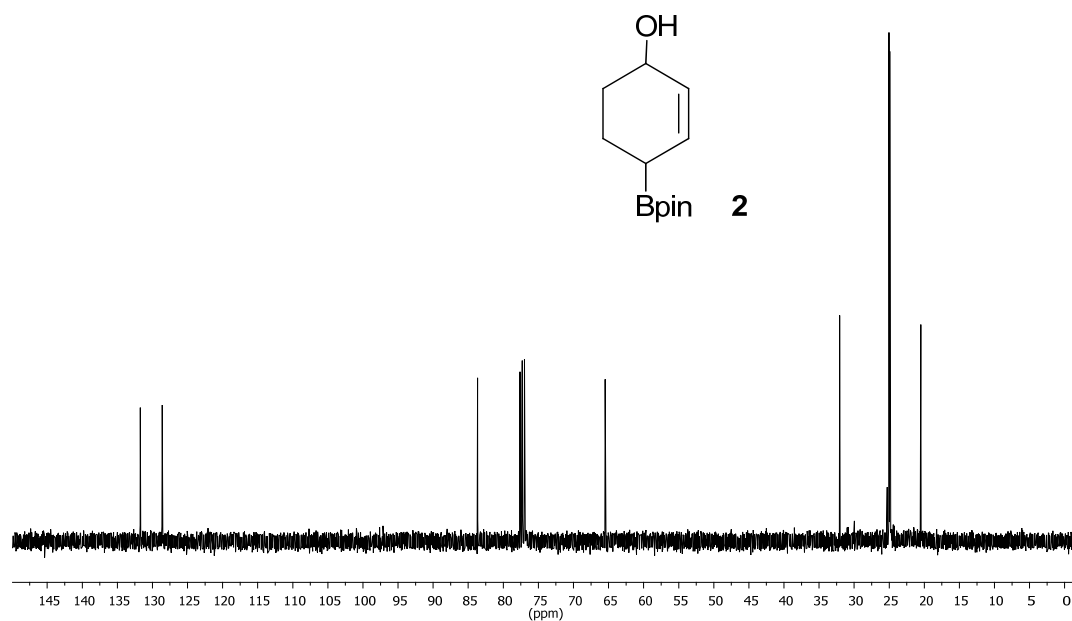
The allyl boronates **2** and **5** obtained in the organocatalytic and copper mediated borylation, respectively, were derivatized with benzaldehyde. To the crude organoboron product (cc. 0.3 mmol) in THF (3 mL), benzaldehyde (100  $\mu$ L, 0.9 mmol) was added. The reaction mixture was stirred vigorously overnight at room temperature. Product **4** was purified by flash chromatography using a silica gel column with ethyl acetate as eluent (R.f.=0.80). The product could be isolated in 56.4 mg (92% yield). Product **6** was purified by flash chromatography using a silica gel column and a mixture of petroleum ether and ethyl acetate (7:3) as eluent (R.f.=0.49). The product could be isolated in 38.6 mg (63% yield). Spectral data for **4** is in accordance with the literature<sup>[2]</sup> Spectral data for **6** is in accordance with the literature<sup>[3]</sup>.

#### 5. NMR spectra

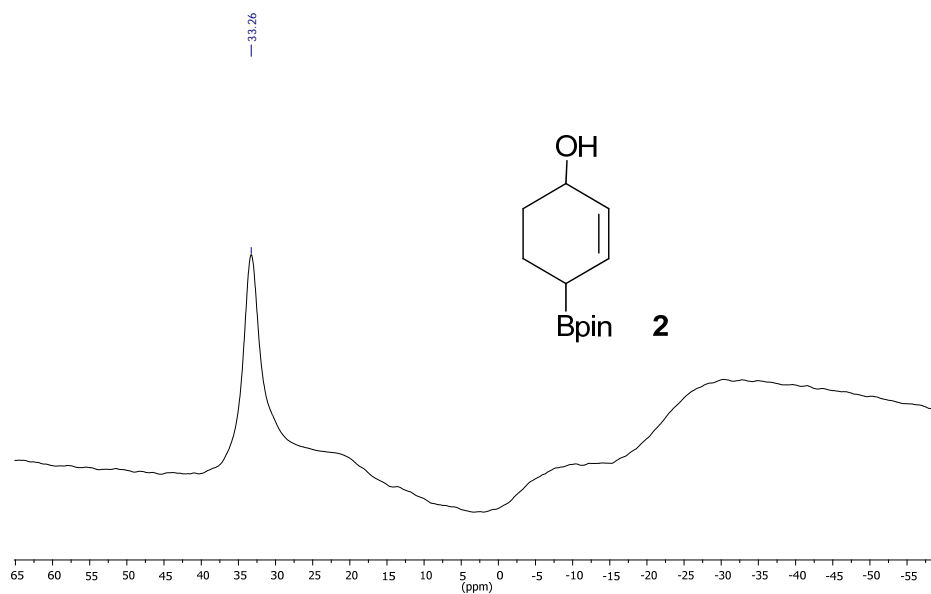
##### <sup>1</sup>H NMR spectra of 1,4-cyclohexenyl hydroxyboronate (**2**) in CDCl<sub>3</sub>



$^{13}\text{C}$  NMR spectra of 1,4-cyclohexenyl hydroxyboronate (**2**) in  $\text{CDCl}_3$

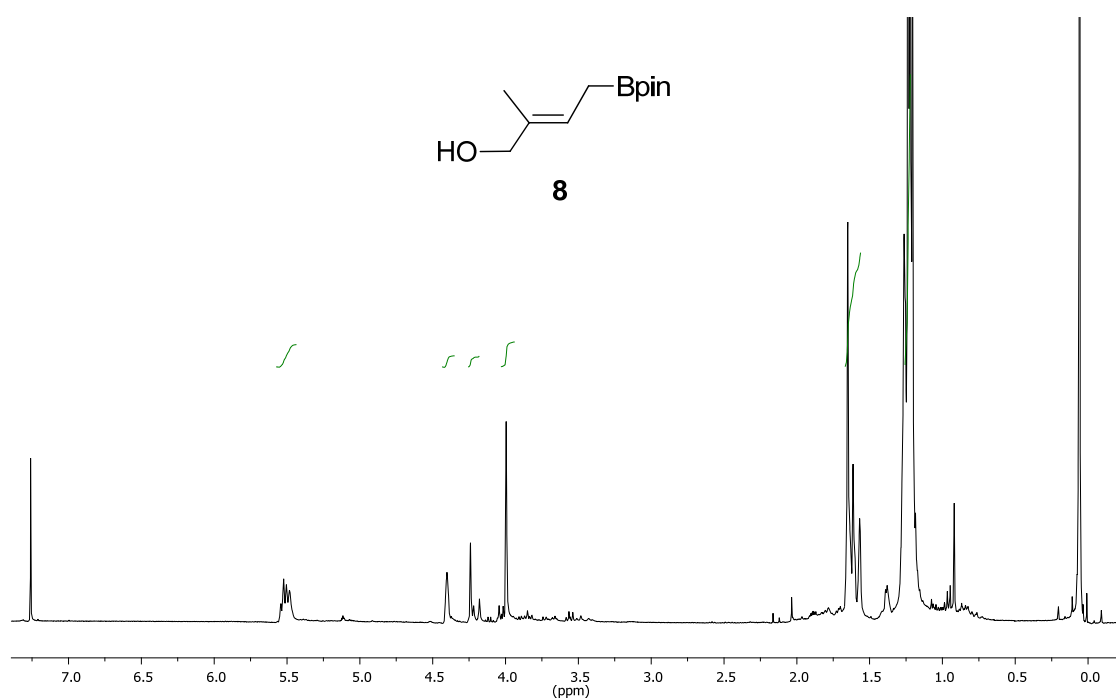


$^{11}\text{B}$  NMR spectra of 1,4-cyclohexenyl hydroxyboronate (**2**) in  $\text{CDCl}_3$

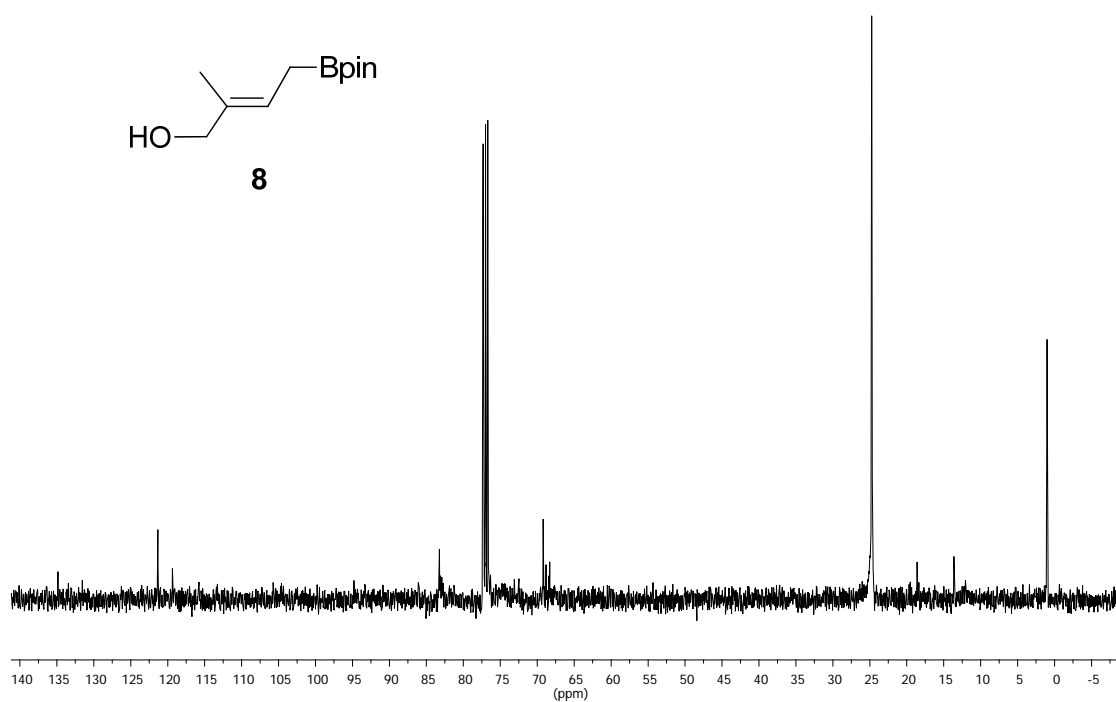




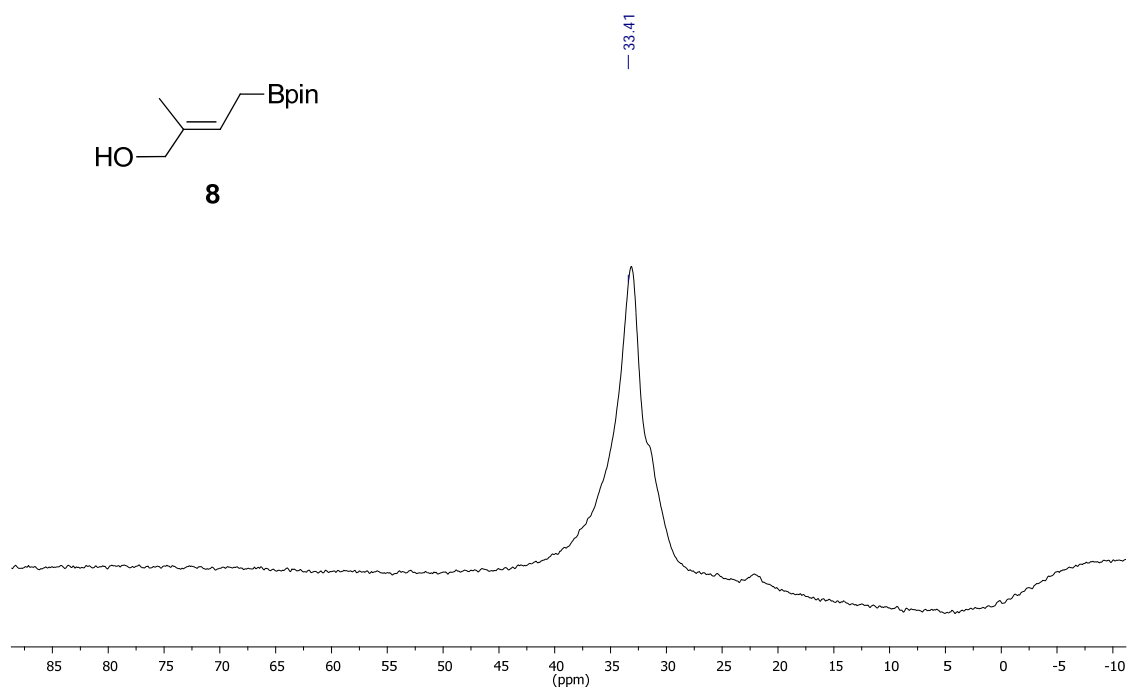
**<sup>1</sup>H NMR spectra of 2-methyl-4-pinacolboryl-butenol (8) in CDCl<sub>3</sub>**



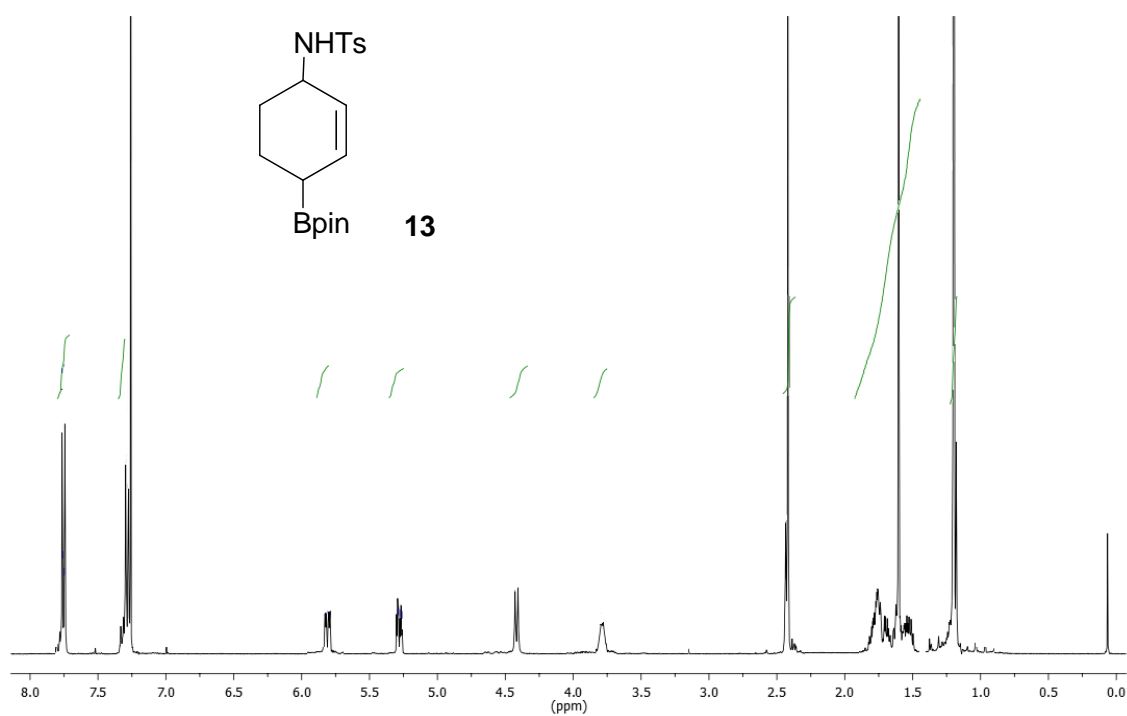
**<sup>13</sup>C NMR spectra of 2-methyl-4-pinacolboryl-butenol (8) in CDCl<sub>3</sub>**



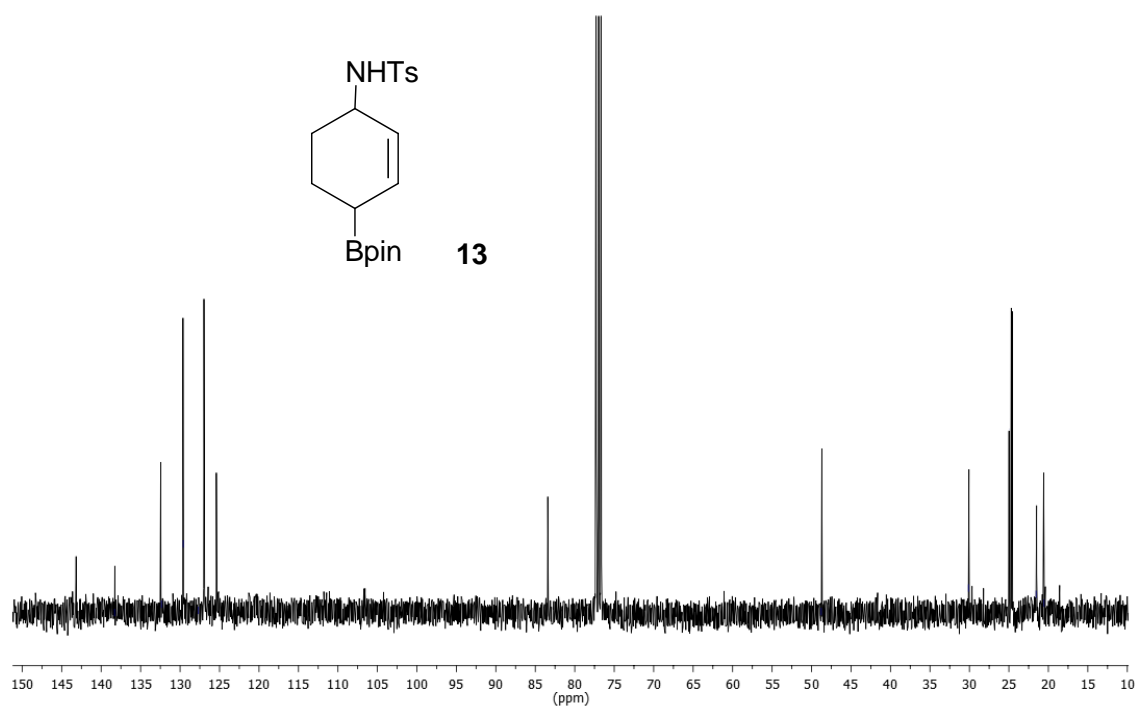
**$^{11}\text{B}$  NMR spectra of 2-methyl-4-pinacolboryl-butenol (**8**) in  $\text{CDCl}_3$**



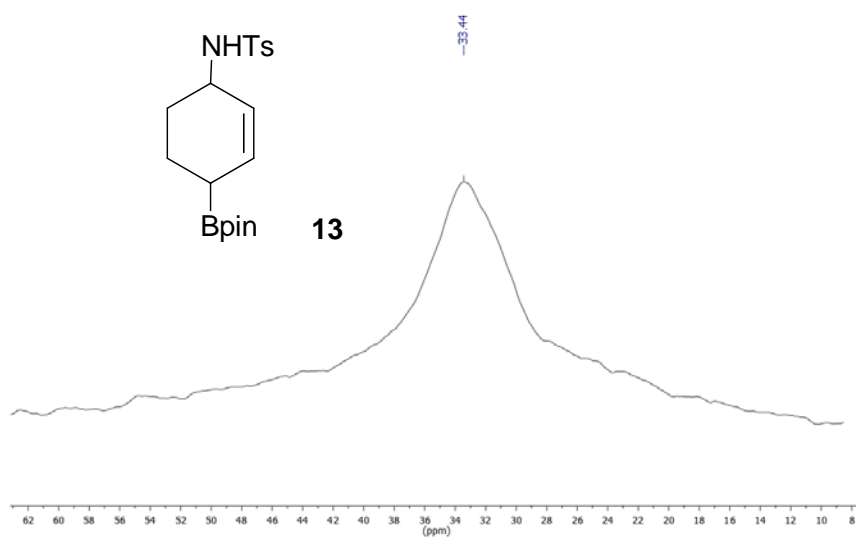
**$^1\text{H}$  NMR spectra of 1,4-cyclohexenyl tosylaminoboronate (**13**) in  $\text{CDCl}_3$**



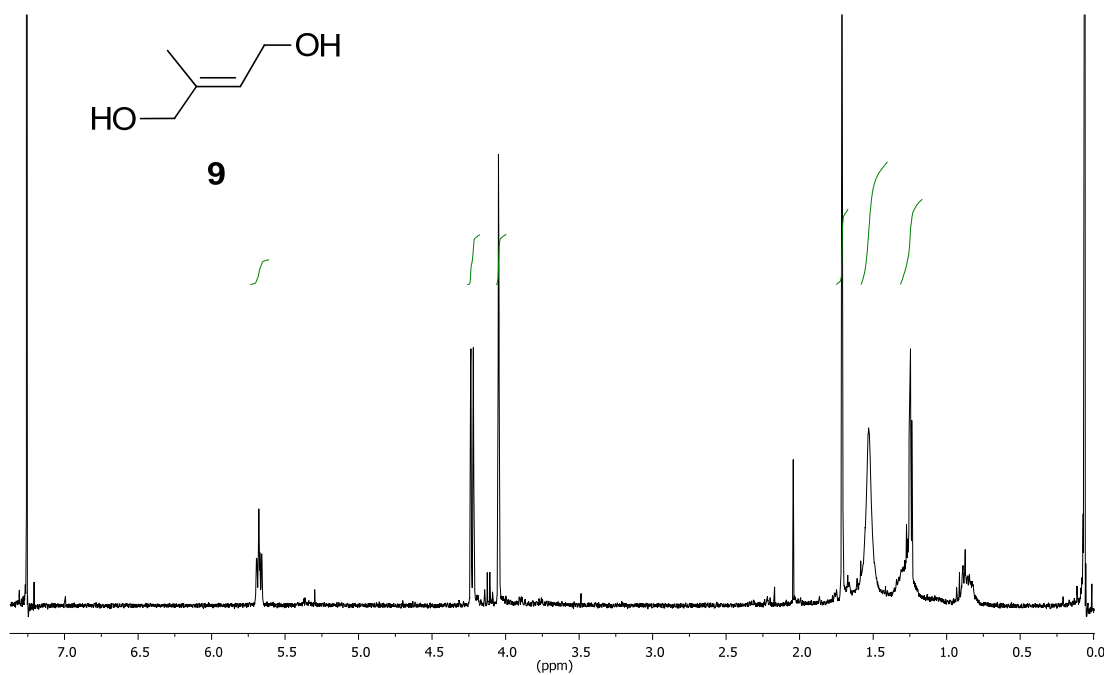
$^{13}\text{C}$  NMR spectra of 1,4-cyclohexenyl tosylaminoboronate (**13**) in  $\text{CDCl}_3$



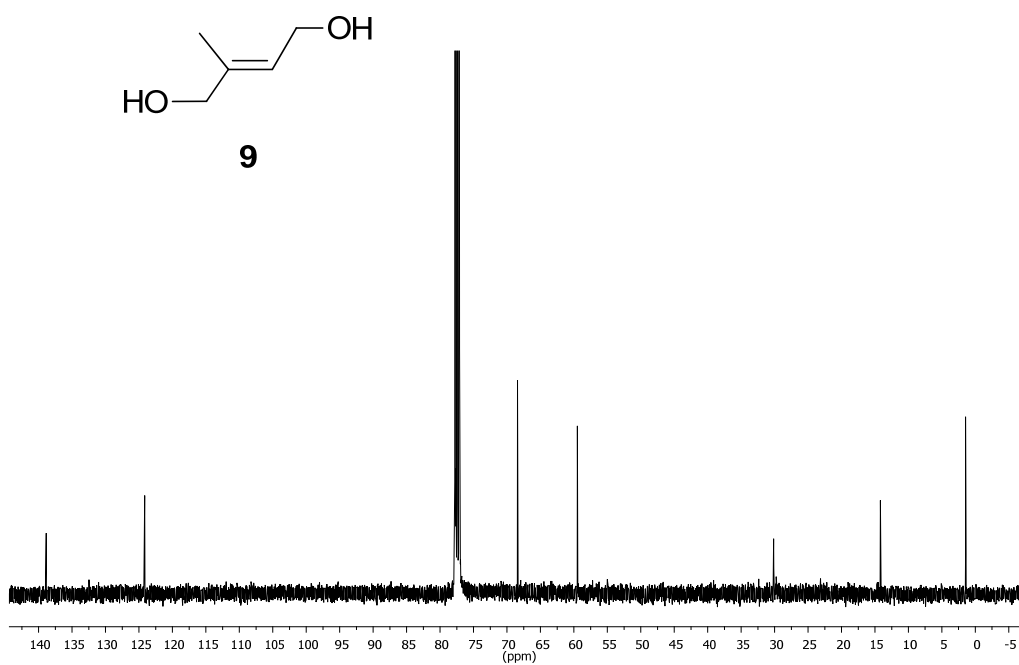
$^{11}\text{B}$  NMR spectra of 1,4-cyclohexenyl tosylaminoboronate (**13**) in  $\text{CDCl}_3$



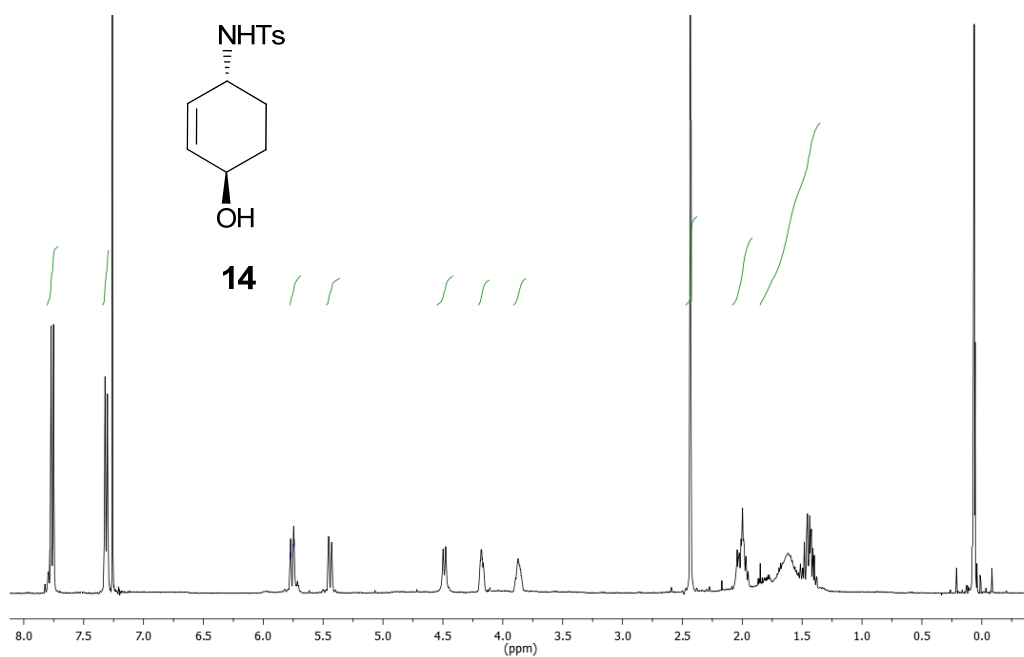
<sup>1</sup>H NMR spectra of 2-methyl-1,4-butendiol (**9**) in CDCl<sub>3</sub>



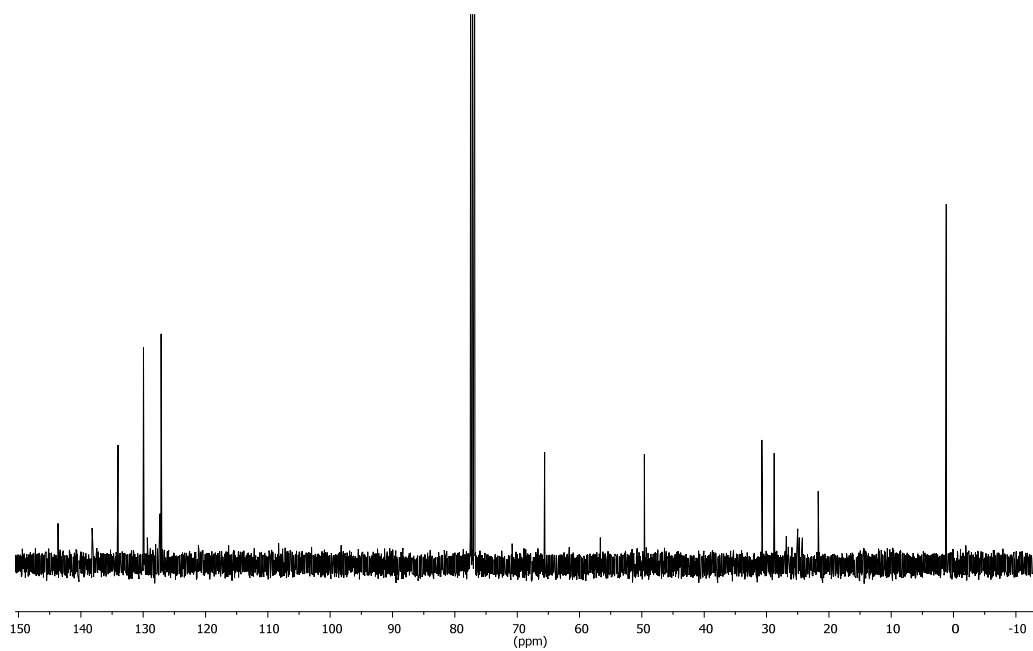
<sup>13</sup>C NMR spectra of 2-methyl-1,4-butendiol (**9**) in CDCl<sub>3</sub>



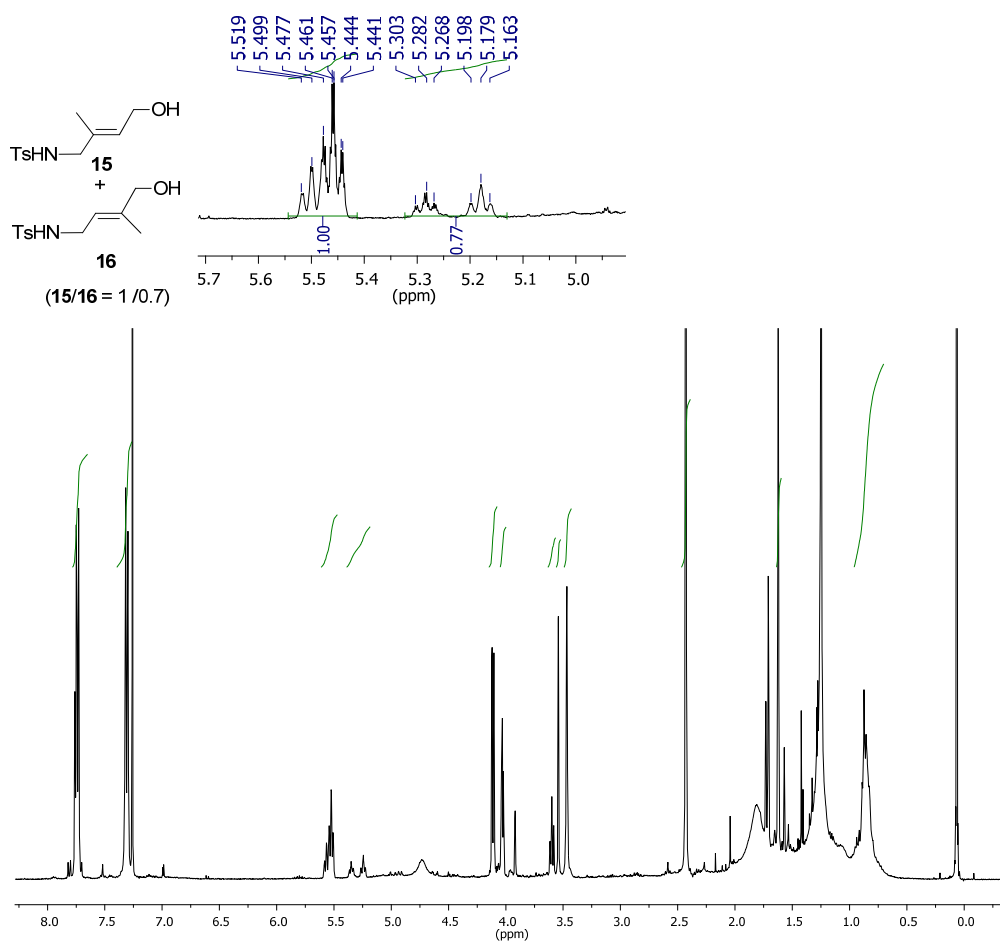
**<sup>1</sup>H NMR spectra of 1,4-cyclohexenyl tosylaminoalcohol (14) in CDCl<sub>3</sub>**



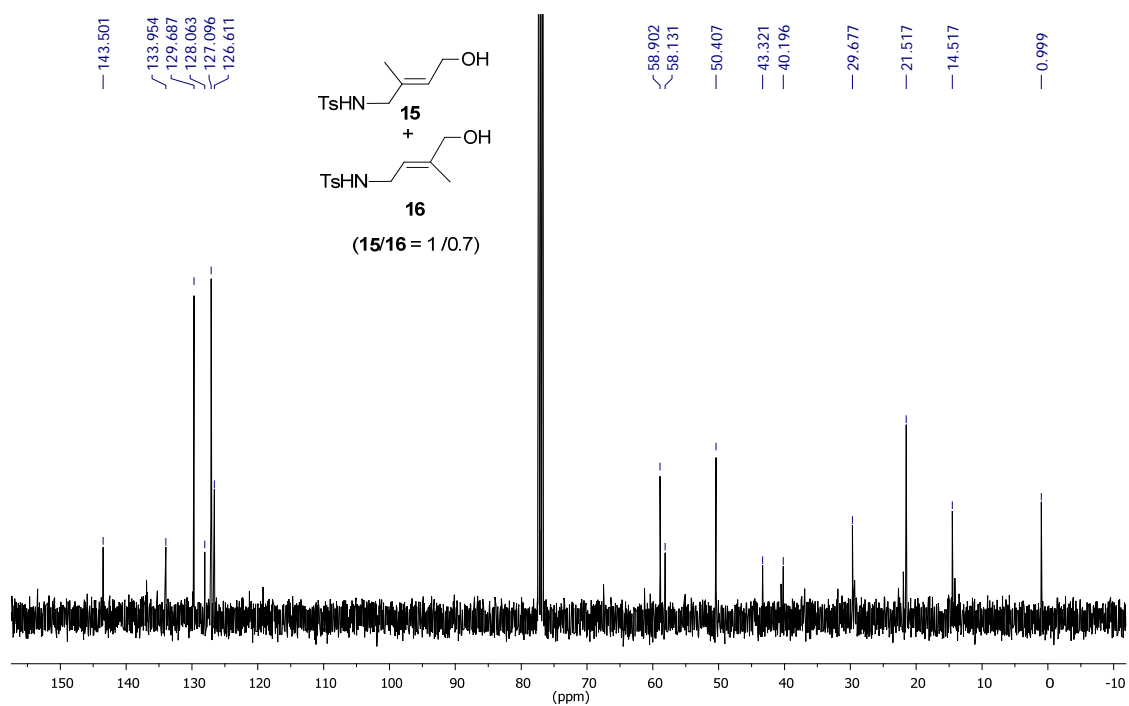
**<sup>13</sup>C NMR spectra of 1,4-cyclohexenyl tosylaminoalcohol (14) in CDCl<sub>3</sub>**



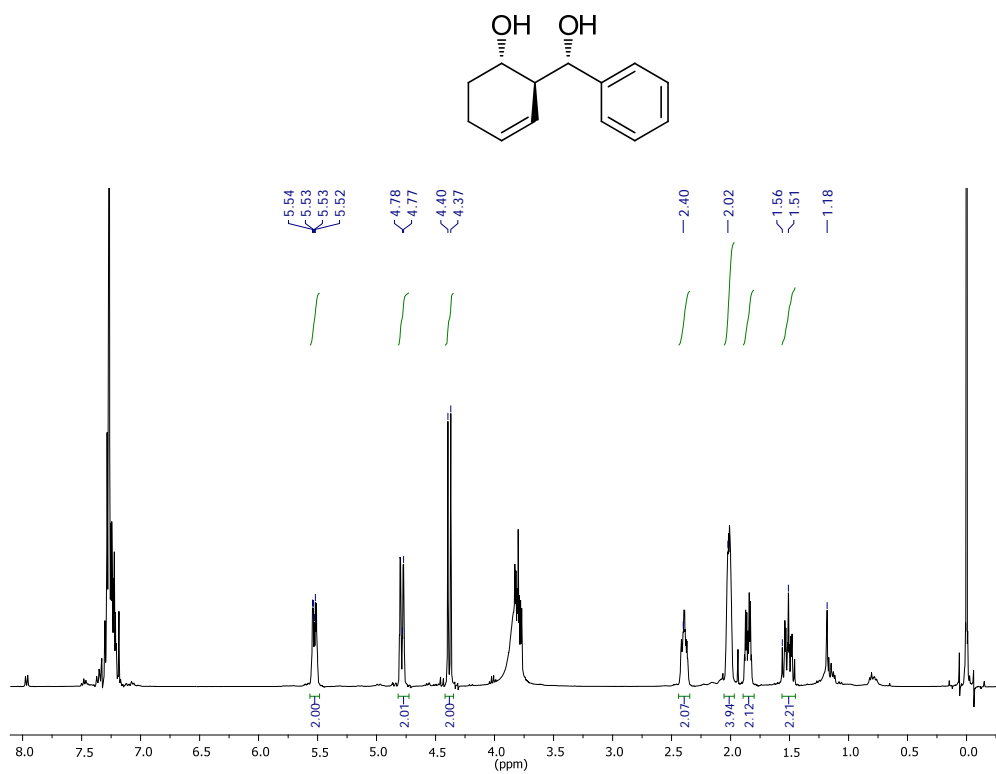
### <sup>1</sup>H NMR spectra of mixture 15/16 in CDCl<sub>3</sub>



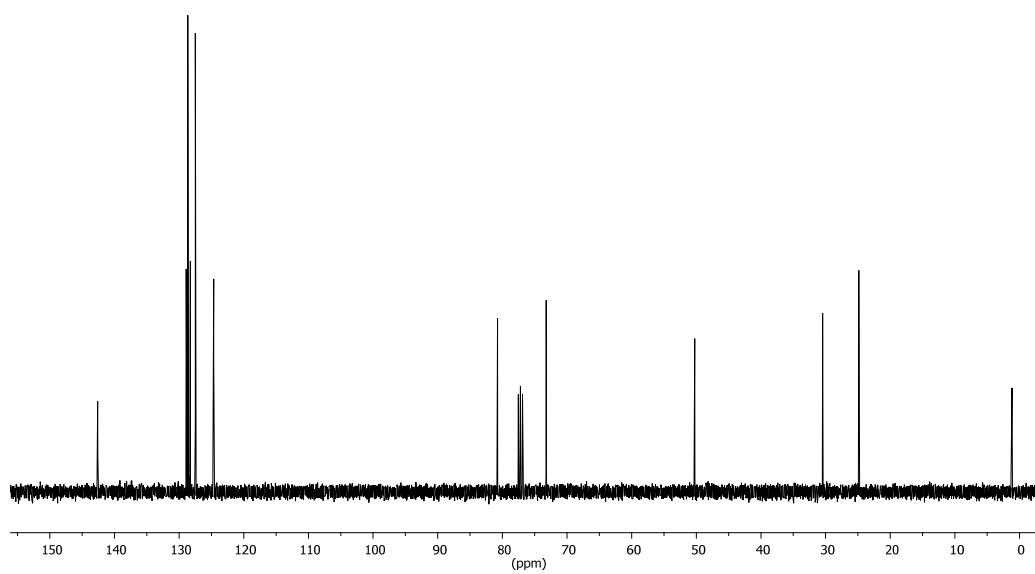
### <sup>13</sup>C NMR spectra of mixture 15/16 in CDCl<sub>3</sub>



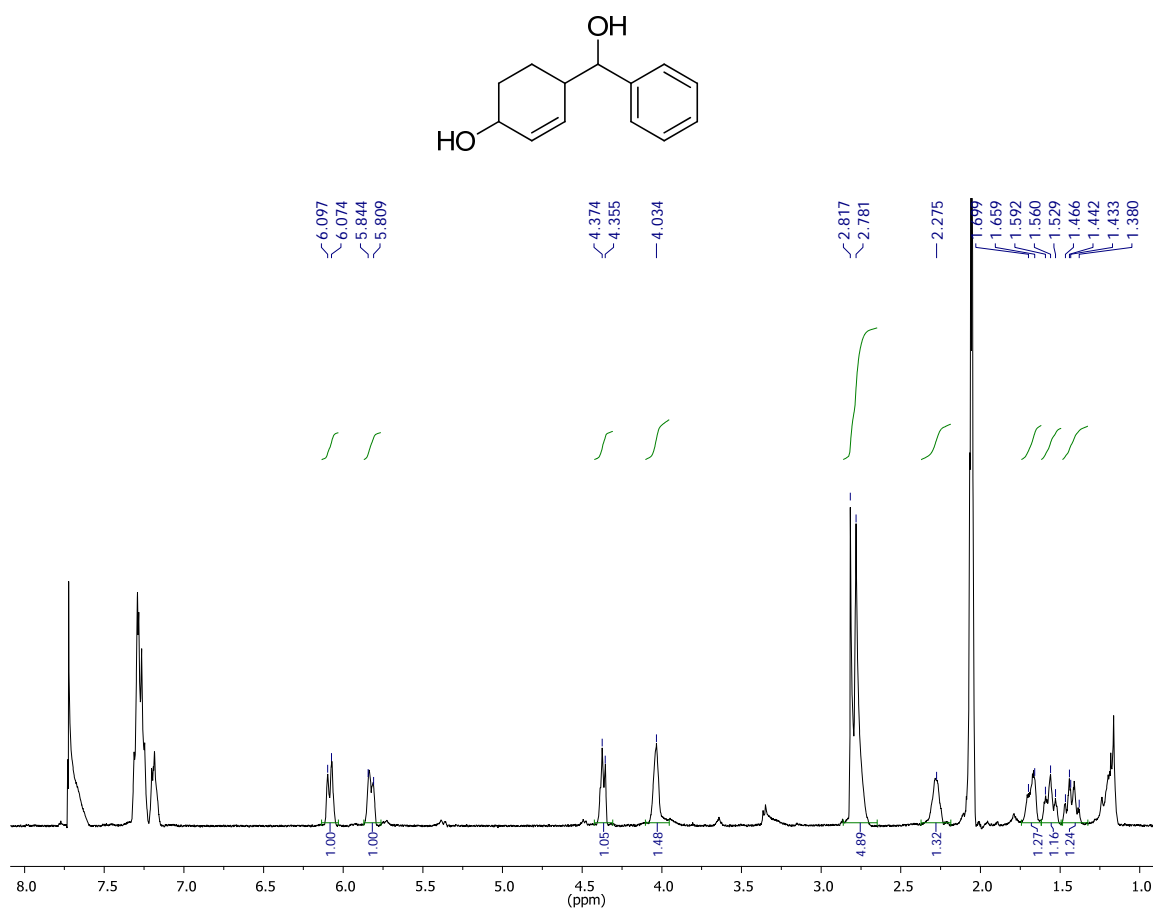
**<sup>1</sup>H NMR spectra of 2-(hydroxybenzyl)-cyclohex-3-enol (4) in CDCl<sub>3</sub>**



**<sup>13</sup>C NMR spectra of 2-(hydroxybenzyl)-cyclohex-3-enol (4) in CDCl<sub>3</sub>**



<sup>1</sup>H NMR spectra of 4-hydroxy-cyclohex-2-enyl-phenyl-methanol (6) in CDCl<sub>3</sub>





## 6. Data of crystal and structure refinement for 2-(hydroxy(phenyl)methyl)cyclohex-3-enol (6)

The data at the Cambridge Crystallographic Data Centre have been assigned the following deposition numbers.

CCDC 947875

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Summary of Data CCDC 947875  
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Compound Name:

Formula: C<sub>13</sub> H<sub>16</sub> O<sub>2</sub>

Unit Cell Parameters: a 9.1921(13) b 14.0304(18) c 9.0659(13) P21/c  
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Table 1. Crystal data and structure refinement for mo\_GL60\_BA\_P21c.

Identification code	mo_GL60_BA_P21c	
Empirical formula	C <sub>13</sub> H <sub>16</sub> O <sub>2</sub>	
Formula weight	204.26	
Temperature	101(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.1921(13) Å	α = 90.00 °.
	b = 14.0304(18) Å	β = 114.463(4) °.
	c = 9.0659(13) Å	γ = 90.00 °.
Volume	1064.3(3) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.275 Mg/m <sup>3</sup>	
Absorption coefficient	0.084 mm <sup>-1</sup>	

F(000)	440
Crystal size	0.12 x 0.05 x 0.01 mm <sup>3</sup>
Theta range for data collection	2.43 to 28.36 °.
Index ranges	-12 ≤h≤10 , -12 ≤k≤18 , -11 ≤l≤12
Reflections collected	2654
Independent reflections	2033 [R(int) = 0.0359 ]
Completeness to theta =28.36 °	0.996 %
Absorption correction	Empirical
Max. and min. transmission	0.9992 and 0.9899
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	2654 / 0 / 138
Goodness-of-fit on F <sup>2</sup>	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0432 , wR2 = 0.1009
R indices (all data)	R1 = 0.0627 , wR2 = 0.1105
Largest diff. peak and hole	0.401 and -0.227 e.Å <sup>-3</sup>

Table 2. Bond lengths [Å] and angles [°] for mo\_GL60\_BA\_P21c.

Bond lengths----

C1-O1	1.4342(15)
C1-C2	1.5146(18)
C1-C8	1.5441(17)
C2-C7	1.390(2)
C2-C3	1.3929(19)
C3-C4	1.3899(19)
C4-C5	1.383(2)
C5-C6	1.385(2)
C6-C7	1.393(2)
C8-C9	1.5125(18)
C8-C13	1.5308(18)
C9-C10	1.326(2)

C10-C11	1.5033(19)
C11-O2	1.4361(16)
C11-C12	1.5190(18)
C12-C13	1.5177(19)
Angles-----	
O1-C1-C2	111.09(11)
O1-C1-C8	106.19(10)
C2-C1-C8	113.83(10)
C7-C2-C3	118.60(12)
C7-C2-C1	121.23(12)
C3-C2-C1	120.16(12)
C4-C3-C2	120.83(13)
C5-C4-C3	120.21(13)
C4-C5-C6	119.43(13)
C5-C6-C7	120.50(14)
C2-C7-C6	120.41(13)
C9-C8-C13	110.03(11)
C9-C8-C1	109.27(10)
C13-C8-C1	112.94(10)
C10-C9-C8	123.38(12)
C9-C10-C11	124.24(12)
O2-C11-C10	110.53(11)
O2-C11-C12	108.49(10)
C10-C11-C12	111.60(11)
C13-C12-C11	110.13(11)
C12-C13-C8	112.15(11)

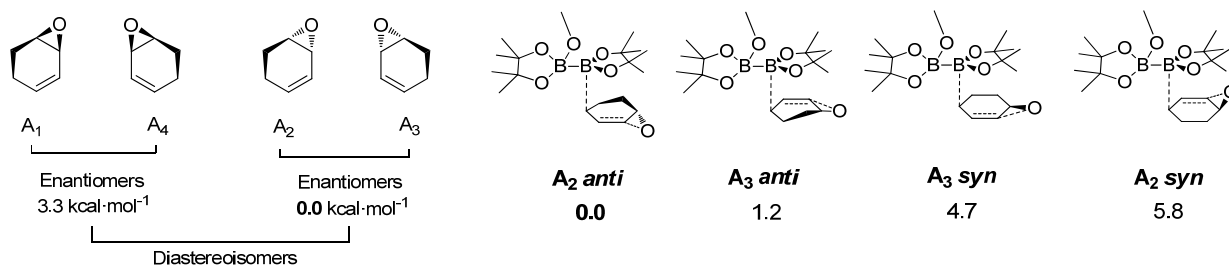
## 7. Computational details

Molecular structures for all species were optimized without constraints using DFT-based methods as implemented in the Amsterdam Density Functional (ADF v2009.01) package.<sup>[4,5]</sup> A triple- $\xi$  plus polarization Slater basis set was used on all atoms. Relativistic corrections were introduced by scalar-relativistic zero-order regular approximation (ZORA).<sup>[6]</sup> For geometry optimizations we used the local VWN correlation potential<sup>[7]</sup> together with the Becke exchange and the Perdew correlation<sup>[8-10]</sup> (BP86) generalized gradient (GGA) corrections. Stationary points in the potential energy hypersurface were characterized either as minima or transition states by means of harmonic vibrational frequency calculations. Solvent effects were introduced by using the continuous solvent model COSMO.<sup>[11]</sup> Single-point energy evaluations at the meta-hybrid M06<sup>[12]</sup> level were performed self-consistently.

## 8. Computed data for the involved species in the conjugate attack

Relative energy barriers for the substrates in different conformations, considering the transition states that come from the most stable species and the addition in *syn* or *anti* in relation to the epoxy/aziridine group. In the figures, the shown energies are in kcal/mol and computed at BP86 level.

### Substrate 1



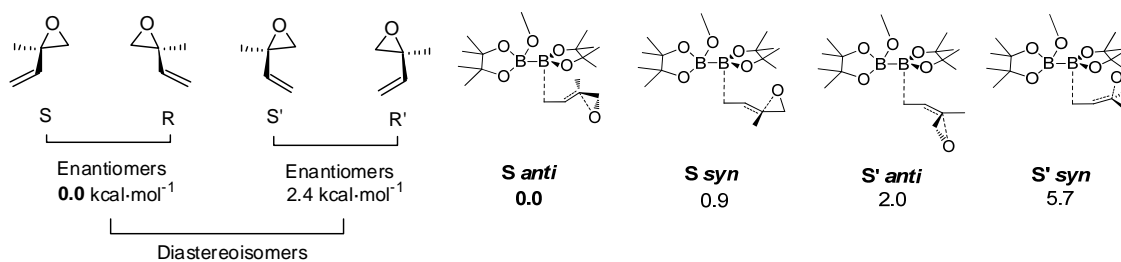
### Transition State

Substrate	BP86				M06			
	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$
$A_2 \text{ anti}$	21.9	35.7	49.8	47.1	20.4	34.2	48.3	34.5
$A_3 \text{ anti}$	23.1	36.1	43.9	43.5	20.4	33.4	41.2	28.2
$A_2 \text{ syn}$	27.7	40.0	52.0	49.3	27.9	40.1	52.2	39.9
$A_3 \text{ syn}$	26.5	40.1	54.4	51.2	25.4	39.0	53.3	39.7

### Intermediate

Substrate	BP86				M06			
	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$
$A_2 \text{ anti}$	-28.7	-29.4	-48.4	-44.3	-30.8	-31.4	-50.4	-49.8
$A_3 \text{ anti}$	-28.7	-29.4	-48.4	-44.3	-30.8	-31.4	-50.4	-49.8
$A_2 \text{ syn}$	-27.8	-28.9	-47.9	-46.8	-30.6	-31.8	-50.8	-49.7
$A_3 \text{ syn}$	-27.8	-28.9	-47.9	-46.8	-30.6	-31.8	-50.8	-49.7

**Substrate 7**



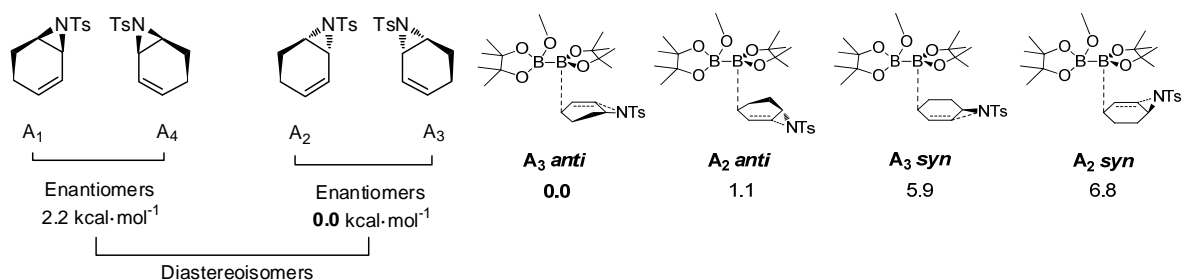
**Transition State**

Substrate	BP86				M06			
	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$
S anti	17.3	31.0	43.2	41.1	16.1	29.8	42.0	28.3
S' anti	19.3	32.8	44.7	39.3	16.1	29.6	41.5	28.0
S syn	18.2	30.7	42.7	40.2	23.0	35.5	47.5	35.0
S' syn	23.0	36.6	48.3	42.5	23.0	36.6	48.4	34.8

**Intermediate**

Substrate	BP86				M06			
	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$
S anti	-30.3	-31.5	-54.0	-50.1	-30.7	-31.9	-54.5	-53.3
S' anti	-29.4	-29.4	-50.9	-50.3	-31.1	-31.1	-52.6	-52.6
S syn	-30.3	-31.5	-54.0	-52.8	-30.7	-31.9	-54.5	-53.3
S' syn	-29.4	-29.4	-50.9	-50.3	-31.1	-31.1	-52.6	-52.6

**Substrate 10**



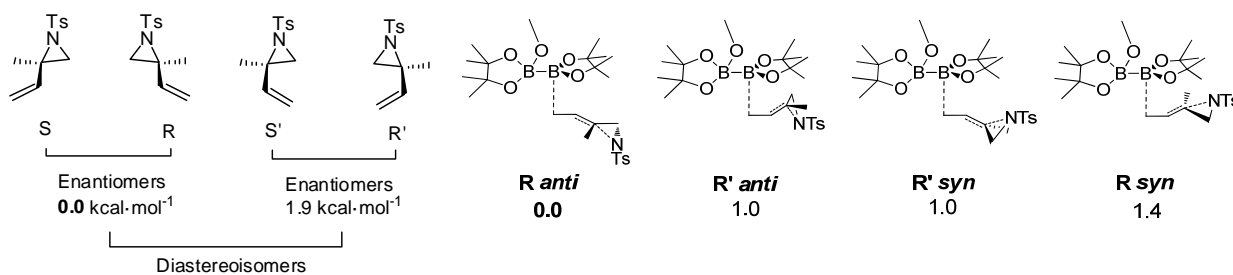
**Transition State**

Substrate	BP86				M06			
	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$
$A_2 \text{ anti}$	13.3	29.0	41.9	41.1	12.2	27.9	40.7	25.0
$A_3 \text{ anti}$	11.2	26.7	39.0	38.2	11.6	27.1	39.4	23.9
$A_2 \text{ syn}$	17.3	33.0	48.1	46.4	18.9	34.6	49.7	34.1
$A_3 \text{ syn}$	18.0	35.6	50.8	47.2	17.7	35.3	50.4	32.8

**Intermediate**

Substrate	BP86				M06			
	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$
$A_2 \text{ anti}$	-56.5	-54.4	-59.2	-56.9	-61.0	-58.9	-63.7	-65.8
$A_3 \text{ anti}$	-56.5	-54.4	-59.2	-56.9	-61.0	-58.9	-63.7	-65.8
$A_2 \text{ syn}$	-50.6	-47.6	-50.7	-53.7	-55.2	-52.2	-49.2	-58.3
$A_3 \text{ syn}$	-50.6	-47.6	-50.7	-53.7	-55.2	-52.2	-49.2	-58.3

### Substrate 11



### Transition State

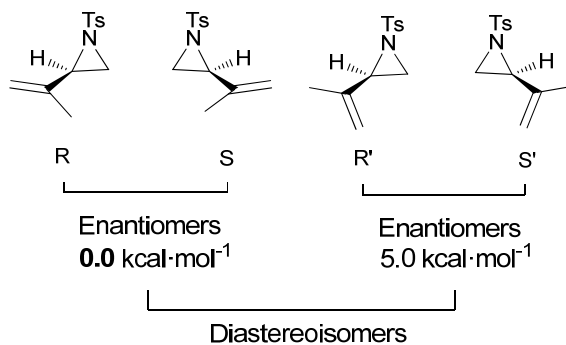
Substrate	BP86				M06			
	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$
R' anti	9.9	26.2	29.3	34.1	12.9	29.3	32.4	16.0
R anti	8.9	25.3	36.9	36.2	10.8	27.1	38.8	22.5
R' syn	9.9	26.2	29.3	34.1	15.9	32.3	35.3	19.0
R syn	10.3	24.1	35.8	33.6	14.6	28.4	40.0	26.3

### Intermediate

Substrate	BP86				M06			
	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$
R' anti	-65.1	-62.7	-68.9	-67.3	-65.1	-62.8	-69.0	-71.4
R anti	-59.4	-56.2	-62.9	-60.9	-59.6	-56.4	-63.0	-66.3
R' syn	-65.1	-62.7	-68.9	-67.3	-65.1	-62.8	-69.0	-71.4
R syn	-59.4	-56.2	-62.9	-60.9	-59.6	-56.4	-63.0	-66.3



**Substrate 12**



**Transition State**

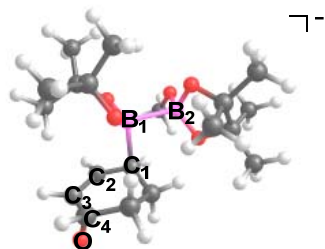
Substrate	BP86				M06			
	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$
R' anti	10.2	27.0	38.4	38.0	14.3	31.0	42.4	25.6
R anti	12.7	29.4	40.7	40.0	17.0	33.7	45.0	28.3
R' syn	12.7	28.0	37.7	38.8	17.8	33.2	42.8	27.5
R syn	16.3	33.1	45.1	44.3	20.6	37.3	49.4	32.6

**Intermediate**

Substrate	BP86				M06			
	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$
R' anti	-64.2	-61.7	-70.2	-67.0	-64.5	-62.0	-70.5	-73.0
R anti	-55.8	-52.0	-60.9	-58.5	-56.5	-52.7	-61.6	-65.4
R' syn	-64.2	-61.7	-70.2	-67.0	-64.5	-62.0	-70.5	-73.0
R syn	-55.8	-52.0	-60.9	-58.5	-56.5	-52.7	-61.6	-65.4

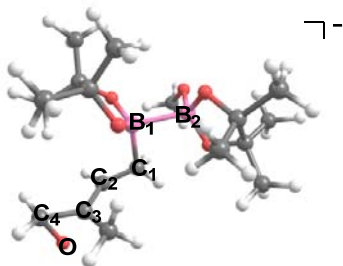
In the left table are shown bond distances (Å) and angles (°) between atoms involved in the reaction for the substrate,  $\text{MeO}^- \rightarrow \text{bis}(\text{pinacolato})\text{diboron}$ , transition state. In the right table is collected the “Voronoi charges” distribution for the atoms involved of the same species of the catalytic cycle.

### Substrate 1



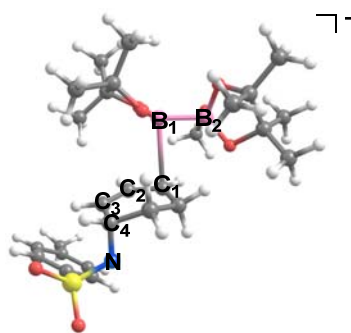
Distances	Substrate	$[\text{B}_2\text{pin}_2 \cdot \text{MeO}]^-$	T.S.	Intermediate	Atoms	Substrate	$[\text{B}_2\text{pin}_2 \cdot \text{MeO}]^-$	T.S.	Intermediate
$d(\text{B}_1\text{-B}_2)$	----	1.755	2.096	----	<b>B<sub>1</sub></b>	----	0.09	0.10	0.21
$d(\text{B}_1\text{-C}_1)$	----	----	1.988	1.577	<b>B<sub>2</sub></b>	----	0.07	0.16	----
$d(\text{C}_1\text{-C}_2)$	1.344	----	1.417	1.521	<b>C<sub>1</sub></b>	-0.05	----	-0.05	-0.15
$d(\text{C}_2\text{-C}_3)$	1.483	----	1.438	1.348	<b>C<sub>2</sub></b>	-0.09	----	-0.14	-0.08
$d(\text{C}_3\text{-C}_4)$	1.480	----	1.476	1.535	<b>C<sub>3</sub></b>	0.00	----	0.01	-0.08
$d(\text{C}_3\text{-O})$	1.475	----	1.624	2.375	<b>C<sub>4</sub></b>	0.00	----	0.00	0.00
$d(\text{C}_4\text{-O})$	1.444	----	1.529	1.351	<b>O</b>	-0.24	----	-0.36	-0.74
$a(\text{C}_3\text{-C}_4\text{-O})$	60.6	----	67.9	110.6					

### Substrate 7



Distances	Substrate	$[\text{B}_2\text{pin}_2 \cdot \text{MeO}]^-$	T.S.	Intermediate	Atoms	Substrate	$[\text{B}_2\text{pin}_2 \cdot \text{MeO}]^-$	T.S.	Intermediate
$d(\text{B}_1\text{-B}_2)$	----	1.755	1.955	----	<b>B<sub>1</sub></b>	----	0.09	0.09	0.20
$d(\text{B}_1\text{-C}_1)$	----	----	2.144	1.561	<b>B<sub>2</sub></b>	----	0.07	0.16	----
$d(\text{C}_1\text{-C}_2)$	1.339	----	1.400	1.527	<b>C<sub>1</sub></b>	-0.05	----	-0.10	-0.18
$d(\text{C}_2\text{-C}_3)$	1.486	----	1.418	1.353	<b>C<sub>2</sub></b>	-0.06	----	-0.15	-0.10
$d(\text{C}_3\text{-C}_4)$	1.485	----	1.477	1.544	<b>C<sub>3</sub></b>	0.03	----	0.04	-0.06
$d(\text{C}_3\text{-O})$	1.472	----	1.865	2.400	<b>C<sub>4</sub></b>	0.02	----	-0.03	0.00
$d(\text{C}_4\text{-O})$	1.438	----	1.396	1.347	<b>O</b>	-0.25	----	-0.33	-0.74
$a(\text{C}_3\text{-C}_4\text{-O})$	60.4	----	80.9	112.1					

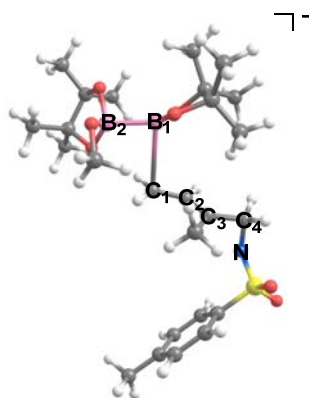
### Substrate 10



Distances	Substrate	[B <sub>2</sub> pin <sub>2</sub> ·MeO] <sup>-</sup>	T.S.	Intermediate
d(B <sub>1</sub> -B <sub>2</sub> )	----	1.755	1.851	----
d(B <sub>1</sub> -C <sub>1</sub> )	----	----	2.853	1.576
d(C <sub>1</sub> -C <sub>2</sub> )	1.343	----	1.384	1.519
d(C <sub>2</sub> -C <sub>3</sub> )	1.483	----	1.399	1.343
d(C <sub>3</sub> -C <sub>4</sub> )	1.495	----	1.485	1.519
d(C <sub>3</sub> -N)	1.516	----	2.118	2.507
d(C <sub>4</sub> -N)	1.490	----	1.418	1.475
a(C <sub>3</sub> -C <sub>4</sub> -N)	61.1	----	91.1	113.7

Atoms	Substrate	[B <sub>2</sub> pin <sub>2</sub> ·MeO] <sup>-</sup>	T.S.	Intermediate
B <sub>1</sub>	----	0.09	0.09	0.20
B <sub>2</sub>	----	0.07	0.10	----
C <sub>1</sub>	-0.06	----	0.06	-0.15
C <sub>2</sub>	-0.08	----	-0.09	-0.07
C <sub>3</sub>	0.02	----	0.04	-0.08
C <sub>4</sub>	0.04	----	-0.03	-0.01
N	-0.17	----	-0.36	-0.41

### Substrate 11









Distances	Substrate	[B <sub>2</sub> pin <sub>2</sub> ·MeO] <sup>-</sup>	T.S.	Intermediate
d(B <sub>1</sub> -B <sub>2</sub> )	----	1.755	1.857	----
d(B <sub>1</sub> -C <sub>1</sub> )	----	----	2.647	1.570
d(C <sub>1</sub> -C <sub>2</sub> )	1.339	----	1.380	1.522
d(C <sub>2</sub> -C <sub>3</sub> )	1.489	----	1.410	1.349
d(C <sub>3</sub> -C <sub>4</sub> )	1.506	----	1.490	1.529
d(C <sub>3</sub> -N)	1.519	----	2.207	2.478
d(C <sub>4</sub> -N)	1.473	----	1.481	1.458
a(C <sub>3</sub> -C <sub>4</sub> -N)	61.3	----	96.0	112.1






Atoms	Substrate	[B <sub>2</sub> pin <sub>2</sub> ·MeO] <sup>-</sup>	T.S.	Intermediate
B <sub>1</sub>	----	0.09	0.01	0.20
B <sub>2</sub>	----	0.07	0.10	----
C <sub>1</sub>	-0.10	----	0.02	-0.18
C <sub>2</sub>	-0.07	----	-0.09	-0.09
C <sub>3</sub>	0.01	----	0.10	-0.05
C <sub>4</sub>	-0.05	----	-0.04	-0.04
N	-0.18	----	-0.37	-0.43

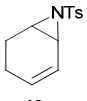
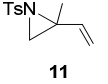
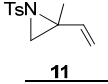
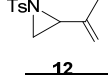
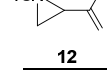
### 9. Computed data for involved species in the direct attack

The next table shows the barriers for the direct addition to the epoxy/aziridine functional groups.

Substrate	Transition State							
	BP86				M06			
	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$
 A <sub>2</sub> anti 4	23.0	36.6	41.7	41.9	21.8	35.4	40.6	27.0
 S anti 7	31.1	45.3	50.2	50.4	29.3	43.4	48.3	34.2
 S' anti 7	33.6	47.5	54.5	50.8	28.5	42.4	49.4	35.5

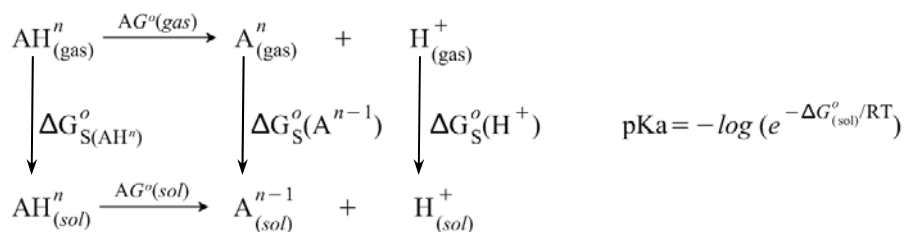
Substrate	Intermediate							
	BP86				M06			
	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$
 A <sub>2</sub> anti 4	-32.3	-33.1	-49.3	-45.7	-34.1	-34.9	-51.1	-50.3
 S anti 7	-27.7	-28.4	-42.9	-39.9	-30.6	-31.3	-45.8	-45.2
 S' anti 7	-26.8	-27.5	-41.5	-41.9	-33.6	-34.3	-48.3	-47.7

Substrate	Transition State							
	BP86				M06			
	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger + \Delta G_{\text{THF}}$	$\Delta E^\ddagger + \Delta G_{\text{THF}}$
 A <sub>2</sub> anti 10	15.5	29.4	39.0	38.9	13.3	27.1	36.7	22.9
 R anti 11	18.3	33.0	42.3	42.5	17.9	32.6	41.9	27.3
 R' anti 11	17.1	32.4	43.3	43.1	16.4	31.7	42.6	27.3
 R anti 12	21.1	37.4	46.5	46.9	20.6	36.8	46.0	29.7
 R' anti 12	17.0	32.1	43.1	42.9	16.4	31.5	42.4	27.4

Substrate	Intermediate							
	BP86				M06			
	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$	$\Delta E$	$\Delta G$	$\Delta G + \Delta G_{\text{THF}}$	$\Delta E + \Delta G_{\text{THF}}$
 <b>10</b> A <sub>2</sub> anti	-56.2	-55.2	-57.9	-56.1	-61.8	-60.8	-63.5	-64.4
 <b>11</b> R anti	-54.5	-53.4	-59.7	-57.2	-59.2	-58.0	-64.3	-65.5
 <b>11</b> R' anti	-61.5	-57.9	-64.5	-62.5	-61.2	-57.6	-64.2	-67.8
 <b>12</b> R anti	-55.9	-53.3	-56.9	-54.8	-60.2	-57.6	-61.1	-63.7
 <b>12</b> R' anti	-60.8	-59.6	-62.8	-60.8	-64.9	-63.7	-66.9	-68.1

## 10. PKa computation details

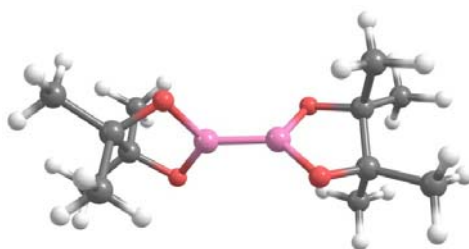
PKa values were obtained based on the Born-Haber cycle using the known solvation energy of the proton ( $\Delta G_{\text{S}}^{\circ}(\text{H}^+) = -265.9 \text{ Kcal} \cdot \text{mol}^{-1}$ ).<sup>[13]</sup>



In this particular case, molecular structures of the intermediates, protonated products were calculated without constraints using Gaussian 09,<sup>[14]</sup> Revision A.02, with the hybrid B3LYP<sup>[15]</sup> functional and 6-31+G(d)<sup>[16]</sup> as a basis set. Solvent effects (dimethylsulphoxide, DMSO) were introduced by using the Polarizable Continuum Model (PCM).<sup>[17]</sup>

## 11. Geometries of the involved species

BISPIN

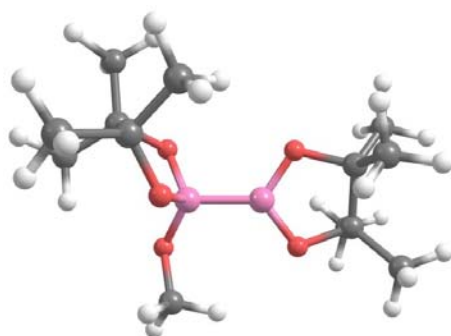


Electronic Energy=-5480.22 kcal/mol

C	-1.980685145	0.549557188	0.478730531
C	-2.518983842	1.369878242	-0.749971365
C	3.041309702	3.933094723	-0.470389308
C	3.416149223	2.742753948	-1.426942132
B	1.263497081	2.484664192	-0.656902419
B	-0.284488374	1.812803190	-0.427120544
O	2.102590954	2.126258702	-1.695164658
O	1.808328805	3.443827668	0.175971848
O	-1.434599222	2.343810088	-0.980105047
O	-0.518363961	0.681157948	0.331305143
C	4.062347767	4.236482741	0.621102665
H	5.016431983	4.564225542	0.180632565
H	3.685235381	5.048209408	1.258643463
H	4.248900014	3.361572920	1.255497887
C	2.655808570	5.215208897	-1.214466066
H	2.216986384	5.921980164	-0.497235213
H	3.531376927	5.690611600	-1.679808172
H	1.908617116	5.011737386	-1.993443329
C	4.031767996	3.150060098	-2.761484117
H	4.997124085	3.655671513	-2.606085832
H	4.211637055	2.252748474	-3.369792630
H	3.370162203	3.818738962	-3.325269894
C	4.267109618	1.662775591	-0.751966369
H	4.312050760	0.784924120	-1.410646917

H	5.293238814	2.013175586	-0.569078194
H	3.825077000	1.349861423	0.203644752
C	-3.808756788	2.144403526	-0.499957490
H	-4.071400308	2.716942718	-1.400389531
H	-4.638991112	1.456080341	-0.279448232
H	-3.703107004	2.848244211	0.334407781
C	-2.631645667	0.542081186	-2.033769931
H	-3.463338264	-0.175222346	-1.979776425
H	-2.812984286	1.221301897	-2.877740851
H	-1.702428465	-0.008767209	-2.232830495
C	-2.333495039	1.175369057	1.831492617
H	-3.403813286	1.067337491	2.059354707
H	-1.758091584	0.667188363	2.617094011
H	-2.073395580	2.242294591	1.854289313
C	-2.327720745	-0.935493053	0.471468668
H	-1.867756448	-1.422342424	1.342657982
H	-3.417017869	-1.080466117	0.535617803
H	-1.958368079	-1.433143504	-0.433309849

BISPIN-OME



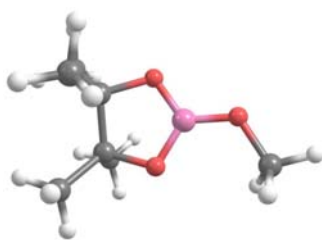
Electronic Energy=-6115.23 kcal/mol

B	-0.862506925	-0.445600549	0.102312124
O	-1.950573999	-1.146444199	-0.463893172
O	-1.297035044	0.842387980	0.480666498
C	-2.622069330	1.075993678	-0.070287271
C	-3.171122471	-0.381558383	-0.243887391
C	-3.820357553	-0.934207501	1.033656088
C	-4.102594297	-0.593317946	-1.437170414
C	-2.432595486	1.809685142	-1.406715576
C	-3.405856097	1.958553008	0.901658450
B	0.790228862	-1.002404323	0.296206800
O	1.645393955	-0.545446923	-0.880476707
O	1.411248687	-0.335200216	1.475694391
C	2.580900170	0.418804520	-0.408674313
C	2.736848514	0.048709085	1.117640518
C	1.980648874	1.829481909	-0.595402032
C	3.870814567	0.303295577	-1.233482530
C	3.692969170	-1.144903451	1.329673493
C	3.167681721	1.211261102	2.022490444
H	-1.851884603	2.724702606	-1.223305591
H	-3.394098692	2.089424881	-1.866363166
H	-3.429363608	1.520524051	1.907472975
H	-4.441281611	2.112558097	0.554829241
H	-3.605093522	-0.337775351	-2.381291822
H	-5.017159707	0.015183551	-1.340679572



H	-3.976090093	-2.014920192	0.907215891
H	-4.792813647	-0.460398567	1.243134280
H	2.687026257	2.633676501	-0.325937228
H	1.705462237	1.947783185	-1.654884883
H	4.655566851	0.982511466	-0.857357210
H	4.253055891	-0.726122342	-1.217448091
H	4.153752360	1.610470819	1.728475092
H	3.239044433	0.855224076	3.062634840
H	3.602296952	-1.473899846	2.375862758
H	3.384900323	-1.981546817	0.690529081
H	-1.864861304	1.186776788	-2.111130439
H	-2.919056236	2.942522774	0.972653546
H	-4.399624909	-1.651543475	-1.485271702
H	-3.156714627	-0.787209357	1.896328514
H	1.069486304	1.927650337	0.008963745
H	3.659549123	0.571515075	-2.281148981
H	2.429314368	2.023887347	1.993629950
H	4.747707233	-0.884478728	1.132090662
O	0.907221393	-2.484317829	0.460359853
C	0.546944576	-3.255816681	-0.661719434
H	0.636219696	-4.327529567	-0.403781047
H	1.204647451	-3.060641575	-1.533677594
H	-0.496344078	-3.070219670	-0.986718071

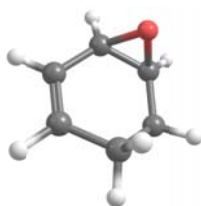
BPIN-OME



Electronic Energy=-3347.68 kcal/mol

C	0.065798618	0.181820185	-0.313269554
C	1.624678614	0.153519552	-0.562367948
B	0.831647485	2.271599590	-0.830691010
O	-0.308888448	1.499846267	-0.873551796
O	1.983438498	1.585793783	-0.501150014
C	-0.307406066	0.215722291	1.172178348
H	-1.382131603	0.441507080	1.261559524
H	-0.113393211	-0.762597232	1.654008561
H	0.254061644	1.000614302	1.710220068
C	-0.725551372	-0.895970176	-1.044747318
H	-0.398739746	-1.904078930	-0.715562255
H	-1.796848713	-0.789535921	-0.807270669
H	-0.601130043	-0.818438453	-2.136898153
C	2.431305226	-0.585898772	0.497497437
H	2.129284482	-1.650566166	0.540877312
H	3.501869798	-0.543586127	0.240816458
H	2.290501554	-0.137474118	1.493639486
C	1.994304550	-0.330659174	-1.968027715
H	3.064209005	-0.138482233	-2.138535544
H	1.810058120	-1.415368798	-2.077958418
H	1.416937560	0.210080866	-2.740809262
O	0.866135753	3.612527675	-1.086280661
C	-0.396273568	4.244901449	-1.383877040
H	-1.098408486	4.135260565	-0.536664142
H	-0.194032748	5.312617175	-1.559778758
H	-0.850262520	3.801199058	-2.289792249

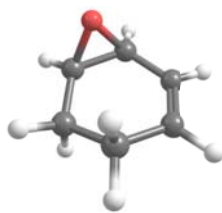
3,4-EPOXY-1-CYCLOHEXENE A<sub>2</sub> (1)



Electronic Energy=-2009.79 kcal/mol

C	-0.517883357	0.617142495	0.285173334
C	0.965401199	0.377249748	0.390343248
C	1.768789029	1.680255429	0.586135086
C	1.132972805	2.616037403	1.589029285
C	-0.339450033	2.594927292	1.739591297
C	-1.119892802	1.637486411	0.919144096
H	2.800183973	1.443294181	0.890005021
H	1.152909217	-0.288755388	1.249172388
H	1.332340387	-0.156629507	-0.499143174
H	-1.114359793	-0.084078742	-0.304383472
H	-2.199925112	1.785438769	0.845967384
H	1.837301200	2.227489613	-0.370568484
O	0.549190021	2.031371574	2.772997610
H	-0.849045677	3.503134351	2.073468162
H	1.659571539	3.561091341	1.770955906

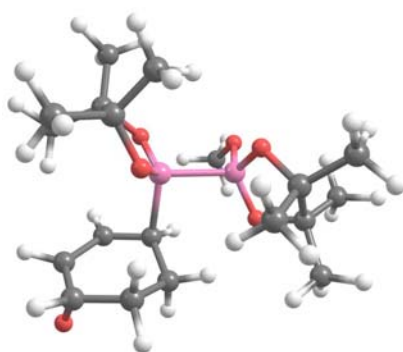
3,4-EPOXY-1-CYCLOHEXENE A<sub>3</sub> (1)



Electronic Energy=-2009.79 kcal/mol

C	-0.506107478	0.772273976	0.307661892
C	0.986883102	0.583139272	0.376457559
C	1.594489283	1.095369150	1.699800314
C	1.031223550	2.432682893	2.125277476
C	-0.357654066	2.769774102	1.738754629
C	-1.123662596	1.790617129	0.929696727
H	1.246669514	-0.476483122	0.233612386
H	1.448874891	1.130070134	-0.462136374
H	-1.088861693	0.069402421	-0.293389846
H	-2.205482529	1.922435216	0.853200173
O	0.799551801	3.417777980	1.096266512
H	2.689960612	1.157529965	1.609956742
H	1.381710212	0.379988992	2.513345163
H	-0.928791516	3.458494917	2.367559965
H	1.425360895	2.848605066	3.060710406

TS ANTI A<sub>2</sub>



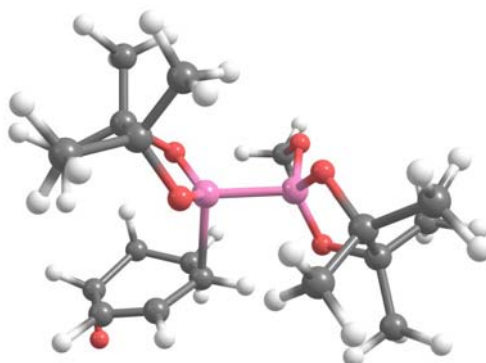
Electronic Energy=-8103.10 kcal/mol

B	-1.113659008	-1.022245065	-0.503360628
B	0.749695959	-0.081795566	-0.310627547
C	0.268855900	1.506376976	-1.404933715
C	1.554387921	2.024085968	-1.702199807
O	1.437258521	4.579690069	-1.051874707
C	2.125899388	3.112398085	-0.956348943
H	2.164918966	1.554745779	-2.476605825
H	-0.244940851	0.997125363	-2.221234225
H	-1.530149095	1.902266566	-0.288927544
C	-0.650751460	2.453753314	-0.637053169
H	-1.006158103	3.204945827	-1.363801188
C	0.037046166	3.191980775	0.522435430
H	0.219392456	2.491227253	1.353544649
H	1.954310560	4.184808799	0.981527831
H	3.203662246	3.287274653	-1.005125801
H	4.223625087	-0.373945510	-1.538142527
C	3.958611409	-0.084809950	-0.510016795
H	4.868737839	-0.124737989	0.108866974
H	3.585582178	0.947174424	-0.534472778
C	2.872708684	-1.039090494	0.004532600
C	2.267851109	-0.602780492	1.394990510
C	3.214315331	0.211117009	2.282448757
H	2.692623940	0.487200193	3.211103814
H	3.536258327	1.134735868	1.784618627

H	4.106834000	-0.376095486	2.555521098
H	4.226622424	-2.629216060	0.656656356
H	3.765565797	-2.689266117	-1.064221125
H	2.596879289	-3.198326729	0.175318907
H	0.962532511	-2.337926477	1.598034840
C	1.696639364	-1.783670239	2.195014879
H	2.491050580	-2.464776896	2.540344173
H	1.170280351	-1.388138351	3.075467570
O	1.150555934	0.242987621	1.016128791
H	-1.418856688	-0.084852312	2.993936434
O	-1.378995459	-1.567192783	0.818221940
C	-2.106036225	0.279149837	2.217614253
H	-2.685737851	-2.168710066	3.108255447
C	-3.299302403	-1.918752830	2.229408455
H	-3.506662781	-2.848034187	1.683641594
H	-4.251215105	-1.492972521	2.588584863
O	-0.817871438	-2.091078021	-1.425087745
C	-0.597617289	-1.758486446	-2.781404662
H	-0.658819465	-2.685126048	-3.376034764
H	-1.358628781	-1.051307245	-3.160299380
H	0.403700873	-1.319498722	-2.927832573
O	-2.231641634	-0.146435586	-0.851604401
C	-4.216390440	0.748016489	0.200757960
H	-4.670434655	0.990830890	-0.772303892
H	-3.651762763	1.626207818	0.538955346
H	-5.029423708	0.551609101	0.919117305
C	-4.107304810	-1.638916403	-0.572269968
H	-3.461132400	-2.519120141	-0.686887580
H	-4.988921617	-1.908792050	0.031995633
H	-4.449799832	-1.332687541	-1.571587421
H	-1.562157451	1.017823626	1.619603294
H	-2.964266640	0.767798627	2.707005647
C	-3.308904180	-0.475151579	0.045712857

C	-2.542595495	-0.914028931	1.352006679
C	3.393632204	-2.478885564	-0.049947879
C	1.381359495	3.777656615	0.130034302
H	-0.618616405	3.997256148	0.900277815
O	1.729451099	-0.944832520	-0.880618628

TS ANTI A<sub>3</sub>



Electronic Energy=-8101.96 kcal/mol

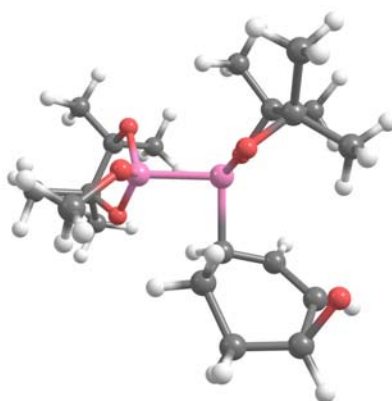
B	0.777820684	-0.325632822	-0.268072459
B	-1.106142191	-0.999020546	-0.474669414
C	1.083818357	2.511789072	-0.556013924
C	0.364852874	1.604638358	-1.360373648
O	2.481904903	4.071615699	-2.639558134
C	2.318333264	3.036244573	-0.936052707
H	2.842920457	3.738197583	-0.286580340
H	0.410573834	0.564838310	-3.262551720
H	0.299778479	2.329947851	-3.329135309
H	0.656580136	2.816476537	0.403729686
H	-0.700177104	1.470164233	-1.172028652
C	0.794879215	1.488374318	-2.808553778
C	2.309608570	1.614544601	-3.029634151
H	2.799634221	0.688413993	-2.689064492
H	2.529029185	1.732864087	-4.104280678
H	4.034006574	2.692224098	-2.256985745
C	2.923390387	2.807032443	-2.276068594
H	-3.235766805	2.039364166	0.373069638

C	-3.931634158	1.222531968	0.142504954
H	-4.406531195	1.442037049	-0.825835580
H	-4.720119569	1.200135895	0.912926858
H	-2.565958988	1.274913179	2.597729511
H	-1.225705797	1.246859495	1.408517014
O	-2.112356510	-0.008453437	-0.873178003
C	-1.812268178	0.638805835	2.106327668
C	-3.202912858	-0.119983281	0.065524347
C	-4.162071903	-1.213291371	-0.438916643
C	-2.460899843	-0.554257863	1.383384666
H	-1.118609111	0.255574302	2.866177511
H	-3.638234508	-2.176676360	-0.491730364
H	-5.049702545	-1.316817870	0.206173995
H	-4.171018955	-0.758103061	2.736378851
H	-2.694685581	-1.614522729	3.251405441
C	-3.312185092	-1.349958213	2.379457039
H	-3.679900400	-2.281679472	1.930394821
O	-1.442747359	-1.428363347	0.877072544
C	-0.703506060	-1.972375888	-2.692245087
H	-0.902555926	-2.922344700	-3.215193257
C	1.618882987	-2.201150772	2.085560912
H	2.390723496	-2.914007591	2.416609771
H	1.037162042	-1.880199246	2.960712872
H	0.922571288	-2.700744477	1.400897212
C	2.235371551	-0.957490462	1.426646370
C	3.131171584	-0.227231558	2.429664536
H	4.010429698	-0.835847194	2.696674126
H	3.473571850	0.736495569	2.031984929
H	2.558372645	-0.033788139	3.348711759
O	1.801813340	-1.050864898	-0.904578416
H	0.348867354	-1.691129787	-2.869493925
H	-1.358408107	-1.193678956	-3.123516159
C	3.396700947	-2.699011142	-0.150541815



C	2.905764467	-1.261430746	0.032325092
H	2.574466763	-3.416395921	-0.038585231
H	4.188312444	-2.944069482	0.576222134
H	3.814528503	-2.813153827	-1.161823222
H	4.895665715	-0.403168039	0.338727674
C	4.025384538	-0.279841860	-0.324952760
H	4.352237996	-0.466945210	-1.357726160
H	3.674517554	0.759426534	-0.262201142
O	1.140061060	-0.076091966	1.072357825
O	-0.955532715	-2.168302904	-1.314393641
H	-4.496588249	-0.946605354	-1.451975325

TS SYN A<sub>2</sub>



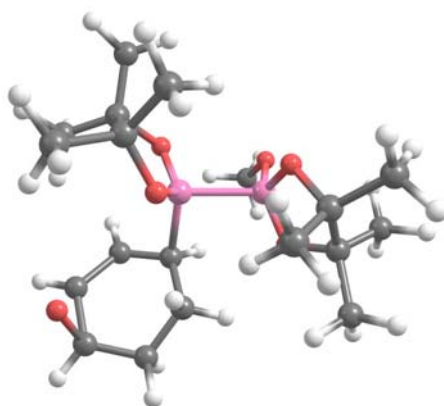
Electronic Energy=-8097.32 kcal/mol

B	0.811931900	-0.042888796	-0.395519485
B	-1.063352549	-0.963885954	-0.544984398
C	0.167297436	1.550822796	-1.219974015
C	1.236853546	2.473200252	-1.018190700
O	2.592311123	2.221632805	-3.309095212
C	1.970821332	3.086098193	-2.098330827
C	1.449395950	3.067356463	-3.475212523
H	1.619981105	3.946184198	-4.124200544
H	2.686439391	3.870160903	-1.836087747
H	1.531993754	2.741487811	-0.001699261
H	-0.716033406	1.687927636	-0.588209094

H	3.484313524	1.161730147	-0.753724960
C	0.092681423	2.412769301	-3.661351712
H	-0.669561519	3.202462083	-3.517154871
H	-0.013658772	2.055457126	-4.701421246
H	4.110682272	-0.009937175	-1.918235812
C	-0.148597658	1.237737252	-2.690437061
H	0.484820783	0.399209366	-3.009940429
H	3.679209404	1.132903882	1.576098335
O	1.285646180	0.174887995	0.936147477
H	2.987611155	0.331039225	3.008546833
C	-3.019843133	-0.450859476	0.651688468
C	-3.658220924	0.782498111	1.296241691
H	-4.306068287	1.285872874	0.562208741
H	-2.892228894	1.497904857	1.621320131
H	-2.026611671	0.030121977	3.356200363
H	-4.276480504	0.503921349	2.165538350
H	-0.560118027	-0.959649533	3.125498308
C	-2.038315441	-1.263306921	1.585299936
C	-4.121478552	-1.341952531	0.048175256
C	2.040650842	-1.914998036	1.879944315
O	-1.099043915	-1.815541239	0.647445679
H	-1.928366510	-2.943466399	2.940040097
H	-3.486261781	-2.080393462	3.013639516
C	-2.692213671	-2.433165818	2.334316418
H	-3.117544561	-3.167658860	1.638287928
H	-4.862207464	-1.653665124	0.801912629
H	-4.642027940	-0.775010655	-0.737338830
H	1.261978041	-2.439295013	1.312439179
H	-3.682561254	-2.238721969	-0.408239202
O	-0.925896419	-1.691026906	-1.776263501
H	2.855104621	-3.092408611	-0.319931550
C	-1.939743832	-1.662824898	-2.759184586
H	-2.671777209	-0.857474105	-2.585942256

H	-1.188960649	0.901688718	-2.780319054
O	1.751327680	-0.824920328	-1.097898352
O	-2.161725232	-0.017856055	-0.419154437
H	3.867067532	-2.397458726	-1.606826677
H	-2.490084754	-2.625150907	-2.782622230
H	-1.484990941	-1.512026602	-3.753906187
C	2.976394378	-0.911299186	-0.323433783
C	3.933922346	0.163699438	-0.847728439
C	2.469892245	-0.634910242	1.146017850
H	4.899815295	0.146411812	-0.317388683
H	1.612021603	-1.636883585	2.853743493
H	4.481824456	-2.448118890	0.066324827
H	4.384994231	-0.397238724	2.174224907
H	2.893785145	-2.588143965	2.060064721
C	3.579194582	-2.300452175	-0.549610039
C	3.444604310	0.157987931	2.022186280
H	-0.800444280	0.463312874	2.112586597
C	-1.322191965	-0.363626103	2.605515146

TS SYN A<sub>3</sub>



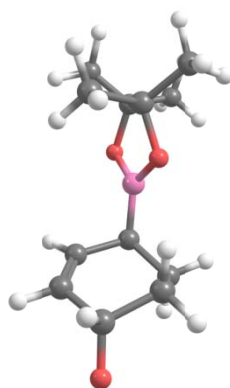
Electronic Energy=-8098.47 kcal/mol

B	-1.138506070	-1.093295622	-0.481634507
B	0.747633477	-0.167468550	-0.264167020
C	0.162655983	1.543619085	-0.969402268
C	1.405248111	2.120274840	-1.361896495

O	2.037880596	3.370011337	0.890672099
C	1.988922266	3.263026519	-0.691219355
C	1.141362200	4.169798709	0.105449823
H	2.919568696	3.665218703	-1.102272502
H	1.982097011	1.674948205	-2.174224993
H	-0.204605337	1.929664968	1.122416530
H	-0.845312316	-1.175122938	3.149177141
H	-0.490795425	1.221432948	-1.781086519
H	-1.127424899	0.270840968	2.175029439
H	-1.640644374	2.073455015	0.095973709
C	-0.334721048	3.820234119	0.134423533
H	-0.793546374	4.278011489	-0.763209193
H	1.365521647	5.250864655	0.115172774
O	1.229078577	-0.068124175	1.061201728
O	1.668509893	-0.927186763	-1.038844255
O	-2.257651019	-0.160723346	-0.403184529
C	-2.245650573	-1.495638682	1.542266493
C	-2.904257513	-2.706411500	2.215285923
H	-1.673724511	-0.367020132	-3.007718810
H	-3.250699011	-3.437084763	1.473183037
O	-0.986693611	-1.848285811	-1.694702912
H	-1.068459601	-1.885281564	-3.737615584
C	-0.905147902	-1.158270109	-2.924564773
H	0.090149968	-0.703122879	-3.063980055
H	-2.167966331	-3.203348371	2.864967060
H	-3.610347032	-2.450785393	-0.659544219
C	-4.160737526	-1.622765551	-0.193623694
H	-4.645320252	-1.041449646	-0.991781949
H	-4.943532885	-2.031606214	0.466215469
C	-3.185512029	-0.697087265	0.557835821
H	-3.757782787	-2.397628215	2.841594142
C	-3.958872184	0.457239859	1.200972224
H	-4.642731586	0.090222709	1.984189958

H	-4.560652822	0.968539279	0.433746142
H	-3.275947235	1.192114181	1.645521994
H	-2.368284365	-0.264797585	3.357446188
C	-1.618776843	-0.599868881	2.622119432
C	2.399654652	-0.906769497	1.219594303
C	2.879594577	-1.143098473	-0.269704971
H	1.525215092	-1.936901251	2.897414333
C	1.945509177	-2.199344836	1.915727157
H	1.153834226	-2.692497566	1.338241491
H	2.588359397	-3.303075182	-0.381161117
H	3.653385816	-2.627450226	-1.633946177
H	2.785122671	-2.894772970	2.075245730
C	3.928210456	-0.123923770	-0.734837863
H	4.103082482	-0.265245523	-1.812463827
H	4.886214245	-0.253169801	-0.207099114
H	4.345336993	-0.719339396	2.206080569
H	3.568952504	0.901230283	-0.575399138
H	2.967763189	-0.042001613	3.113408721
H	3.606777497	0.842287080	1.714506843
C	3.399630232	-0.160373450	2.108357190
C	3.374249638	-2.561552615	-0.571316433
H	4.261741064	-2.813937822	0.032043742
H	-0.823771517	4.278828471	1.012169637
O	-1.218577173	-1.982058807	0.660381926
C	-0.569985948	2.296091101	0.153557407

BORANE CY6 1,4-ANTI (Intermediate)

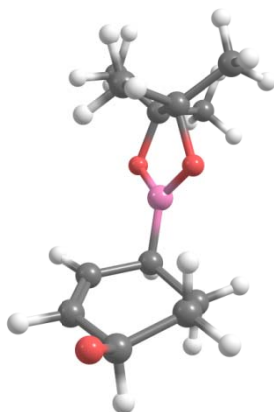


Electronic Energy=-4779.27 kcal/mol

C	-0.141398759	0.559185613	-0.642833905
C	1.374495915	0.541867245	-0.327869684
C	1.702463812	1.579435330	0.752803201
C	0.767165274	2.082960864	1.589376355
C	-0.740531158	1.824465446	1.507000164
C	-0.993562219	0.548714693	0.634410573
H	2.742354198	1.931780290	0.788171670
H	-0.371394626	1.496795372	-1.178897131
H	-0.401606013	-0.283426564	-1.309935207
H	1.051564847	2.877680071	2.290168098
H	-0.783542928	-0.367989165	1.216616568
H	-2.065273023	0.554343900	0.376356202
H	1.938121331	0.817343754	-1.239958256
H	-1.062119688	1.511882533	2.560077095
O	-1.340234145	2.950667273	1.052103644
C	2.256342738	-2.725437622	1.440556456
C	3.518577590	-2.499921710	0.532015201
B	1.973569728	-0.813879258	0.192044369
O	1.274313861	-1.843796680	0.820910522
O	3.341284956	-1.122303948	0.088248549
C	2.457618220	-2.233303816	2.879601003
H	1.482935877	-2.222861714	3.386196436
H	3.142607812	-2.885933783	3.442860292

H	2.847411642	-1.205981347	2.889810037
C	1.693483801	-4.145436371	1.441435881
H	2.425309156	-4.860969892	1.848911463
H	0.795292349	-4.176157190	2.074621624
H	1.407261776	-4.465332328	0.431544964
C	4.863000127	-2.618761848	1.247798258
H	5.001045680	-3.632937018	1.655997703
H	5.678098044	-2.423947729	0.535337692
H	4.944192619	-1.893839007	2.067044077
C	3.511648419	-3.378426724	-0.726825256
H	4.297444672	-3.024253647	-1.408823847
H	3.703875149	-4.436087705	-0.490039444
H	2.546742627	-3.302144146	-1.246395335

BORANE CY6 1,4-SYN (Intermediate)



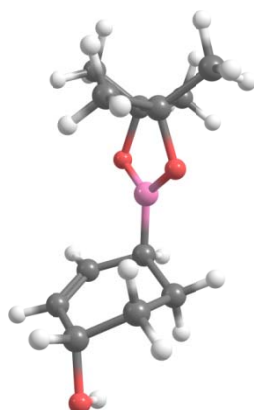
Electronic Energy=-4778.32 kcal/mol

C	-0.149185511	0.490764812	-0.551869660
C	1.375392045	0.509129282	-0.272217445
C	1.709494107	1.542346198	0.808300359
C	0.766949070	2.169618091	1.544056585
C	-0.742908295	1.886974664	1.548427206
C	-0.975745358	0.566343707	0.740395324
H	2.778228030	1.746609341	0.967135653
H	-0.389989552	1.371295705	-1.177481581
H	-0.415242832	-0.402054282	-1.148939045
H	1.068153016	2.904267180	2.301998748
H	-0.708474469	-0.262020953	1.416611306
H	-2.054071698	0.474658272	0.525562604
H	1.916364861	0.802046065	-1.194238948
C	2.285131348	-2.795582461	1.394646499
C	3.557037485	-2.526656571	0.510823201
B	1.992283353	-0.858488563	0.200752399
O	1.297833493	-1.916716809	0.778184873
O	3.363117170	-1.138719326	0.103020102
C	2.452527185	-2.329178233	2.846242734
H	1.467891699	-2.335279396	3.333059910
H	3.133086922	-2.985879603	3.409881837
H	2.830898175	-1.298346492	2.885954609
C	1.751640153	-4.226003556	1.356507039



H	2.493819263	-4.933308729	1.759223894
H	0.846756305	-4.288970282	1.977453645
H	1.486207428	-4.531303412	0.336408535
C	4.892922810	-2.640213078	1.242286959
H	5.044943047	-3.661960847	1.624731171
H	5.713714394	-2.409797316	0.547015206
H	4.947418943	-1.936453004	2.081839866
C	3.581394518	-3.369783916	-0.771278839
H	4.367091453	-2.981951195	-1.435035158
H	3.792604650	-4.429122341	-0.560558413
H	2.620518686	-3.299694350	-1.299241252
H	-1.197727306	2.703545117	0.875456002
O	-1.228957464	1.861092984	2.805792181

BORANE CY6 1,4-ANTI

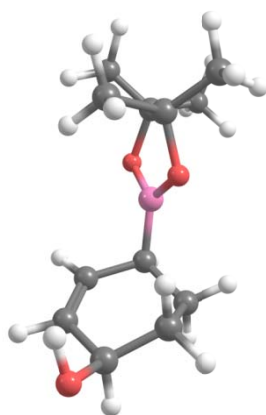


Electronic Energy=-4866.48 kcal/mol

C	-0.017940759	0.566547164	-0.654024154
C	1.456831226	0.601456231	-0.204358375
C	1.670991539	1.637067384	0.877525089
C	0.680064737	2.165692243	1.617785196
C	-0.771828127	1.802751382	1.444306620
C	-0.963177571	0.565821315	0.554784216
H	2.704052685	1.941261763	1.070064734
H	-0.225604725	1.453317194	-1.278916285
H	-0.208352427	-0.315120150	-1.282960672

H	0.908470829	2.921395439	2.375406928
H	-0.773096264	-0.337569167	1.157995768
H	-2.014893164	0.529908958	0.235070224
H	2.093719636	0.888926515	-1.062721601
H	-1.220721860	1.605289094	2.430207886
O	-1.525524449	2.953624977	0.958745217
H	-0.974249014	3.363888469	0.265040042
C	2.119991322	-2.947753868	1.070477490
C	3.579612212	-2.374250895	0.915295368
B	2.036093040	-0.790920942	0.294905283
O	1.315677401	-1.969152104	0.315438361
O	3.336055822	-0.932115368	0.744110526
C	1.605099107	-2.912118158	2.512517000
H	0.529517975	-3.135244630	2.511307463
H	2.112588327	-3.659193298	3.139449605
H	1.749221914	-1.920005773	2.962020838
C	1.894581542	-4.326266449	0.459012200
H	2.520951045	-5.079744688	0.960115753
H	0.843129065	-4.617298926	0.590581462
H	2.120942299	-4.336748317	-0.613989025
C	4.482355923	-2.566188619	2.129671666
H	4.639244054	-3.636459851	2.332765145
H	5.462766283	-2.110234653	1.933384768
H	4.059530589	-2.095352995	3.025378120
C	4.285164134	-2.851066823	-0.357460500
H	5.199649309	-2.259342041	-0.498911128
H	4.565723617	-3.911894108	-0.289425143
H	3.646947650	-2.713454796	-1.241042315

BORANE CY6 1,4-SYN

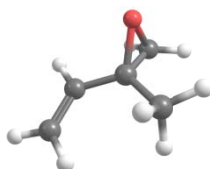


Electronic Energy=-4866.09 kcal/mol

C	-0.170453299	0.433445926	-0.513044627
C	1.352749190	0.492928103	-0.255817706
C	1.694383516	1.579815407	0.744065513
C	0.784702244	2.213429486	1.503731055
C	-0.692456209	1.905639169	1.476396598
C	-0.973497274	0.565680107	0.788910928
H	2.751882433	1.845883588	0.839118585
H	-0.447334188	1.257241474	-1.193240878
H	-0.439965368	-0.502695577	-1.024105780
H	1.094965200	3.003865693	2.194421266
H	-0.685285527	-0.248552726	1.474428174
H	-2.053127924	0.466637440	0.602167326
H	1.873883402	0.743908043	-1.197640363
C	2.293482591	-2.829740525	1.394552235
C	3.564911069	-2.527178275	0.516206265
B	2.000601858	-0.867865768	0.243412446
O	1.296220463	-1.901723816	0.830395866
O	3.356502134	-1.119075806	0.136273699
C	2.468517179	-2.438984195	2.865177529
H	1.491623105	-2.489524737	3.364993871
H	3.157876837	-3.120752489	3.383489717
H	2.850400687	-1.413218299	2.961049137
C	1.747174478	-4.248848430	1.282623589

H	2.487208455	-4.978575864	1.644713742
H	0.845472434	-4.343875739	1.903512832
H	1.479476338	-4.501215417	0.249521806
C	4.899197900	-2.635722468	1.246639877
H	5.063595095	-3.663312826	1.604959680
H	5.716326524	-2.381823358	0.557067159
H	4.948519012	-1.951667656	2.102468730
C	3.601968079	-3.329684467	-0.787830345
H	4.389168302	-2.920052216	-1.435054819
H	3.823422681	-4.390344809	-0.601304624
H	2.645638895	-3.260813317	-1.324190080
H	-1.222635406	2.712884623	0.942817142
O	-1.261851431	1.962532100	2.808536173
H	-0.763272727	1.315409509	3.344760042

2-METHYL-2-VINYLOXIRANE R (7)

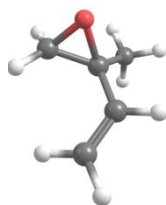


Electronic Energy=-1804.92 kcal/mol

C	-1.210397399	0.246499610	-0.245295897
C	0.184259323	-0.184327263	0.030906181
O	-0.231964004	1.223979005	0.148352697
H	-1.542870624	0.310249361	-1.287316647
H	-1.995380060	0.049708145	0.492797731
C	0.458676739	-0.811468018	1.349845351
H	-0.184619988	-0.453821029	2.160235486
C	1.400881026	-1.729343436	1.599326522
H	2.065434670	-2.104358468	0.818818066
H	1.533099690	-2.140019727	2.600498221
C	1.111911675	-0.467816594	-1.127208656

H	2.146837301	-0.200797911	-0.869009996
H	1.087700879	-1.534124323	-1.398084436
H	0.809768171	0.122189387	-2.001640588

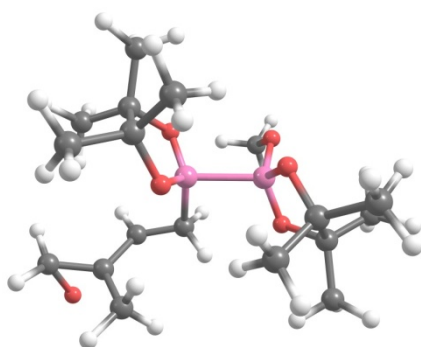
2-METHYL-2-VINYLOXIRANE R' (7)



Electronic Energy=-1802.55 kcal/mol

C	-1.230288783	0.324091148	-0.245882119
C	0.135475678	-0.139423459	0.063004766
O	-0.193026504	1.293940672	0.035896636
H	-1.574156870	0.304408150	-1.285851770
H	-2.015296489	0.260736381	0.513613965
C	0.467578625	-0.671175665	1.420294430
H	1.519386209	-0.565187648	1.710636067
C	-0.389648396	-1.259116418	2.260364405
H	-1.440527340	-1.405186649	2.001095096
H	-0.066046173	-1.618087763	3.237960976
C	1.064981546	-0.566472133	-1.052133482
H	2.099920023	-0.279750885	-0.812233126
H	1.038285964	-1.658444218	-1.188305873
H	0.781970446	-0.080787272	-1.994916027

TS ANTI R



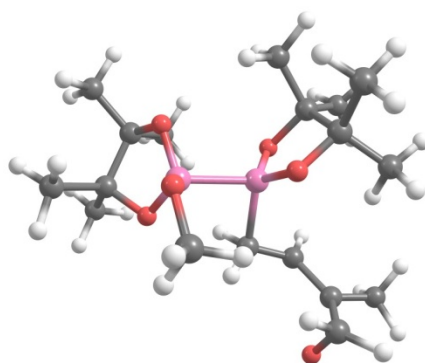
Electronic Energy=-7902.87 kcal/mol

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C	-0.123884738	1.357797418	-1.260032108
C	0.926542986	2.314850379	-1.304203472
O	1.573160988	4.727225921	-0.858416710
C	1.182919719	3.325748042	-0.281323353
C	2.523686803	3.942111755	-0.129149383
H	3.360951527	3.548554204	-0.723910572
H	1.696885733	2.222694513	-2.076404121
H	2.826775258	4.349285371	0.849126603
H	-0.405995299	0.930021452	-2.224021351
H	-1.020497682	1.605802880	-0.687461093
C	0.220937626	3.458280814	0.877006051
H	0.231479008	2.535469363	1.476308841
H	0.501586719	4.311939730	1.510240081
H	-0.803487928	3.621896433	0.510131038
H	-1.562940979	0.778293765	1.702104024
H	-1.259920741	-0.366490535	3.013262516
C	-2.027674588	0.001153750	2.319033113
H	-2.852682928	0.441117708	2.902524590
O	-2.368685015	-0.290699403	-0.724627553
H	-1.558561841	-1.027120698	-3.149663161
O	-1.379210357	-1.782015228	0.799907292
O	-0.920700547	-2.149087582	-1.499527377

H	0.219006781	-1.231289374	-2.983789162
H	-0.797235665	-2.611987331	-3.489133703
H	-2.486684506	-2.502625360	3.152543414
C	-3.173775694	-2.227644357	2.337788253
C	-2.507532659	-1.171400380	1.448700924
H	-4.102275360	-1.841120590	2.789978261
H	-3.404802642	-3.136826522	1.767719025
C	-3.373990123	-0.691055366	0.223530807
C	-4.291153452	0.501728148	0.501748361
H	-3.713793729	1.375998960	0.828849042
H	-5.038931553	0.258969204	1.274895756
H	-4.827493267	0.773648654	-0.420342990
C	-4.184590410	-1.844802909	-0.396936064
H	-3.524910516	-2.698336832	-0.601785810
H	-5.012796123	-2.172024709	0.252678831
H	-4.605474696	-1.499872714	-1.352759265
O	1.614205533	-0.829895041	-0.981503841
O	0.990976829	0.191620327	1.004256782
C	2.177658534	-0.577476268	1.303549506
C	2.778438331	-0.885256379	-0.125371694
C	1.728861108	-1.842623553	2.052598833
H	2.582312632	-2.481275664	2.331144616
H	2.671643141	-3.062106279	-0.070769012
H	1.210576698	-1.535406619	2.972467125
H	1.011755848	-2.414321247	1.451654587
C	3.408152589	-2.273985767	-0.270387293
H	4.263877018	-2.399230966	0.413301102
H	4.025698729	-0.274581416	2.434144231
H	4.693727912	0.197581826	-0.024093231
C	3.086830976	0.258919570	2.210617553
H	4.019821013	-0.028017172	-1.663249088
H	2.570481855	0.450941948	3.163171810
H	3.298436538	1.178996511	-0.573903154

H	3.329403776	1.226713533	1.753566688
C	3.763780696	0.185055538	-0.614407887
C	-0.757414991	-1.722962724	-2.838043142
H	3.772231736	-2.401445285	-1.301097293

TS ANTI R'



Electronic Energy=-7901.74 kcal/mol

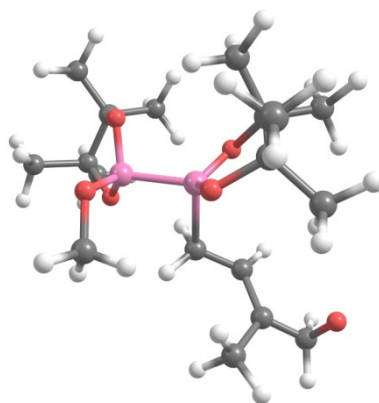
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B	0.643649487	-0.781467696	0.128145230
C	0.549529932	0.979733195	-0.669806857
C	1.826963256	1.551573504	-0.532709449
O	2.356592917	2.389811399	-2.905906826
C	2.828464529	1.717137032	-1.582664090
C	4.169868468	2.279335443	-1.152769561
H	4.754844886	2.594061923	-2.027828594
H	4.749597815	1.530080696	-0.587650415
H	4.024148471	3.153341960	-0.499145735
C	2.817435654	-1.046911570	2.955060445
H	3.352272817	-0.193063296	2.519230943
H	3.704801624	0.791966598	-3.415108803
H	3.555255049	-1.792094492	3.295516946
H	2.262781311	-0.688296919	3.835117306
C	2.766103440	1.016413149	-2.882998759
C	3.799238247	-1.444591053	0.258103021
H	4.602000310	-1.671017695	0.977550918
H	4.123714206	-1.771177426	-0.740976143



H	3.639122768	-0.357812381	0.225436618
H	1.970206725	0.280133546	-3.048127822
C	1.829101056	-1.654110431	1.952545891
C	2.486475830	-2.158160514	0.602995799
C	2.680642096	-3.675307027	0.513084803
H	3.376156101	-4.037160436	1.288338321
H	3.102691924	-3.928698565	-0.470945259
H	1.724110286	-4.202400317	0.616971722
H	1.589569077	-3.567502689	3.017758863
O	1.512580795	-1.773361066	-0.397484583
C	0.978277515	-2.727041473	2.651674725
H	0.475823746	-2.263780322	3.513416135
H	0.196041944	-3.096665787	1.977167363
O	0.931698324	-0.610841577	1.516918745
H	0.164270695	0.848385231	-1.682921740
H	-0.235803225	1.335240530	-0.002107552
H	2.134736441	1.892307643	0.461059495
O	-1.178077008	-2.171952058	-1.439137162
C	-0.700649369	-1.729342295	-2.691733486
H	0.382001270	-1.512799867	-2.655988610
H	-1.229740037	-0.822475181	-3.041334700
H	-0.865831847	-2.532663420	-3.429117082
O	-1.797497198	-1.825733113	0.831883110
H	-1.589768963	-0.612613787	3.164496186
H	-1.366689597	0.632864582	1.933692404
C	-2.116131545	-0.004168215	2.416716681
C	-2.780669298	-0.941981984	1.394102244
C	-3.289153479	-0.164993483	0.122995772
H	-2.857887478	0.628469297	2.931011208
C	-3.881460468	1.219925358	0.394883876
H	-3.140176591	1.880101817	0.863735346
H	-4.190358807	1.678576570	-0.557122144
H	-4.767347354	1.155888486	1.048521943

C	-4.279650200	-1.006886647	-0.705112185
H	-4.439051907	-0.507176318	-1.671839676
C	-3.839955105	-1.794678786	2.102414659
H	-3.380347064	-2.303898887	2.963488855
H	-3.855036255	-2.000459079	-0.899550587
H	-4.245534931	-2.562372910	1.430709956
H	-4.668283459	-1.170664894	2.477685183
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TS SYN R



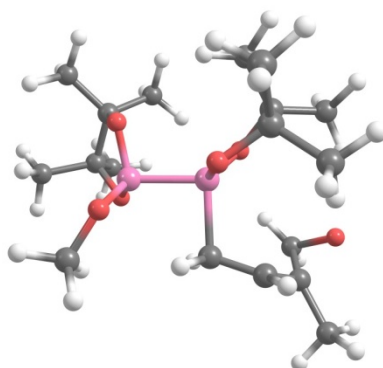
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C	1.143810911	2.569764291	-1.344564626
O	3.742052223	3.227826098	-2.102799039
C	1.937863182	2.921730341	-2.464977361
C	2.752611797	4.153015545	-2.441668306
H	2.486015640	4.893370505	-1.658710305
H	1.297957502	3.164082436	-0.438182544
H	2.878196825	4.669836764	-3.418823107
H	-0.678829557	1.698524982	-0.626453216
H	-0.172560182	1.161241007	-2.285125192
C	1.878403020	2.141068855	-3.749708384

H	0.927062205	2.339509254	-4.274415157
H	2.708490024	2.431505227	-4.405724609
H	1.934631626	1.059094111	-3.565271598
H	-1.254805164	0.742807080	1.823364354
H	-1.130334220	-0.559891844	3.010029926
C	-1.824592589	-0.042033994	2.333680601
H	-2.625896420	0.415470613	2.936436695
O	-2.119497690	0.043903449	-0.726271815
H	-1.371278768	-0.618422912	-3.293156468
O	-1.296079498	-1.695274945	0.629561807
O	-0.919114036	-1.903652633	-1.701347983
H	0.369756521	-0.999910231	-3.069888709
H	-0.743505681	-2.241589910	-3.710244027
H	-2.518192631	-2.576423027	2.865123363
C	-3.159835592	-2.146339782	2.080960611
C	-2.380595392	-1.062788195	1.325542886
H	-4.057283952	-1.727186627	2.565984681
H	-3.463310661	-2.958319045	1.407600346
C	-3.174872240	-0.373252495	0.152610673
C	-3.990623820	0.858107094	0.555089558
H	-3.344520076	1.636732450	0.981365228
H	-4.769726732	0.599999549	1.291432369
H	-4.485484006	1.276139352	-0.335108170
C	-4.071206257	-1.371575987	-0.604479759
H	-3.485334070	-2.252315375	-0.897835167
H	-4.940728440	-1.691045737	-0.007073575
H	-4.436795563	-0.883629082	-1.520008765
O	1.780124297	-0.931782993	-0.947413811
O	1.138371254	0.184584107	0.966493071
C	2.315174791	-0.589887108	1.331893004
C	2.945113772	-0.949184371	-0.067349055
C	1.818744242	-1.822770404	2.104105972
H	2.652406998	-2.465777917	2.427939568

H	2.833253878	-3.128009099	0.069644758
H	1.276098016	-1.482147464	2.997671068
H	1.114578257	-2.404383610	1.495648214
C	3.570179008	-2.344665915	-0.147907554
H	4.413951336	-2.440749609	0.555072453
H	4.124526054	-0.268114039	2.506075865
H	4.855716596	0.114507621	0.024278406
C	3.200973993	0.269216557	2.234871567
H	4.216174290	-0.160122073	-1.614771766
H	2.656551794	0.499880726	3.163020078
H	3.506037078	1.106140470	-0.604609655
H	3.472067157	1.214060138	1.747721368
C	3.936589087	0.096528641	-0.582945708
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H	3.955236275	-2.510042392	-1.165026830

TS SYN R'



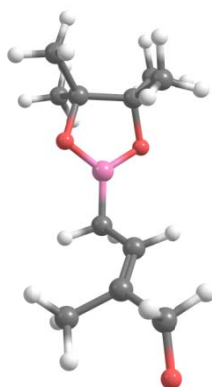
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C	1.496103320	1.946444290	-1.755186278
O	2.882344139	2.984618264	0.270389129
C	1.972214726	3.120191661	-1.042315847
C	1.534947187	3.469709127	0.319426788
H	1.425085709	4.533795596	0.590656393
H	0.823258113	2.805303796	0.826312064
H	3.024202362	5.000003345	-1.262597184
H	1.856073453	4.650993926	-2.581406617
H	3.406710886	3.785293807	-2.509560124
C	2.596443431	4.208883972	-1.895014043
H	2.129812055	1.618252671	-2.587285796
H	-0.069834028	0.640469319	-2.315493472
H	-0.428309043	1.632859582	-0.838442080
O	1.728260931	-1.233779527	-1.160108116
O	1.438680505	-0.067337627	0.820258256
C	2.982267483	-1.380635267	-0.445342261
C	2.636567604	-0.870362439	1.015910631
C	3.701638359	0.024178003	1.656061614
H	3.813616322	0.959806499	1.093564778
H	3.381559282	0.287357972	2.676256672
C	4.026748195	-0.512802724	-1.159094487

H	5.020025196	-0.604058506	-0.692020317
H	4.671430402	-0.495773840	1.728542379
H	3.727241649	0.543511082	-1.147559214
C	3.390237897	-2.855811464	-0.533244999
H	3.572398989	-3.114139259	-1.587185919
H	4.314033252	-3.053748923	0.034501717
H	2.592327478	-3.509468590	-0.158851731
C	2.277626907	-2.014822114	1.973383516
H	1.951106782	-1.582259635	2.929359785
H	1.452805010	-2.613932717	1.567739452
H	3.145691423	-2.663811755	2.169629392
C	-1.033500582	-1.242800638	2.715763409
H	-0.305922731	-1.994620527	3.048329932
H	-0.474166606	-0.352289467	2.404445266
H	-1.685766256	-0.998457371	3.569530508
C	-1.837387163	-1.817685785	1.539064873
C	-2.827375608	-0.754507665	0.924171321
C	-2.492609791	-3.135433605	1.976530988
O	-1.206196474	-1.465935077	-1.884175775
H	-1.711747419	-3.813341653	2.353606623
H	-3.224497456	-2.973878581	2.786050373
H	-2.991516319	-3.632746451	1.134797364
O	-0.963343616	-2.117529357	0.434257065
C	-2.094658415	-0.802912566	-2.760475812
H	-1.564267517	-0.470560738	-3.672084752
H	-2.899201979	-1.494412086	-3.082126642
H	-2.568345930	0.073177669	-2.290456003
O	-1.987540736	-0.044624997	-0.005376641
C	-3.975898414	-1.421455851	0.142418644
H	-4.518749617	-0.646826749	-0.418650130
H	-4.688680756	-1.931573346	0.810520314
H	-3.575652654	-2.151170710	-0.573696554
C	-3.405158203	0.250798639	1.923808689

H	-2.607120568	0.844054454	2.388191972
H	-4.085259972	0.940562307	1.400482348
H	-3.977815154	-0.259285684	2.716150912
H	4.101481654	-0.844589333	-2.205913871

BORANE MV E (Intermediate)



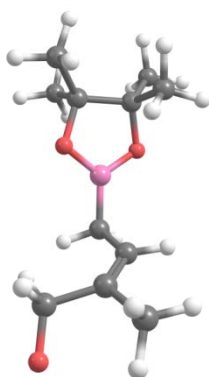
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C	0.557179908	1.976613704	0.319160627
H	0.787086159	2.336082895	1.331563426
C	1.662697732	2.167301971	-0.720221802
H	2.503284499	1.473669154	-0.508864781
H	1.288669999	1.916720948	-1.722873880
C	3.170273549	5.561893846	0.115226705
C	2.857104003	5.727993053	-1.418725985
C	2.117836700	6.214236699	1.019932645
H	2.292203392	5.887751161	2.054368197
H	2.176840079	7.312965262	0.984904630
H	1.104332889	5.900738025	0.735420696
C	4.571917817	5.995627844	0.541316437
H	4.723524520	7.071220821	0.358809915
H	4.697765186	5.811077612	1.617689402
H	5.347580575	5.432953418	0.006801095

C	2.117478026	7.010464421	-1.793749933
H	2.724557263	7.897166480	-1.550557004
H	1.921069192	7.017564095	-2.875626917
H	1.155644923	7.085752627	-1.272305235
C	4.095822471	5.555215794	-2.307936181
H	3.768877107	5.477447978	-3.354180399
H	4.786461967	6.407427292	-2.219648295
H	4.635946480	4.633998854	-2.049638377
B	2.230353950	3.624441209	-0.708720534
O	1.987149020	4.586763857	-1.689990448
O	3.058683749	4.118063515	0.300067447
O	-2.099470164	-0.048631087	1.411182905
H	-2.502903301	1.972382215	0.986867333
C	-1.072919694	0.789247174	-1.200451177
H	-1.361287250	1.564866788	-1.933968658
H	-0.286560500	0.172600782	-1.667638307
H	-1.933911159	0.136067189	-0.983452747



BORANE MV Z (Intermediate)

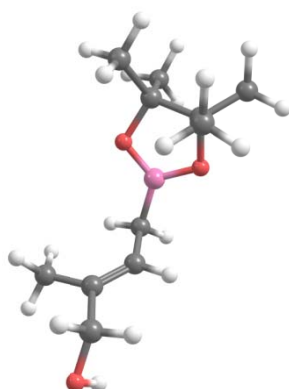


Electronic Energy=-4575.99 kcal/mol

C	-0.722196222	1.680702835	-0.000572045
C	-1.118630143	1.188804268	-1.409441370
H	-1.802666168	2.026523179	-1.809058574
H	-0.202281146	1.288764898	-2.071469260
O	-1.669202187	-0.039728244	-1.381349383
C	0.524690363	1.979108197	0.431226127
H	0.672719731	2.229037356	1.493373258
C	1.804053800	1.990984724	-0.402688060
H	2.577670532	1.377071811	0.094434790
H	1.592900631	1.552951090	-1.389296935
C	3.078442621	5.534054502	0.100823605
C	2.790226848	5.528977624	-1.447624550
C	1.948594678	6.170093036	0.920596009
H	2.127886684	5.962514274	1.984941684
H	1.903826328	7.260696905	0.779132145
H	0.977404426	5.733496228	0.649897186
C	4.425563668	6.128081357	0.508156402
H	4.486578113	7.192045445	0.229666554
H	4.542066369	6.053507470	1.599044800
H	5.259892576	5.591566585	0.038968492
C	1.948056341	6.699454595	-1.953049439
H	2.461843208	7.658575634	-1.779430343
H	1.782449326	6.589587982	-3.034357819

H	0.967607673	6.725857510	-1.462307740
C	4.060767509	5.388113384	-2.297254327
H	3.764733747	5.181036217	-3.334959153
H	4.670160156	6.304578252	-2.282595504
H	4.674673835	4.548001506	-1.944571017
B	2.307904819	3.461056233	-0.547312154
O	2.030235271	4.299944347	-1.625429559
O	3.083137358	4.110320207	0.421737425
C	-1.874749475	1.682304319	0.973741243
H	-2.638848913	2.419087930	0.661156983
H	-2.355281139	0.692776560	0.934950407
H	-1.560819947	1.917589595	2.004087991

BORANE MV E

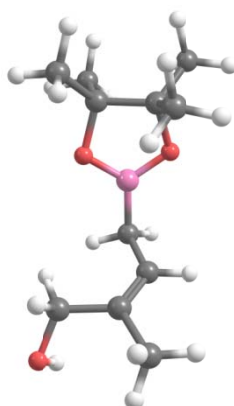


Electronic Energy=-4663.73 kcal/mol

C	-0.575467264	1.653655655	0.140256118
C	-1.034578344	1.630922604	-1.297423756
H	-1.742561324	2.455121583	-1.477945081
H	-0.192058348	1.765188382	-1.992705640
O	-1.783883368	0.435712743	-1.635595959
C	0.721413164	1.757772858	0.499430183
H	0.938097738	1.806997766	1.572887971
C	1.939246018	1.876673379	-0.391483081
H	2.767741452	1.311144365	0.064660813
H	1.760468801	1.454283936	-1.389466877

C	2.935130947	5.526402662	0.076261472
C	2.775341730	5.438426587	-1.489923436
C	1.708855968	6.119077618	0.777206207
H	1.811785295	5.966973040	1.860267625
H	1.617086795	7.197887602	0.585528416
H	0.785078094	5.623202276	0.448813947
C	4.208239415	6.212114326	0.560332648
H	4.228638158	7.264180311	0.237638234
H	4.238806928	6.193541022	1.658642685
H	5.107902136	5.710245998	0.184286585
C	1.895771754	6.516892598	-2.114349775
H	2.329931015	7.515266215	-1.952776955
H	1.823819093	6.348844435	-3.198055293
H	0.881321852	6.501686935	-1.697936997
C	4.111563737	5.341758569	-2.231954933
H	3.916932979	5.076971005	-3.280112196
H	4.654443685	6.297622176	-2.210947655
H	4.753090334	4.564381200	-1.794848233
B	2.364737523	3.391883904	-0.533596891
O	2.106260667	4.138457685	-1.666598797
O	2.994696072	4.106642904	0.467796766
C	-1.673188041	1.567080988	1.173891706
H	-2.354225164	2.431633407	1.095962620
H	-2.291713208	0.670533363	1.018424718
H	-1.265936445	1.540206195	2.193063690
H	-1.197245240	-0.318983576	-1.438624514

BORANE MV Z



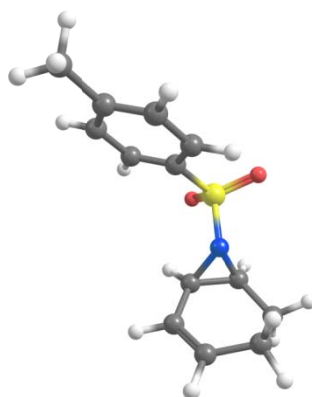
Electronic Energy=-4664.82 kcal/mol

C	-0.517342975	1.546819531	0.068935982
C	-1.495661872	1.477879301	1.216821399
H	-0.998919921	1.773740242	2.156949783
C	0.782641174	1.795048426	0.332839676
H	1.058301952	1.943000751	1.384340195
C	1.919265220	1.963548614	-0.645889029
H	2.773517438	1.347146491	-0.317516668
H	1.637649513	1.635525125	-1.654726279
C	3.088340343	5.505204584	0.128307614
C	2.739107993	5.622271075	-1.405673592
C	1.978913856	6.029780722	1.045753947
H	2.207365966	5.738066617	2.079982470
H	1.904373924	7.126095562	1.003244979
H	1.004194377	5.600176218	0.776562739
C	4.435922819	6.093984380	0.533536273
H	4.456897631	7.178611603	0.347834939
H	4.598663585	5.930622963	1.607930766
H	5.264065292	5.626653731	-0.012726257
C	1.820659832	6.783509928	-1.774703243
H	2.298084379	7.747214535	-1.541431499
H	1.614429656	6.758364090	-2.853816774
H	0.863271330	6.726005832	-1.242769091
C	3.973189208	5.607464395	-2.312757576

H	3.645600091	5.488846269	-3.354502297
H	4.543588492	6.544132010	-2.233107473
H	4.638310655	4.769173372	-2.064528241
B	2.374990005	3.476876810	-0.670982442
O	2.017232761	4.365163677	-1.665024225
O	3.139894750	4.046528520	0.330202057
O	-2.118993767	0.177709566	1.361467187
H	-2.341187570	2.163245982	1.048840548
C	-1.104987283	1.329545333	-1.302637536
H	-1.789152474	2.155078236	-1.563558681
H	-0.342640030	1.266940374	-2.087956507
H	-1.705056139	0.406965085	-1.319959348
H	-1.388198590	-0.466305436	1.426678377

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3,4-AZIRIDINE-1-CYCLOHEXENE A<sub>2</sub> (10)

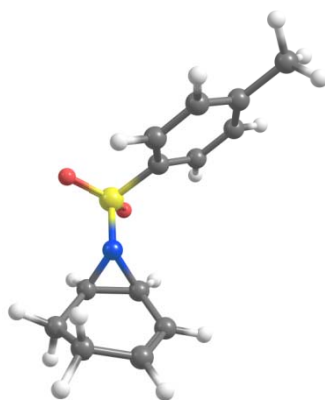


Electronic Energy=-4427.95 kcal/mol

C	-0.102409750	0.100033191	0.811616652
C	1.229832270	0.646834048	0.363572007
C	1.264451401	2.189806975	0.318757746
C	0.593469734	2.828025588	1.514094465
C	-0.523640151	2.096300673	2.185896599
C	-0.902919174	0.761276437	1.663783489
H	2.301963809	2.544585179	0.234346167
H	2.006549567	0.291578604	1.061091475
H	1.496318351	0.242864544	-0.624382956
H	-0.402050416	-0.885290911	0.445454382
H	-1.853013421	0.334226501	1.990501343
H	0.727784862	2.545463209	-0.576898348
H	-1.291699273	2.710541269	2.659464642
H	0.520551744	3.919166117	1.514992060
S	1.016365473	3.302364244	4.124084501
O	2.389736667	3.791069483	4.026927257
O	-0.104047677	4.251634116	4.167667163
C	0.880636561	2.219337310	5.541751209
C	1.932218435	1.347865176	5.844637811
C	-0.255167848	2.284915887	6.351152482
C	1.830713173	0.529369094	6.967350951
H	2.816901566	1.321296383	5.209503950
C	-0.336554717	1.461042491	7.475416873

H	-1.052646494	2.984488024	6.103971351
C	0.699420801	0.572772107	7.801242951
H	2.647631796	-0.155285001	7.204923856
H	-1.222033209	1.512493048	8.112271268
C	0.618894927	-0.292487284	9.036028817
H	1.115388231	0.199423152	9.887185723
H	-0.422298893	-0.481275041	9.326813696
H	1.116550346	-1.258820208	8.881771256
N	0.843778161	2.184619299	2.834360883

3,4-AZIRIDINE-1-CYCLOHEXENE A<sub>3</sub> (10)



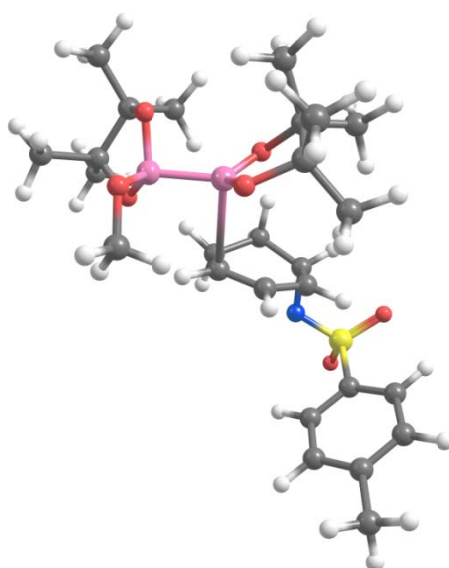
Electronic Energy=-4427.95 kcal/mol

C	-0.608146101	0.712575775	0.604580403
C	0.805243971	0.668668969	0.080176561
C	1.835040937	1.252957521	1.071184678
C	1.356345763	2.523861179	1.736124081
C	-0.111972509	2.719707445	1.937590406
C	-1.034528107	1.667108705	1.448006152
H	1.085677834	-0.363450622	-0.177458241
H	0.847834970	1.242867105	-0.860318617
H	-1.309343734	-0.049097246	0.253981094
H	-2.068912146	1.689965874	1.796244472
H	2.793567312	1.431135779	0.562346505
H	2.027712469	0.523910916	1.876208534
H	-0.408900337	3.314343832	2.803463588

H	2.006925619	2.955401876	2.501926903
N	0.632220210	3.492667975	0.866682950
S	0.995718469	5.133463316	1.210269946
O	0.844841732	5.431756537	2.640919821
O	2.265765074	5.393684240	0.536818192
C	-0.318483806	5.968876128	0.328366202
C	-0.312232920	5.976815037	-1.071140591
C	-1.303728009	6.647592507	1.046964399
C	-1.314764459	6.666572326	-1.748081748
H	0.476818896	5.458687506	-1.614929582
C	-2.297896375	7.338905998	0.350576939
H	-1.273373160	6.645413789	2.135798399
C	-2.323296706	7.356912184	-1.051397663
H	-1.310535144	6.679069148	-2.840108618
H	-3.063285297	7.880710667	0.909867950
C	-3.412284449	8.086985856	-1.800419761
H	-3.010159808	8.615860523	-2.675053243
H	-4.172919657	7.380839405	-2.168211491
H	-3.920264901	8.817761160	-1.158858446



TS ANTI A<sub>2</sub>



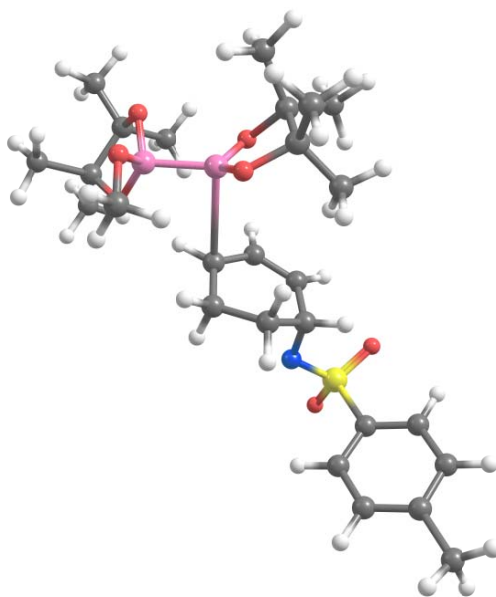
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B	-1.083250834	-1.115102546	-0.535076838
B	0.650688880	-0.524167659	-0.145730005
C	0.077289442	1.750193284	-1.506139653
C	1.423573384	2.036738708	-1.708215601
C	2.059771545	3.031057310	-0.972849461
N	1.162912359	5.029188436	-1.004513367
C	1.356046383	3.931126684	-0.024326243
H	1.986128795	4.233185844	0.824899092
C	0.027240905	3.351236575	0.466276791
H	-0.581350156	4.156266196	0.904718184
H	0.261145396	2.627615028	1.262886787
C	-0.759552726	2.622573019	-0.632714524
H	-1.223477531	3.365072885	-1.313043710
H	-1.588036260	2.021565620	-0.231539216
H	-0.445359213	1.071253046	-2.177056216
H	1.987907733	1.482286786	-2.460129306
H	3.108959124	3.261077404	-1.166805460
S	2.397380502	6.053397565	-1.213286486
O	1.828755126	7.373574787	-1.532642820
H	1.393760085	5.581022181	-3.902099752

C	2.457398585	5.341999722	-3.914833114
O	3.450073323	5.973040905	-0.171500849
C	3.213979366	5.510076361	-2.747599152
C	3.060422959	4.835508403	-5.064269077
H	2.457640298	4.687785566	-5.964448777
C	4.571703277	5.185762175	-2.747687353
H	5.144430334	5.317157692	-1.829185464
C	5.166656400	4.677543429	-3.908840652
H	6.227437100	4.412367034	-3.896409565
H	5.255127328	4.727987065	-7.071759623
C	5.062979807	3.932200438	-6.334237344
H	6.023520699	3.448097436	-6.111841515
C	4.423629189	4.487161625	-5.081052238
H	4.413005043	3.190109716	-6.820272088
C	3.144571144	0.279619641	2.287732758
H	2.621114915	0.569964302	3.210015962
H	3.444166986	0.840396306	-0.518832968
H	3.358935443	1.190898630	1.715775869
H	4.099177876	-0.191395000	2.572284803
H	4.088716846	-0.478208588	-1.524305917
H	4.812609048	-0.139901509	0.070851566
C	3.867190935	-0.170330391	-0.492189087
C	2.880974517	-1.167841061	0.120363731
C	3.510449772	-2.562695619	0.133603630
H	4.368391873	-2.604484977	0.823808917
H	3.874413512	-2.802532502	-0.876421344
H	2.780474775	-3.328780964	0.421683249
H	2.693402613	-2.442693208	2.755414377
C	1.833266560	-1.859441470	2.391762850
H	1.296809736	-1.451994451	3.260162294
H	1.140064189	-2.520078179	1.854694316
O	1.701264506	-1.228141455	-0.742065709
C	2.272861735	-0.692905385	1.495934930

O	1.048481019	-0.000363876	1.090754019
C	-0.635302091	-1.597994641	-2.896787305
H	0.354225329	-1.105160731	-2.933403749
O	-0.922253599	-2.097180159	-1.610301344
H	-0.616880441	-2.444037510	-3.602588874
O	-1.380676745	-1.838267240	0.717396861
C	-2.512054414	-1.199145818	1.335753518
O	-2.191359997	-0.156817730	-0.728881252
C	-2.035568375	-0.077184587	2.274859303
H	-1.314775667	-0.493700696	2.991218570
H	-1.521931922	0.710432102	1.712080012
H	-2.874121454	0.365824496	2.835697384
C	-3.280135524	-0.633673205	0.087734882
C	-3.266183994	-2.256305107	2.148437175
H	-2.636807055	-2.583882008	2.989929014
H	-3.498892495	-3.135951179	1.534948623
H	-3.349853401	-2.586776095	-0.869966691
H	-4.201865452	-1.846056290	2.562509764
C	-4.027273972	-1.747021369	-0.671368981
H	-4.906357423	-2.108274983	-0.113560121
H	-4.368192599	-1.345929817	-1.636832335
C	-4.233674541	0.527781326	0.372707927
H	-3.707157557	1.383232768	0.815550527
H	-4.697106549	0.861821967	-0.568313486
H	-5.040055072	0.218007049	1.057402641
H	-1.400375368	-0.875683488	-3.243893530

TS ANTI A<sub>3</sub>



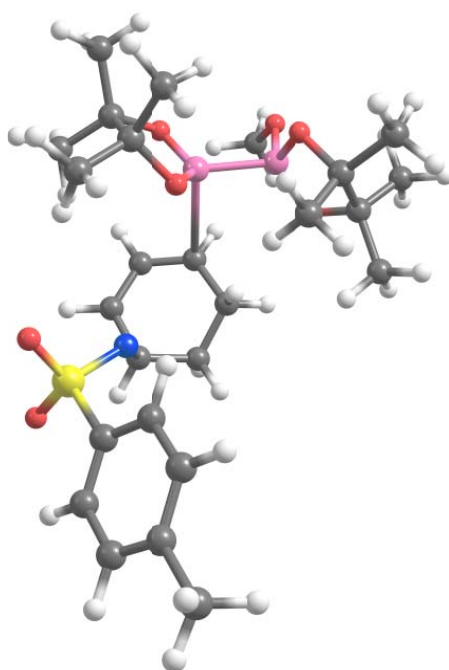
Electronic Energy=-10531.98 kcal/mol

B	-1.135539745	-1.110479956	-0.421501992
B	0.659977919	-0.673071170	-0.061933478
C	0.304297254	1.716481794	-1.375848935
C	1.011970601	2.498370997	-0.469998142
C	2.216180007	3.106471937	-0.816331066
N	2.295853345	4.293360672	-2.641613881
C	2.821969362	2.991638472	-2.172063941
H	3.922757898	2.942316341	-2.131618131
H	2.775283037	0.899079422	-2.640510441
C	2.269763783	1.815370907	-2.981676260
C	0.756887632	1.629536695	-2.799375228
H	0.221233029	2.441881988	-3.329459754
H	0.601320289	2.664128044	0.528386011
H	0.412509975	0.690128177	-3.254077435
H	2.721063830	3.785661702	-0.128623982
H	-0.697718353	1.347147810	-1.137324726
S	3.304914726	5.543459779	-2.467572483
O	4.130345353	5.510478441	-1.235622537
O	2.558433687	6.771754358	-2.769671142
C	4.510020751	5.367205901	-3.822742549

C	4.057216397	5.243153711	-5.141862473
H	2.984762370	5.230322000	-5.339767886
H	4.617817212	5.029944373	-7.210762125
C	5.881276117	5.367279990	-3.555206336
H	6.212951967	5.459255888	-2.520833893
C	6.795410910	5.258787352	-4.607607760
H	7.867084257	5.262975368	-4.390136282
H	7.693389059	6.069237016	-7.375705186
C	7.356620415	5.064489948	-7.072243846
H	8.250853520	4.495298768	-6.783064603
H	6.917562113	4.583357543	-7.956580580
C	6.361847068	5.144091999	-5.936257599
C	4.978242718	5.131549542	-6.183601950
C	3.876258497	-0.268902239	-0.171361531
H	3.423018591	0.729026908	-0.101505141
H	4.770658821	-0.294297494	0.469913449
H	4.196012094	-0.431663647	-1.210268435
H	3.941771460	-0.818485867	2.884970608
C	3.019163191	-0.283148072	2.609213954
H	3.288527401	0.700282396	2.204368189
H	2.429907406	-0.126585098	3.524473411
C	2.191462408	-1.093480999	1.613647380
C	2.876670587	-1.357754032	0.222897825
O	1.017086824	-0.312673216	1.244499448
C	3.518663567	-2.736305923	0.064775868
H	3.945535425	-2.824418790	-0.945183719
H	4.332585014	-2.880495926	0.793434467
H	2.779037503	-3.536165291	0.192674858
H	2.485568129	-3.019124217	2.633478711
C	1.666489241	-2.374383669	2.278924972
H	1.041492758	-2.091402727	3.136967361
H	1.031340225	-2.939875216	1.584363083
H	0.401298165	-1.782518403	-2.676612285

C	-0.649273058	-2.116055535	-2.603358286
O	-1.040781280	-2.309253342	-1.258660202
H	-0.740726052	-3.079038496	-3.131382169
O	-1.643239373	-1.506504336	0.900662975
O	-2.065282418	-0.067149744	-0.917060013
C	-1.974138117	0.631405051	2.020307612
H	-1.319217749	1.185488449	1.338021915
H	-2.721152176	1.323337394	2.440710886
H	-1.347544776	0.243462265	2.833886778
C	-2.638968170	-0.554333053	1.296648209
C	-3.245874899	-0.129137064	-0.088436836
C	-3.607674026	-1.253646456	2.255630823
H	-3.071785783	-1.516132623	3.180651375
H	-4.450279782	-0.595717087	2.524155117
H	-3.999337337	-2.180259534	1.816540708
H	-3.695058480	-2.187786816	-0.626953528
C	-4.189249870	-1.208180440	-0.650240359
H	-4.422651673	-0.963478649	-1.696593924
H	-5.134696634	-1.262659718	-0.086323428
C	-3.938769414	1.234325024	-0.110284422
H	-3.245868660	2.040215865	0.164346579
H	-4.317279786	1.441082056	-1.123065353
H	-4.795380575	1.253142699	0.583390357
H	2.519796683	1.959708217	-4.042906856
H	-1.291771635	-1.374893062	-3.115078939
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TS SYN A<sub>2</sub>



Electronic Energy=-10525.87 kcal/mol

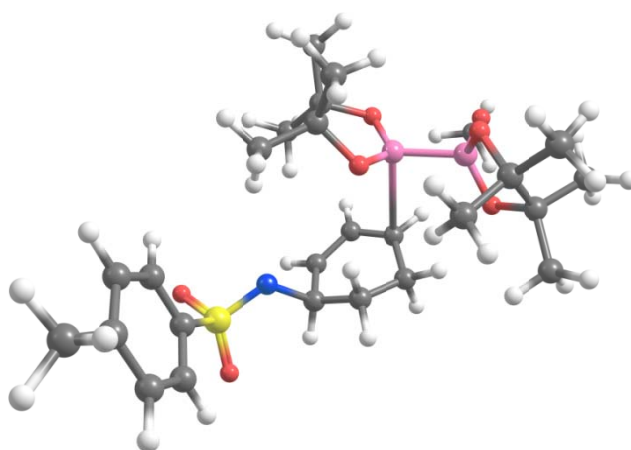
B	0.674715460	-0.026998727	-0.256855231
B	-1.024673116	-0.901622047	-0.604862683
C	-0.448268674	2.294310566	-0.703751321
C	0.741602557	3.032999050	-0.791939042
C	1.042498358	4.056277403	0.096397887
N	0.768128396	3.674323269	2.268434702
C	0.123439141	4.458275418	1.206689606
H	0.170982862	5.544121411	1.389303256
C	-1.317020526	4.024878968	0.925248194
H	-1.921772861	4.142615649	1.836078148
H	-1.727019529	4.712153446	0.164162774
H	-1.199411710	1.889724751	1.236630044
C	-1.417422431	2.578981983	0.406244878
H	-2.435650323	2.336539354	0.079261012
S	1.754682705	4.460106156	3.265886115
O	1.967988031	5.892482107	2.935034538
C	0.847436690	4.457703608	4.844067162
O	2.950380244	3.644453210	3.542287750

C	0.303964426	3.265735955	5.346581275
C	0.726751397	5.638191688	5.579206957
H	1.148531848	6.556390087	5.170031167
H	0.001690855	6.550577475	7.396556753
C	0.082124889	5.623363186	6.822205972
C	-0.455896239	4.441620496	7.347320080
C	-1.134695800	4.422126434	8.699141624
H	-1.177953552	5.428631830	9.136508250
H	-0.597060870	3.772604663	9.407756586
H	-2.164614150	4.039938869	8.629827341
C	-0.339553413	3.265137143	6.582860575
H	-0.761360686	2.331606624	6.966045815
H	0.383627558	2.350767141	4.759089597
H	-1.033250174	-0.078745431	2.248113202
C	-1.347838219	-1.087482698	2.536573871
H	-0.453367674	-1.612346291	2.898052793
H	-2.073786453	-1.022801687	3.362387475
C	-1.928187033	-1.858694593	1.340496621
O	-0.922844494	-2.026515356	0.321760312
C	-2.359363565	-3.254449708	1.805262798
H	-1.513515633	-3.743922970	2.311144269
C	-3.034067214	-1.040055685	0.576894737
C	-3.934024355	-0.182724165	1.468941237
H	-3.349196031	0.555468137	2.031688141
H	-4.494798371	-0.807676499	2.182933949
H	-4.662758185	0.359120639	0.846656430
H	-3.194557606	-3.191753232	2.521898049
C	-3.894801829	-1.939444208	-0.328650091
H	-2.659592284	-3.883555650	0.957677429
H	-3.251755574	-2.560358719	-0.965842625
H	-4.568121018	-2.590120435	0.252387024
H	-4.506498324	-1.297402452	-0.979026966
O	-0.909067378	-1.391915791	-1.967812108



H	-1.844354824	0.215514668	-2.932923256
C	-0.968999266	-0.456619108	-3.021737264
H	-0.050963980	0.156367927	-3.070889193
H	-1.057160888	-1.010466188	-3.970289073
H	2.006561113	-1.994254714	2.445546756
O	1.173773444	0.059366820	1.033626479
H	-0.786880783	1.723180114	-1.562762067
C	2.443253264	-1.941812843	1.438537892
H	3.434142381	-2.420790865	1.467972156
O	1.695829836	-0.231418161	-1.187275927
H	1.783011816	-2.498089542	0.760509026
C	2.542399102	-0.465495808	1.028332265
C	3.362228046	0.314354704	2.052701592
H	2.989310947	0.091442883	3.062129937
H	2.001990164	4.575339082	0.041796856
H	3.280686536	1.398398657	1.912866203
H	4.423125486	0.017638345	2.011354581
H	3.147424696	1.895483643	-0.292552119
C	3.700039646	1.055821656	-0.729381198
H	4.712496226	1.048275755	-0.298298729
H	3.786943548	1.211803486	-1.815045582
C	2.980906609	-0.270841969	-0.475673734
C	3.793223587	-1.423775629	-1.068404554
H	4.744676135	-1.555391992	-0.528613328
H	4.025325591	-1.202543674	-2.120906188
H	3.231331060	-2.365411571	-1.034882669
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TS SYN A<sub>3</sub>



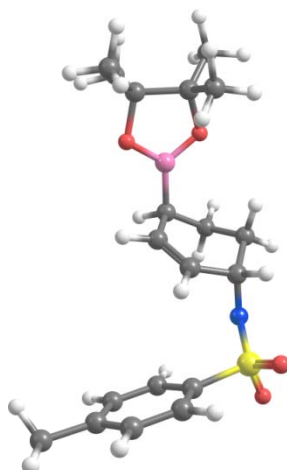
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B	-0.996918148	-1.098006887	-0.675580860
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C	-0.102951415	2.211291706	-0.579355586
C	1.133270230	2.848996663	-0.691694149
C	1.587857108	3.676189940	0.332039379
N	2.221504452	3.176261063	2.425253379
H	-3.458623401	0.393661092	1.893715259
C	1.026548084	3.662933041	1.716552415
C	-0.124956771	2.656418494	1.895040310
C	-0.959192008	2.450776423	0.617723108
H	-1.669234101	1.617886736	0.709637503
H	1.707120664	2.758590697	-1.616624428
H	-0.543881426	1.716393011	-1.443624876
H	-1.564384327	3.357353227	0.403911944
H	-0.765281448	2.965974457	2.734123946
H	0.329184740	1.690992202	2.158895615
H	0.730935168	4.677947713	2.041073467
H	2.457971219	4.318957206	0.181403353
C	-4.027924073	-0.240671796	1.201714566
H	-4.719896690	-0.866567062	1.788646079
H	-4.630105341	0.413426950	0.552335271
O	-2.160632563	-0.250168676	-0.339309451

O	-1.092694781	-2.287282588	0.187162319
O	-0.932032960	-1.542563137	-2.070850952
O	1.761258319	-0.671438639	-1.200266588
O	1.229696892	-0.507022851	1.030542796
H	-1.174640921	-0.409496639	2.183489780
H	-2.353803319	-1.307847750	3.190263649
H	3.859041190	0.811212330	-1.690802669
C	3.773457398	0.561834272	-0.622805914
H	3.237776374	1.370443198	-0.111725011
H	4.788133772	0.503051676	-0.200057367
C	3.416289174	-0.412420550	2.082177703
H	3.361535812	0.681839695	2.020032657
H	3.030516432	-0.708147895	3.068199183
H	4.468759399	-0.734860629	2.018468131
C	2.580923535	-1.077823549	0.992223518
H	-0.761550265	-2.014949050	2.794922679
C	3.039425521	-0.773393903	-0.483681626
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H	4.095635827	-1.577228108	-2.184730001
H	3.281755744	-2.819866471	-1.206955100
H	4.794585212	-2.063196435	-0.619323545
C	2.423535645	-2.578419311	1.274743256
H	1.953849676	-2.701295327	2.260417820
H	3.397455005	-3.092300667	1.286900845
C	-2.750798735	-3.426131796	1.505000922
H	-3.031509824	-3.991148354	0.606935426
H	-2.005072069	-4.015615013	2.059767852
C	-3.929709178	-1.866745325	-0.710900446
H	-3.269987068	-2.493193770	-1.324529945
H	-4.707426111	-2.496440959	-0.249122871
H	-0.906470468	-1.020058411	-4.047503966
H	-4.419675838	-1.135037528	-1.369707781
C	-0.862747887	-0.538379060	-3.057419906

H	-1.705711657	0.176447861	-2.981723291
H	0.086104060	0.026970877	-2.996354851
C	-3.103185072	-1.104807804	0.341887091
C	-2.148346752	-2.065045821	1.138570698
C	-1.584894141	-1.400641156	2.406521600
O	2.170262177	5.384888550	3.800319936
S	3.002625406	4.233794678	3.367526919
O	4.358769607	4.541431063	2.868680578
C	3.248478763	3.195506010	4.831293424
C	2.461152872	3.391733775	5.969815983
C	2.636269100	2.568750723	7.084044363
C	3.585320348	1.533232617	7.081529785
C	4.371262472	1.360250192	5.931557207
C	4.213871982	2.184049996	4.815587885
H	4.834476751	2.050297730	3.930485831
H	5.120516733	0.564499783	5.909188716
C	3.740115956	0.620518249	8.277691955
H	2.894838952	-0.081904135	8.354171923
H	4.659626042	0.024169614	8.208134925
H	3.774282112	1.190148919	9.217973252
H	2.021607684	2.732712284	7.973458926
H	1.724690973	4.195516329	5.969332881
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BORANE ANTI (Intermediate)

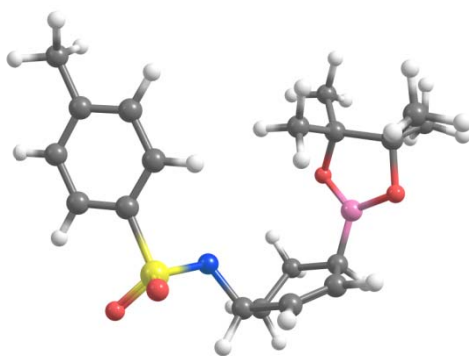


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C	0.566637665	2.778663029	1.751587225
C	0.238548499	1.572168210	2.607035274
C	0.407851195	0.294366604	2.229571267
H	1.182749325	3.194303950	-0.268893945
H	2.543661302	1.278902959	0.559050145
H	1.700628664	0.848395126	-0.947313232
H	0.169847035	-0.517059375	2.925304188
H	-0.288382512	2.195198935	-0.156230134
H	-0.101060609	1.780795878	3.626122780
H	-0.279496867	3.487342464	1.830050780
S	1.730804394	4.381609282	3.445390085
O	2.933640819	5.241731840	3.489366209
O	0.415093432	5.048235819	3.671464432
C	1.923661054	3.338160376	4.946856540
C	2.968604046	2.404372490	5.006436163
C	1.017889426	3.412480043	6.008002162
C	3.094406878	1.557368553	6.106063450
H	3.662071083	2.338191549	4.166639602
C	1.147050685	2.554178770	7.108404561

H	0.207820868	4.140719914	5.948651383
C	2.179412969	1.609788401	7.174857219
H	3.909786878	0.827582719	6.133318504
H	0.425818665	2.616977063	7.929578837
C	2.296473378	0.652873964	8.341296349
H	3.314553917	0.645240075	8.760388530
H	1.601635296	0.922932271	9.148649877
H	2.065708030	-0.381717730	8.038161800
N	1.816286928	3.439673550	2.189026293
H	1.681522955	-0.900373884	1.003764850
C	-2.207735499	-1.104982874	-1.122499968
C	-1.932376157	-2.404384030	-0.268694204
B	-0.307933024	-0.814039547	0.142058892
O	-0.899629036	-1.963354342	0.663234882
O	-0.942135461	-0.376901226	-1.013281447
C	-3.121994219	-2.906397471	0.548630451
H	-3.956834159	-3.202770779	-0.105385909
H	-2.815365649	-3.785747970	1.133173371
H	-3.474846431	-2.139936359	1.249326426
C	-3.289007884	-0.201447185	-0.518704126
H	-3.297851743	0.752189045	-1.064036888
H	-4.287639328	-0.657184977	-0.595304528
H	-3.076897875	0.017181441	0.536745479
C	-2.490173614	-1.348229477	-2.603263645
H	-3.410193424	-1.938330031	-2.736653838
H	-2.627545061	-0.381906487	-3.108641510
H	-1.659244601	-1.872561905	-3.091454285
C	-1.331500280	-3.553618899	-1.086902731
H	-0.998271998	-4.340728797	-0.396248342
H	-2.066857320	-3.987276012	-1.781090104
H	-0.460175001	-3.213206925	-1.662718240

BORANE SYN (Intermediate)



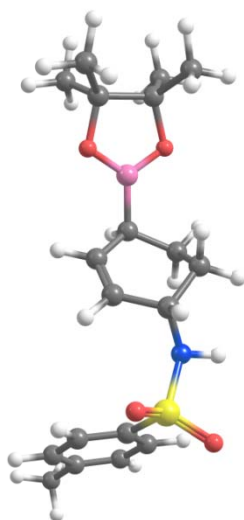
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C	1.130814677	2.707317439	-1.058184572
C	1.722276934	3.404894104	-2.043014026
N	2.642597936	2.311934570	-4.049494174
C	1.515594465	3.114135935	-3.513548818
C	0.173510272	2.377485099	-3.695140314
C	0.080839707	1.140781518	-2.791943943
H	0.869727261	0.444799022	-3.109852119
H	-0.881917330	0.623635679	-2.940383645
H	-0.711434259	1.632691748	-0.790739696
H	1.335026958	2.959750084	-0.012397104
H	2.422066756	4.209169329	-1.797525712
H	1.427494644	4.084902666	-4.036740512
H	0.075457004	2.081392704	-4.750236550
H	-0.645262938	3.083285897	-3.461754085
O	1.459103621	0.456895273	0.812509003
O	1.652936924	-0.753668256	-1.141346031
C	2.813592297	-1.128837204	-0.332781825
C	4.000425088	-0.365755829	-0.930464300
H	3.827929132	0.719388918	-0.896406676
H	4.095136359	-0.640569441	-1.989055684
H	4.943686043	-0.599380214	-0.414803856
H	3.891324214	-2.959481421	0.135967249

C	3.029940657	-2.633370547	-0.467289832
H	2.144555443	-3.204626609	-0.160654340
C	2.401710922	-0.624227988	1.106692771
C	1.655032972	-1.676547509	1.931372614
H	0.822451688	-2.109337552	1.360800295
H	1.245512821	-1.199563500	2.832782037
H	2.328293530	-2.489274448	2.244127811
H	3.163020186	0.317424357	2.896071878
C	3.545109375	-0.020572654	1.921723448
H	3.976254420	0.845491285	1.404764193
H	4.341601559	-0.759525942	2.099708111
S	3.745649694	3.153694019	-4.798412343
O	3.375266709	3.701755793	-6.140550623
C	4.955207935	1.836455794	-5.143495306
O	4.477350200	4.154118683	-3.960463112
H	5.196205660	1.288837169	-3.080548125
C	5.532861510	1.103759876	-4.099751385
C	6.522862386	0.158848100	-4.371091019
H	6.967954694	-0.408181094	-3.547450247
C	6.968327215	-0.072133464	-5.685373163
H	7.611699098	-2.132944892	-5.951288172
C	8.029281539	-1.112650637	-5.974193063
H	8.840594404	-1.079410429	-5.231711925
H	8.474467663	-0.962758021	-6.967691175
C	6.387998504	0.678277906	-6.716769474
H	6.723816427	0.522573725	-7.746501981
C	5.389977690	1.624527856	-6.451858798
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BORANE ANTI

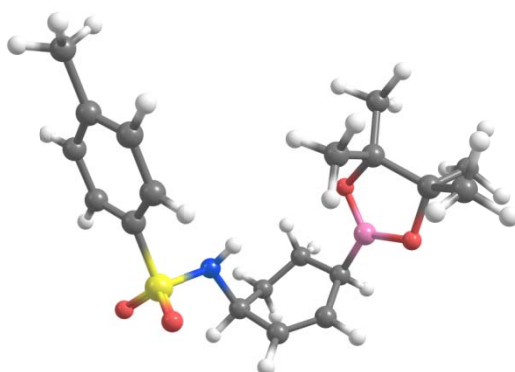


Electronic Energy=-7279.81 kcal/mol

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C	0.993661140	2.007544596	0.337069252
C	0.515552624	2.716218885	1.614544759
C	-0.463110456	1.853215395	2.377720292
C	-0.661813925	0.553978347	2.107936863
H	1.839866341	2.558645947	-0.105686527
H	2.147936458	0.519189633	1.387131994
H	1.780505472	0.082014173	-0.295197057
H	-1.447970219	0.016729770	2.645760305
H	0.174834904	2.053699860	-0.399642165
H	-1.067401518	2.353390353	3.136648407
H	0.002222969	3.653158227	1.340696225
S	1.655791116	4.190278398	3.665258824
O	2.737271713	5.142656419	3.399805707
O	0.265101102	4.613755553	3.828246995
C	2.123047655	3.296221453	5.151804129
C	3.471451628	2.987683291	5.368336876
C	1.157435333	2.978339887	6.106879873
C	3.843784485	2.348287174	6.547534602
H	4.220165781	3.264232259	4.626573503

C	1.549661761	2.342693239	7.288570980
H	0.116378155	3.245215287	5.930761229
C	2.892010793	2.018976546	7.529697431
H	4.896261406	2.109268127	6.715870657
H	0.795396101	2.101629363	8.040426942
C	3.319660635	1.362471889	8.820857256
H	3.846779519	2.080587297	9.467922539
H	2.458417018	0.978533816	9.381426351
H	4.009551120	0.527543834	8.635080530
N	1.745073709	3.055719179	2.414632911
H	0.486321193	-1.149929207	1.621796034
C	-1.270965924	-1.669139579	-2.180245895
C	-2.505080104	-1.878305260	-1.179958305
B	-0.755140698	-0.830484063	-0.080965377
O	-2.061208825	-1.238525537	0.066298131
O	-0.235725150	-1.059971076	-1.336114977
H	2.485943875	3.405315210	1.798655852
C	-0.673234071	-2.960926233	-2.741002335
H	-1.390684845	-3.488845634	-3.385709312
H	0.209759342	-2.710750468	-3.345135625
H	-0.353550283	-3.639530383	-1.940730732
C	-1.541392480	-0.690923067	-3.325831902
H	-0.608512873	-0.530958904	-3.883664663
H	-2.292631174	-1.089994326	-4.022701254
H	-1.887625576	0.282566708	-2.957141991
C	-2.799824260	-3.341295030	-0.839780806
H	-3.589423473	-3.376226845	-0.076862792
H	-3.151112387	-3.894842789	-1.722722146
H	-1.915611267	-3.850208214	-0.435765183
C	-3.797617425	-1.180837206	-1.606514301
H	-4.187286365	-1.603545313	-2.544315203
H	-4.556444909	-1.325183551	-0.825338130
H	-3.651768161	-0.102173551	-1.740475571

### BORANE SYN

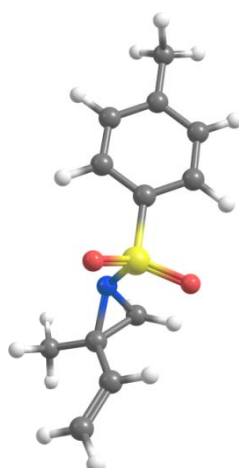


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C	1.099714939	2.800991080	-1.239258748
C	1.565039192	3.510475198	-2.279684930
N	2.519842883	2.267053152	-4.249404795
C	1.353508743	3.063457245	-3.708686195
C	0.080893123	2.209566239	-3.807712065
C	0.117320145	1.035809278	-2.819317201
H	0.896655809	0.328564000	-3.141364178
H	-0.828021028	0.475727686	-2.870874328
H	-0.570133161	1.570044526	-0.799660790
H	1.270536709	3.167479169	-0.222724525
H	2.126999931	4.431275984	-2.110204113
H	1.260953531	3.933851817	-4.372618732
H	-0.033390864	1.838736338	-4.836198033
H	-0.775048541	2.868998883	-3.590443817
O	1.572784836	0.544729220	0.785587892
O	1.909278888	-0.642399778	-1.167028503
C	2.904724755	-1.160216427	-0.213269749
C	4.243292126	-0.528714347	-0.608032874
H	4.206972118	0.566133586	-0.521624110
H	4.459034355	-0.785399212	-1.654234800
H	5.067045980	-0.902513174	0.016671990

H	3.672895777	-3.111081272	0.358677029
C	2.968718080	-2.676300065	-0.366626173
H	1.985430724	-3.140712018	-0.225106985
C	2.350085771	-0.645758266	1.172365767
C	1.364519374	-1.614057639	1.830924405
H	0.579138836	-1.922585192	1.127656992
H	0.885450571	-1.108581462	2.680180252
H	1.873866297	-2.513545960	2.205358721
H	2.940715093	0.152100715	3.088741616
C	3.420235145	-0.213646515	2.170347355
H	4.046539457	0.591720439	1.767786189
H	4.066648642	-1.063079624	2.438634454
S	3.853122552	3.207161009	-4.733817607
O	3.437457207	3.910585473	-5.946357242
C	5.013873554	1.904138910	-5.153304484
O	4.433536909	3.970824904	-3.624024042
H	5.744553810	1.748945741	-3.128320270
C	5.823575030	1.368988602	-4.146677326
C	6.747644537	0.376167340	-4.471639880
H	7.382823192	-0.041136739	-3.687311960
C	6.891197002	-0.076759435	-5.793231235
H	7.414242973	-2.150742472	-6.104303444
C	7.889407047	-1.157633035	-6.133637110
H	8.723369803	-1.170995733	-5.420131748
H	8.300125609	-1.021263822	-7.142394877
C	6.077972659	0.493456683	-6.787048234
H	6.190618774	0.170021415	-7.823951669
C	5.135738070	1.474934150	-6.476769850
H	4.513338778	1.926507995	-7.248532570
H	3.323119236	-2.925766087	-1.376408744
H	2.861512318	1.631478989	-3.515050299

2-METHYL-2-VINYLAZIRIDINE R (11)

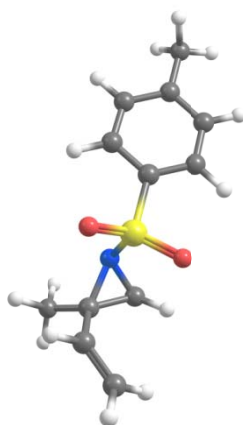


Electronic Energy=-4220.29 kcal/mol

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H	1.199175770	-2.598789442	-1.440380423
H	1.445098087	-3.667265026	0.058290054
C	1.730150298	-0.209894983	-0.319219860
H	1.302456417	-0.152708334	-1.323174991
C	2.499889836	0.789728287	0.128853447
H	2.945061684	0.786585632	1.124927109
H	2.707176231	1.654034289	-0.502096821
C	1.957714655	-1.573751942	1.853211122
H	3.057747472	-1.569740326	1.836010213
H	1.615005195	-0.739926877	2.481267846
H	1.614693952	-2.511465768	2.307458446
N	0.023404337	-2.056777990	0.331001233
S	-1.188165652	-1.306447629	-0.626688046
C	-2.477145402	-2.546497053	-0.516787854
C	-2.815363869	-3.285508272	-1.651144852
C	-3.168473311	-2.719034619	0.687963629
C	-3.857987135	-4.212062063	-1.573308621
H	-2.275086672	-3.119020245	-2.582074981
C	-4.201352126	-3.650721127	0.748260961
H	-2.900607725	-2.121787493	1.558951251

C	-4.565830603	-4.409523904	-0.379315106
H	-4.128050183	-4.787920337	-2.460752618
H	-4.741831460	-3.788967203	1.687142892
C	-5.712290354	-5.389310619	-0.307320110
H	-6.677318441	-4.859207752	-0.314081769
H	-5.705722059	-6.078324409	-1.160880340
H	-5.674730063	-5.982342192	0.616571202
O	-0.793118227	-1.212535810	-2.039008688
O	-1.609364007	-0.123194362	0.114993655

2-METHYL-2-VINYLAZIRIDINE R' (11)

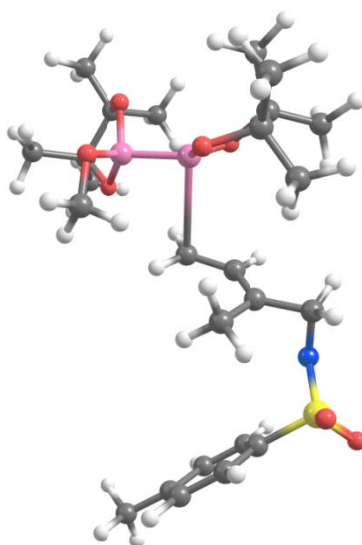


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H	1.269368309	-2.262382606	-1.595487848
H	1.627715127	-3.511764551	-0.270029472
C	1.546202584	0.009146104	-0.043534862
H	1.074320352	0.781879086	0.570953432
C	2.280152438	0.357312492	-1.103420465
H	2.768620108	-0.385150492	-1.737936440
H	2.406861907	1.405124904	-1.377912138
C	1.882745779	-1.648065265	1.841776306
H	2.974263992	-1.509791641	1.862386099
H	1.433759166	-0.941205760	2.554144923
H	1.639603609	-2.668395959	2.165725325

N	0.039681882	-2.112310774	0.216293063
S	-1.218179509	-1.322746937	-0.650937770
C	-2.509289326	-2.560097114	-0.516672259
C	-2.847738401	-3.325651723	-1.632932655
C	-3.194667417	-2.711441453	0.693804413
C	-3.884261288	-4.256960152	-1.530565112
H	-2.313355034	-3.176213972	-2.570248570
C	-4.222842627	-3.646366874	0.778795437
H	-2.927032839	-2.092921342	1.549714176
C	-4.586698643	-4.432383198	-0.329915002
H	-4.154614988	-4.853790445	-2.404023097
H	-4.759735385	-3.765702812	1.722406941
C	-5.725660151	-5.418611497	-0.229539983
H	-6.693577468	-4.894763097	-0.201858716
H	-5.741342132	-6.102843827	-1.086835232
H	-5.655311237	-6.017774091	0.688795978
O	-0.896309472	-1.177779573	-2.073703058
O	-1.603527420	-0.171930267	0.165030335

TS ANTI R



Electronic Energy=-10326.58 kcal/mol

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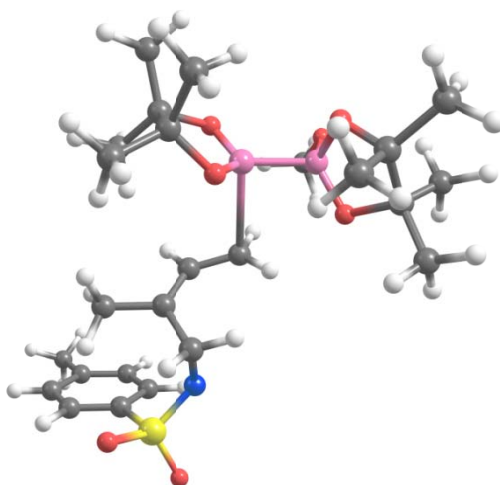
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C	0.254330016	1.612621710	-1.129957821
C	1.476344033	2.213135476	-0.930578503
C	2.535074647	2.189834979	-1.861238411
N	3.637591666	4.147107571	-1.926761176
C	3.860048357	2.762423376	-1.480370098
H	4.699681779	2.256131601	-1.978988982
H	-0.524734186	1.592673936	-0.372126957
H	1.692311339	2.645970385	0.050832348
S	4.324001499	4.587922251	-3.324827249
O	5.082635718	5.829974042	-3.083146202
H	2.228375482	6.551434556	-2.940836564
C	2.065890175	6.098367454	-3.918760927
O	5.015469107	3.497832299	-4.057532231
C	2.938749890	5.097755167	-4.368367361
C	0.998715814	6.493792814	-4.720329766
H	0.317877285	7.269723665	-4.360309747
C	2.740794483	4.508033826	-5.617016892
H	3.433167465	3.736269489	-5.953098677
C	1.664976877	4.916659471	-6.414372508
H	1.513019655	4.449319177	-7.390827977
H	-0.333084977	7.409020685	-7.090360411
C	-0.394043372	6.340439231	-6.834541524
H	-0.432451885	5.771340660	-7.771895164
C	0.776995259	5.908754836	-5.981272343
H	-1.349887088	6.185297477	-6.308498165
C	3.271018254	-0.284828567	2.314471321
H	2.792926827	0.029009918	3.253653304
H	3.431589114	0.284996984	-0.522052768
H	3.510214776	0.615863054	1.735841270
H	4.210707263	-0.802253956	2.565620991
H	4.027992631	-1.049339711	-1.535446063
H	4.808331040	-0.707890166	0.031178461



C	3.844448698	-0.731252286	-0.499499880
C	2.857531419	-1.700889742	0.150621005
C	3.439131715	-3.115191576	0.130063758
H	4.330998664	-3.185989085	0.773359196
H	3.741152456	-3.363182736	-0.898036293
H	2.701808713	-3.858781211	0.455917888
H	2.705205980	-2.984368284	2.781885572
C	1.861189825	-2.358644881	2.452703740
H	1.373913111	-1.934341610	3.341735884
H	1.123294403	-2.984213006	1.933186695
O	1.642296587	-1.709104479	-0.663472425
C	2.325091803	-1.208734931	1.549157831
O	1.127954086	-0.448067291	1.190065559
C	-0.751422351	-1.526522201	-2.875955408
H	0.256444086	-1.065853235	-2.851848466
O	-1.077892132	-2.128803662	-1.647102590
H	-0.748079207	-2.303670247	-3.657230480
O	-1.523745122	-2.075017498	0.698862620
C	-2.577755764	-1.371849332	1.379428639
O	-2.054995516	-0.130527674	-0.530734409
C	-1.975709103	-0.474436764	2.474761035
H	-1.366728543	-1.096782393	3.145251571
H	-1.316304032	0.283601660	2.036311770
H	-2.757765189	0.022074856	3.071388156
C	-3.218422134	-0.533127855	0.214149382
C	-3.505850448	-2.408688546	2.022382818
H	-2.962242836	-2.943082835	2.816433102
H	-3.844706844	-3.148451663	1.285866527
H	-3.581717038	-2.308909447	-0.992656773
H	-4.386069646	-1.925174533	2.477779322
C	-4.118263964	-1.402225641	-0.685787078
H	-5.057767827	-1.684463879	-0.183412313
H	-4.366619769	-0.828830304	-1.590706173

C	-3.975600953	0.723779051	0.646204619
H	-3.317434414	1.417765248	1.185412307
H	-4.359393501	1.242252443	-0.245920362
H	-4.833842184	0.472794907	1.290849446
H	-1.479348616	-0.742375725	-3.161452519
H	4.024420281	2.759459800	-0.392367013
C	2.369685801	1.595212576	-3.223111356
H	1.445272978	1.928659884	-3.717025812
H	3.230102240	1.826694659	-3.861760740
H	2.296353976	0.496723614	-3.116581110
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TS ANTI R'



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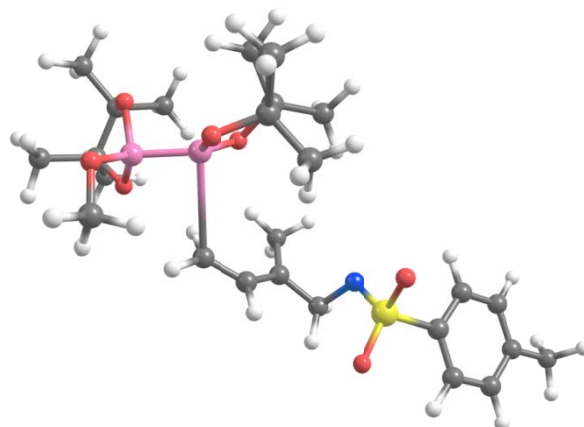
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C	1.575989545	2.103983672	-1.285495215
C	1.891238379	3.083489724	-0.320912728
N	0.725230334	4.934130169	-0.617875841
C	0.860935224	3.874982749	0.408048614
H	1.206247276	4.237597349	1.387484284
H	0.204101649	0.827230626	-2.306759109

H	2.396445718	1.799436174	-1.944555183
S	1.561854665	6.303419493	-0.443492711
O	0.666380660	7.423824469	-0.781205252
H	1.329566572	5.709154010	-3.280994450
C	2.375484432	5.951642708	-3.092385413
O	2.354091498	6.413970756	0.808447031
C	2.781605204	6.279563532	-1.791732692
C	3.315085823	5.908359215	-4.121202416
H	2.991737949	5.637683400	-5.129982196
C	4.123815972	6.568532711	-1.536348416
H	4.426876776	6.815928200	-0.518733669
C	5.058051842	6.520580243	-2.577616742
H	6.109223848	6.734842242	-2.365635436
H	5.678426073	7.081248400	-5.587594453
C	5.681613205	6.142983147	-5.009501949
H	6.701212102	5.995539463	-4.628125652
C	4.673013050	6.187970124	-3.883187720
H	5.460403959	5.327936399	-5.713090955
C	3.105944425	-0.097528085	2.412806146
H	2.572515034	0.245100195	3.311044041
H	3.420889334	0.422067520	-0.421016022
H	3.392102492	0.786860423	1.831319115
H	4.020826786	-0.619572277	2.736315254
H	4.050707346	-0.928837867	-1.389574201
H	4.770548282	-0.567884920	0.204107906
C	3.829215591	-0.593801344	-0.366043201
C	2.811731594	-1.554447009	0.256026686
C	3.395310477	-2.966244974	0.309187765
H	4.250525105	-3.015832569	1.002359384
H	3.750577039	-3.247490245	-0.693020987
H	2.640445127	-3.698825892	0.619772874
H	2.501155022	-2.777391272	2.903262959
C	1.680042428	-2.156193314	2.513354899

H	1.151326895	-1.705830118	3.365093143
H	0.964542205	-2.788723190	1.971720597
O	1.647186714	-1.584894024	-0.627519762
C	2.199936582	-1.029497512	1.609872275
O	1.033112943	-0.273169570	1.161838457
C	-0.744905299	-1.388221090	-2.992406319
H	0.334887624	-1.144343941	-3.019611008
O	-1.115094146	-1.974519568	-1.769838423
H	-0.942554548	-2.111724190	-3.800648940
O	-1.480776003	-2.062763613	0.562209328
C	-2.569622513	-1.473233736	1.294321858
O	-2.068190140	-0.038500744	-0.500347827
C	-2.014128356	-0.721948864	2.515522293
H	-1.422829272	-1.426145716	3.118251652
H	-1.348255458	0.090726988	2.202782879
H	-2.819903894	-0.316424519	3.147831874
C	-3.217119020	-0.505451207	0.231045047
C	-3.481863311	-2.612126839	1.768355094
H	-2.935914663	-3.239121399	2.489785280
H	-3.786663230	-3.249421028	0.928461360
H	-3.631588406	-2.116092354	-1.175109505
H	-4.383224393	-2.220633670	2.268440749
C	-4.150466395	-1.251852142	-0.741238054
H	-5.079635436	-1.588025636	-0.253084887
H	-4.415808948	-0.566729312	-1.559602130
C	-3.946260214	0.702674028	0.822822949
H	-3.266782239	1.321767224	1.422743827
H	-4.346517360	1.325892355	0.008922559
H	-4.790518399	0.385314724	1.456997362
H	-1.319897653	-0.466537807	-3.210195628
H	-0.102698756	3.364494099	0.520183087
C	3.328629609	3.401289140	-0.052652874
H	3.959127462	3.278252215	-0.944878164

H	3.458985144	4.405564044	0.368908272
H	3.692784569	2.685596058	0.708621257
H	-0.525540458	1.701113512	-0.860335882

TS SYN R



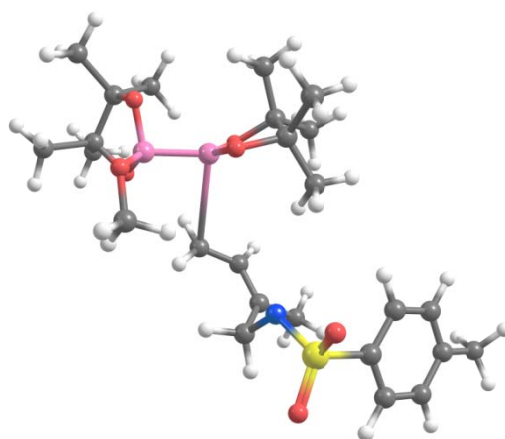
Electronic Energy=-10325.18 kcal/mol

B	1.967907572	3.859426459	-1.465376906
B	0.665325335	2.756010095	-0.809785780
C	2.693167738	0.644963606	-1.048913719
C	2.374129601	-0.636400575	-0.643085222
N	0.809796930	-2.580507881	1.169619672
C	2.397645215	-1.082321359	0.688848599
C	2.264337809	-2.544673419	1.006812946
H	2.634241614	-3.179482647	0.185979600
H	2.786203275	-2.813268974	1.942390072
C	2.503687911	-0.162272768	1.855923874
H	1.675126496	-0.390493939	2.545938356
H	2.453146523	0.897716437	1.587126034
H	3.437314495	-0.374235634	2.410020033
H	2.167469418	-1.395969025	-1.404407165
H	2.803879381	0.857822706	-2.109728848
H	3.017054075	1.438104543	-0.378237526
H	-1.106613770	0.616853349	1.687423596
C	-1.435376648	1.646531068	1.871284691

H	-2.529241322	1.647641503	2.005679312
H	-0.980080533	1.998856036	2.808782317
C	-1.038972010	2.582120445	0.732809166
O	-0.484912150	2.590585985	-1.568900410
C	-1.576573396	2.167936545	-0.686700115
O	0.418746371	2.520821184	0.548992813
C	2.081803611	2.845389934	-3.705353589
H	1.872321586	3.086677247	-4.759845150
H	1.457735556	1.973430080	-3.425975577
C	-1.367771645	4.036070809	1.100654199
H	-2.447394292	4.181819042	1.258522915
H	-1.015860832	4.723264918	0.319225653
H	-0.843936437	4.290907187	2.032956504
H	-3.112131939	2.564026775	-2.148252018
H	-3.682933519	2.702879273	-0.465664511
C	-2.836158560	2.907612785	-1.140746004
H	-2.667609873	3.991432061	-1.186170883
H	-1.913961228	0.437024322	-1.919554804
H	-2.628683740	0.291533288	-0.296627932
C	-1.756100064	0.658943013	-0.855076231
H	-0.875318262	0.100083574	-0.517930394
H	3.146809720	2.548914163	-3.620553499
O	1.779926491	3.970491247	-2.918787505
O	1.543467116	5.143434072	-0.857019156
O	3.360410420	3.640508058	-1.012908438
C	2.603172148	5.618947029	-0.010605322
C	3.870238794	4.938666510	-0.647897352
C	2.362526144	5.151394359	1.435634563
H	1.371229682	5.498977272	1.758507663
H	2.367991554	4.056816478	1.494428676
H	3.116331570	5.561251783	2.127039703
C	5.057380888	4.759780232	0.300195721
H	4.791328130	4.131010778	1.159978926

H	5.887275776	4.274560755	-0.236098394
H	5.415791592	5.734570465	0.670694963
C	4.330715401	5.671703386	-1.922688469
C	2.588300713	7.151813185	-0.058966253
H	1.658538312	7.519345206	0.401791150
H	3.484624368	5.804402937	-2.608402792
H	2.618641438	7.514467610	-1.094337250
H	4.777293942	6.653487672	-1.696159525
H	3.437878540	7.579522564	0.498894451
H	-1.261177811	-3.780043341	2.787723836
S	0.010840923	-3.603464138	0.201989038
O	-1.325314095	-3.061964523	-0.082511208
O	0.806504817	-4.149323819	-0.924334760
C	-0.293643103	-5.014436197	1.309021600
C	-0.950138488	-4.792079086	2.528372696
H	0.629714529	-6.460465035	0.017233104
C	0.121469318	-6.302857782	0.968927526
C	-1.183755146	-5.855810122	3.395135576
H	-1.688458252	-5.670396252	4.347406380
C	-0.125798594	-7.366851260	1.846709820
C	-0.776180863	-7.163580795	3.070449929
H	0.196067621	-8.375223844	1.572124153
C	-1.046976622	-8.308662384	4.020492775
H	-2.125918683	-8.516728908	4.098557871
H	-0.552337483	-9.230821359	3.687705841
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TS SYN R'



Electronic Energy=-10321.75 kcal/mol

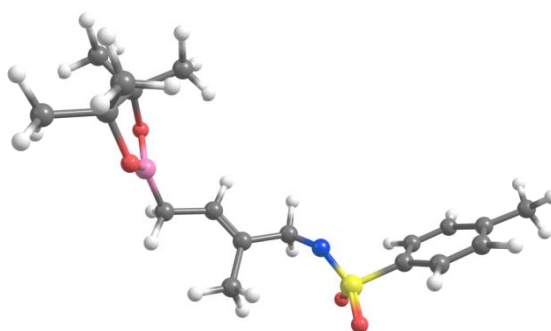
B	-1.162425466	-1.364321425	-0.450927868
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C	1.769674271	2.004052768	-1.480065920
C	2.733867156	2.219275782	-2.485659294
N	3.546585463	0.333221267	-3.440458893
C	2.714434637	1.494836394	-3.795828763
H	3.126311706	2.107085285	-4.617087648
H	-0.173276868	1.266490756	-0.857152652
H	1.945324874	2.506390083	-0.522388452
S	4.859929235	0.073716835	-4.339823563
O	5.220308002	-1.342092495	-4.163982551
H	6.099748648	-0.057329974	-1.704753702
C	6.626350073	0.714240635	-2.266696853
O	4.769266773	0.617232276	-5.717718049
C	6.245441740	0.982393141	-3.589570907
C	7.662826159	1.439920948	-1.682546148
C	6.923264364	1.961800929	-4.319854119
H	6.624596833	2.141047710	-5.352828840
C	7.965734306	2.680485863	-3.724922209
H	8.493589609	3.441632315	-4.306033985
H	10.071398268	2.639462015	-1.094051124



C	9.433642754	3.259716781	-1.739369324
H	10.073651781	3.746995960	-2.486905361
C	8.345285303	2.442160932	-2.397417662
H	9.004881990	4.052898606	-1.105473248
C	2.884983387	-0.096191437	2.647535631
H	2.312496713	0.410598819	3.438599348
H	3.302829326	-0.053589039	-0.255043199
H	3.256700491	0.662992894	1.948561688
H	3.747417213	-0.595612136	3.117541786
H	3.929297502	-1.543405396	-0.958884321
C	3.693101062	-1.048805299	-0.007782519
C	2.653863457	-1.880576831	0.745862870
C	3.225999280	-3.255226616	1.088170538
H	4.039206599	-3.170053352	1.827195841
H	3.639945416	-3.708579585	0.176430220
H	2.452862048	-3.926104178	1.483251164
H	2.103237011	-2.618430315	3.536058894
C	1.345181406	-2.051890962	2.973449871
H	0.759010022	-1.452436516	3.684222754
H	0.660864900	-2.754724848	2.479142545
O	1.514997568	-2.079687744	-0.155988638
C	1.989353526	-1.112899536	1.944741277
O	0.894750123	-0.390556982	1.283727675
C	-0.611688643	-1.645152372	-2.838806266
H	0.450294167	-1.361294867	-2.712918013
O	-1.143533823	-2.194951821	-1.657114640
H	-0.665656945	-2.404507005	-3.633984739
O	-1.735862407	-2.180875728	0.643369998
C	-2.812684878	-1.450119370	1.251443383
O	-1.977054773	-0.129581458	-0.506704139
C	-2.288441539	-0.729621838	2.505616753
H	-1.842322090	-1.479444654	3.174858933
H	-1.505924204	-0.009442556	2.237625116

H	-3.094976208	-0.214249189	3.051782371
C	-3.238055315	-0.446211361	0.113237276
C	-3.893502989	-2.460939388	1.658143899
H	-3.493625068	-3.124262813	2.440222751
H	-4.190966053	-3.085226242	0.806007540
H	-3.681520879	-2.039952902	-1.302566946
H	-4.785709030	-1.953759338	2.062237832
C	-4.145123736	-1.114605239	-0.937383834
H	-5.148465980	-1.339033878	-0.540267018
H	-4.253308197	-0.427907177	-1.789588364
C	-3.886368899	0.848416747	0.608576245
H	-3.204491750	1.408535352	1.261837191
H	-4.139215898	1.486704837	-0.251794908
H	-4.816568532	0.638279510	1.162365252
H	-1.175864138	-0.749929872	-3.169836554
H	1.704747215	1.172062908	-4.094544003
C	3.829622214	3.207625172	-2.244542967
H	3.942823901	3.450824152	-1.179293618
H	4.794477774	2.855106886	-2.637261194
H	3.598730353	4.144980700	-2.785060976
H	0.375599463	0.765305197	-2.549641631
H	4.618446674	-0.938056994	0.580010192
H	7.950219597	1.227924890	-0.648992785

BORANE E (Intermediate)

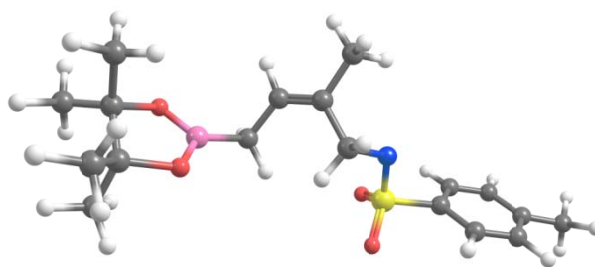


Electronic Energy=-7024.56 kcal/mol

C	-0.802689093	1.523831072	-0.102354495
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H	-2.006297695	0.648973664	1.433746893
C	0.319349207	2.202820840	0.210804498
H	0.299918276	2.804426627	1.128896601
C	1.642673431	2.208211426	-0.544172535
H	2.365255818	1.539327088	-0.038215402
H	1.504803945	1.816898137	-1.561418864
C	3.181171881	5.606229227	0.193318875
C	2.963887527	5.703375035	-1.365171473
C	2.086852153	6.310001068	1.003659492
H	2.197901405	6.030313200	2.060452902
H	2.160579611	7.404623249	0.922726960
H	1.087142799	5.996678762	0.673768198
C	4.561033911	6.038524428	0.683237050
H	4.736082121	7.104268143	0.468913995
H	4.622284239	5.895163058	1.771315276
H	5.359482596	5.448711615	0.216031750
C	2.236057721	6.959834072	-1.836998138
H	2.814266135	7.863251497	-1.587019697
H	2.112708183	6.923927901	-2.928626844
H	1.239963217	7.039975128	-1.385437621
C	4.253195426	5.505660724	-2.171124406
H	3.990166594	5.388944920	-3.231483232

H	4.931079618	6.366663152	-2.073074125
H	4.784777820	4.599665883	-1.849265965
B	2.266061466	3.647040978	-0.594261316
O	2.115912466	4.543483942	-1.642703340
O	3.029826061	4.171918667	0.443683944
H	-1.892304273	2.426574854	1.512003025
C	-0.967583135	0.643541504	-1.309910162
H	-1.832472344	0.994351920	-1.892240008
H	-0.074248364	0.604110734	-1.947131870
H	-1.223558061	-0.382113188	-0.994228568
N	-3.265804508	1.673862912	0.064529808
S	-4.407327835	0.638159694	0.374020843
O	-4.028606250	-0.481594161	1.284378804
O	-5.129515555	0.275488629	-0.866820716
C	-5.699575168	1.537509324	1.306122185
C	-5.774834807	1.461381121	2.702249122
C	-6.626723812	2.333995803	0.619793419
C	-6.765204238	2.164858424	3.395819656
H	-5.063561744	0.825498273	3.231236265
C	-7.612259316	3.032229731	1.318664729
H	-6.573585675	2.376379450	-0.468568663
C	-7.706185689	2.956074025	2.718824403
H	-6.817123941	2.086458068	4.486527425
H	-8.334920556	3.640920705	0.765772085
C	-8.819541434	3.660447503	3.463479795
H	-9.700047991	3.006342808	3.583293081
H	-8.502707207	3.965123685	4.471397426
H	-9.155133561	4.559569029	2.926920409

BORANE Z (Intermediate)

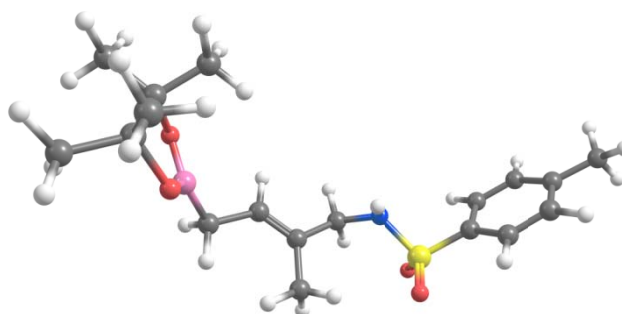


Electronic Energy=-7020.50 kcal/mol

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H	-2.031900743	1.829581179	-1.736694343
H	-0.359809207	1.472425355	-2.161160522
C	0.462527669	1.904309366	0.373238222
H	0.602208633	2.140099020	1.437327557
C	1.730035281	1.962880518	-0.460975899
H	2.503030014	1.346776462	0.030905796
H	1.559505838	1.529644953	-1.454882942
C	3.024166493	5.496751075	0.108049349
C	2.744895051	5.510994668	-1.442564543
C	1.902213204	6.142957365	0.929703424
H	2.073800288	5.924232012	1.992928240
H	1.877669602	7.235004514	0.797352062
H	0.923531391	5.728976108	0.651175255
C	4.378111357	6.064536913	0.527428587
H	4.455522402	7.129560700	0.258182987
H	4.488571532	5.979716316	1.617983679
H	5.206570058	5.520689281	0.057157429
C	1.912219286	6.689819971	-1.941104989
H	2.433867603	7.643278424	-1.762708490
H	1.746859280	6.586428836	-3.022765269
H	0.931880784	6.723382227	-1.450492612
C	4.016478616	5.365927446	-2.287484229
H	3.724833137	5.170137939	-3.328291605

H	4.631129286	6.278221288	-2.261168519
H	4.624435849	4.519263942	-1.940582764
B	2.242725595	3.440181086	-0.570485692
O	1.972507804	4.287072594	-1.636833817
O	3.002739777	4.066706126	0.417648066
C	-1.918748716	1.505433467	0.949500010
H	-2.715302753	2.219210657	0.673181406
H	-2.368417810	0.500821589	0.915689349
H	-1.595010107	1.725068682	1.977435486
N	-1.554453174	-0.219793677	-1.552447477
S	-0.707614185	-1.097849502	-2.549232794
C	-1.890594889	-2.450884299	-2.846375448
C	-1.808603620	-3.632891045	-2.105748430
C	-2.852290188	-2.337034026	-3.854825962
C	-2.683196074	-4.690921675	-2.373064743
H	-1.039231655	-3.712289801	-1.337284124
C	-3.718280222	-3.400217970	-4.121428292
H	-2.899432561	-1.412582588	-4.431874967
C	-3.645128967	-4.598165841	-3.390163711
H	-2.608958989	-5.612792212	-1.787742198
H	-4.463000950	-3.303147992	-4.917543966
C	-4.540862514	-5.771549207	-3.725023676
H	-4.086444686	-6.412771849	-4.499294369
H	-4.721203103	-6.404577148	-2.844357670
H	-5.515445760	-5.439023181	-4.110744272
O	0.491095160	-1.794449269	-1.996273089
O	-0.456910517	-0.468619252	-3.884309329

BORANE E



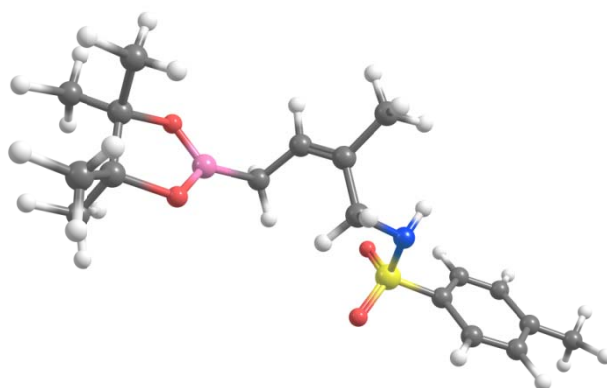
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C	-1.593033397	0.993063168	1.199471704
H	-1.863167472	-0.065795895	1.305908636
C	0.567228238	1.810628187	0.307433298
H	0.761133736	2.135112121	1.335741842
C	1.703300787	2.058236110	-0.663160647
H	2.570384474	1.427547277	-0.372860014
H	1.424831032	1.755778511	-1.681151575
C	2.958073345	5.571329984	0.124977323
C	2.744735488	5.651707982	-1.435758549
C	1.817265130	6.208094874	0.926055609
H	1.941733548	5.944917415	1.986696378
H	1.823667246	7.306139397	0.836120313
H	0.839902004	5.828325728	0.593670984
C	4.306002010	6.088775482	0.622417410
H	4.422544869	7.163296182	0.393421964
H	4.362797226	5.964830126	1.715264153
H	5.143639651	5.538036302	0.170415017
C	1.941418446	6.857254478	-1.918024680
H	2.460589912	7.798724978	-1.667451958
H	1.829863728	6.808421031	-3.012230669
H	0.937955191	6.875658260	-1.471828306
C	4.049675934	5.533124969	-2.232044465
H	3.802485659	5.393994717	-3.295119504
H	4.668595322	6.441203837	-2.133394871

H	4.640720506	4.666121747	-1.899479687
B	2.177238798	3.557292263	-0.664444328
O	1.971541814	4.437570360	-1.717351571
O	2.897363403	4.127263909	0.377962282
H	-1.119048088	1.311740691	2.142118331
C	-1.051614733	0.668487068	-1.280616984
H	-2.061296389	1.028373978	-1.534822998
H	-0.365243351	0.948864716	-2.089548493
H	-1.124387450	-0.432297669	-1.258959207
N	-2.894851325	1.714991619	1.087926150
S	-4.299244270	0.914933955	0.471111955
O	-4.097375611	-0.468254099	0.947421599
O	-4.418592293	1.170786678	-0.981905877
C	-5.638450358	1.658813239	1.260853834
C	-5.838357996	1.473390933	2.664956508
C	-6.535894436	2.506991728	0.547066761
C	-6.897660670	2.099277762	3.298731836
H	-5.157327538	0.832522531	3.221763724
C	-7.589767171	3.113643800	1.211381664
H	-6.388967599	2.647640534	-0.521657437
C	-7.808300863	2.935104607	2.602969755
H	-7.036792475	1.939266923	4.372054308
H	-8.277429017	3.744707699	0.640906829
C	-8.998563050	3.542768708	3.296739033
H	-9.871073563	2.858528164	3.334168818
H	-8.768959770	3.811904058	4.340131507
H	-9.339707970	4.457357515	2.787717577
H	-2.802085234	2.614665041	0.607762360



BORANE Z



Electronic Energy=-7081.70 kcal/mol

C	-0.744981769	1.592612135	-0.037604531
C	-1.179382947	1.338949560	-1.459124123
H	-1.979875577	2.054632714	-1.720623269
H	-0.368511363	1.503387273	-2.176637857
C	0.534807180	1.811866828	0.345150224
H	0.714097497	1.989955110	1.412325238
C	1.770353616	1.888343139	-0.523820362
H	2.565663272	1.274008562	-0.069654935
H	1.580546880	1.478235284	-1.523366317
C	2.997617664	5.441006158	0.106256777
C	2.706670195	5.479251302	-1.442162833
C	1.869313673	6.048221884	0.947732021
H	2.051621001	5.811240066	2.005761936
H	1.830865718	7.143654302	0.837866005
H	0.894065017	5.626883864	0.664751986
C	4.342913025	6.026373939	0.526617165
H	4.399140384	7.097393785	0.264661797
H	4.457565491	5.935826971	1.617251572
H	5.180288797	5.501638770	0.047848191
C	1.852628710	6.653832431	-1.911396693
H	2.362772588	7.610851291	-1.706827645
H	1.689368305	6.576987492	-2.996293203
H	0.872583144	6.662096732	-1.417194379

C	3.973610905	5.369615837	-2.297697389
H	3.678672815	5.190565701	-3.340935746
H	4.570350387	6.294609027	-2.255450460
H	4.600461014	4.528421338	-1.969234049
B	2.253592193	3.385021162	-0.606486042
O	1.952026622	4.239436640	-1.654404654
O	3.005866143	3.998983083	0.387789787
C	-1.853714515	1.583679079	0.991252185
H	-2.640214978	2.315754207	0.736862564
H	-2.355901206	0.602273413	1.056156019
H	-1.471930119	1.823208901	1.993381765
N	-1.740890952	-0.033869454	-1.719793396
S	-0.720425078	-1.149705089	-2.592183679
C	-1.767018748	-2.477885674	-2.937420091
C	-1.710206677	-3.671193492	-2.149535311
C	-2.792400957	-2.360071005	-3.931709782
C	-2.621346398	-4.692083155	-2.372637756
H	-0.931708023	-3.767602909	-1.392758388
C	-3.686643110	-3.399639077	-4.127040147
H	-2.850585480	-1.452276361	-4.532434438
C	-3.638974925	-4.595881080	-3.360728710
H	-2.548524765	-5.603220555	-1.768847599
H	-4.455966113	-3.293613413	-4.899829746
C	-4.577415504	-5.742598532	-3.635296782
H	-4.181425636	-6.453605290	-4.391844460
H	-4.774554942	-6.332849524	-2.724999580
H	-5.549404847	-5.388990893	-4.016944364
O	0.378461520	-1.613227894	-1.717191270
O	-0.391054364	-0.374221743	-3.804540498
H	-1.968167948	-0.504361877	-0.837215397

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