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ELECTRONIC SUPPORTING INFORMATION

A DFT Examination of the Role of Proximal Boron Functionalities on the S-Alkylation of Sulfenic Acid Anions

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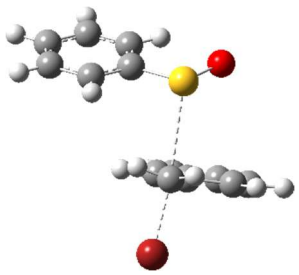
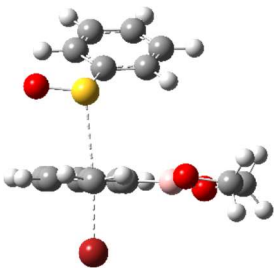
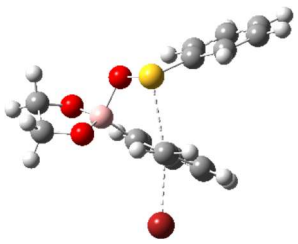
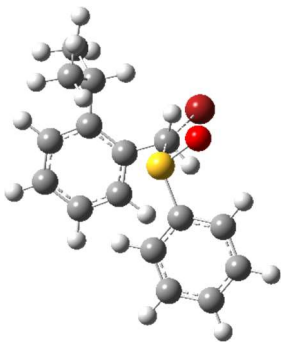
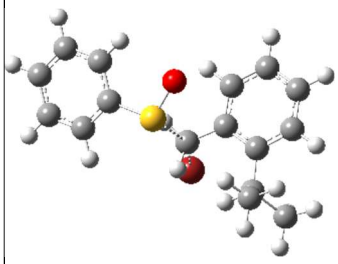
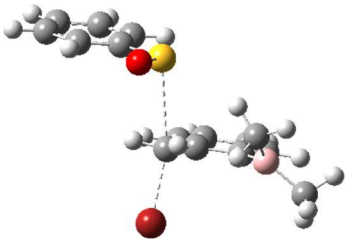
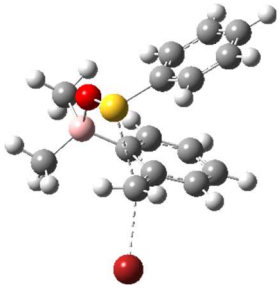
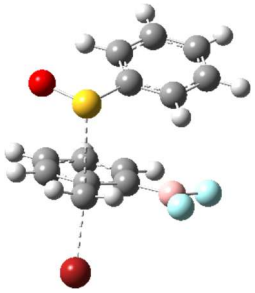
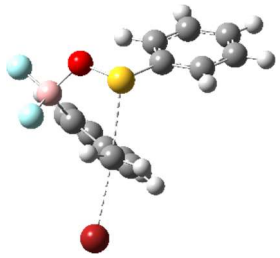
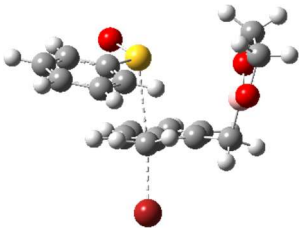
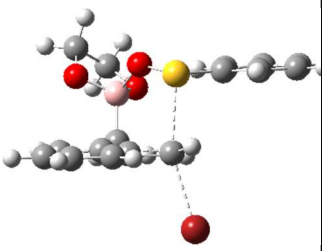
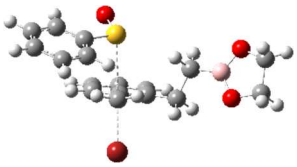
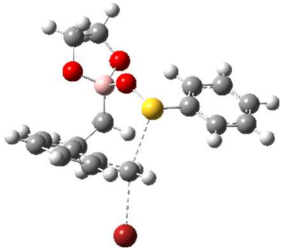
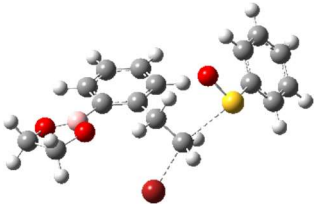
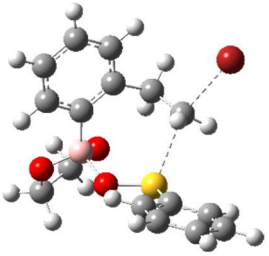
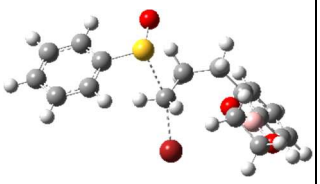
 1.2.TS	 1.2a.TS	 1.2a.C.TS	 1.2iP.TSa
 1.2iP.TSb	 1.2b.TS	 1.2b.C.TS	 1.2c.TS
 1.2c.C.TS	 1.2Ca.TS	 1.2Ca.C.TS	 1.2C₂a.TS
 1.2C₂a.C.TS	 1.3a.TS	 1.3a.C.TS	 1.4a.TS

Table S1. Alkylation transitions states, continued

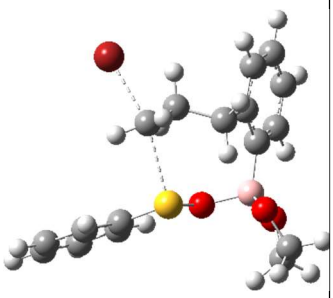
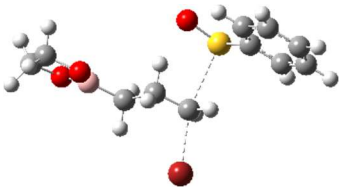
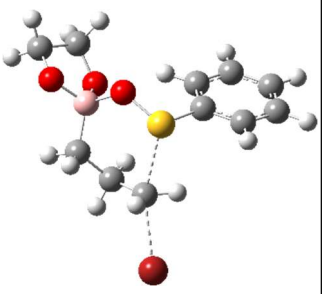
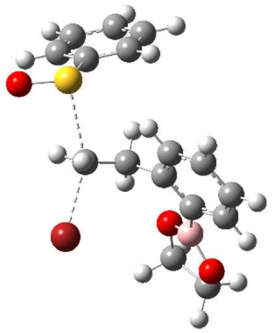
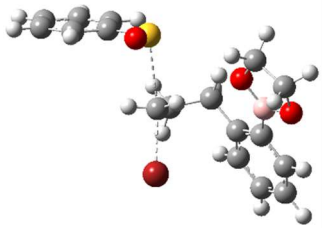
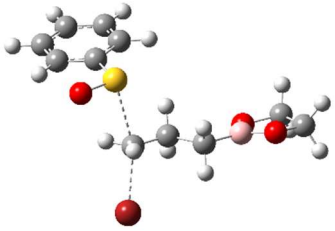
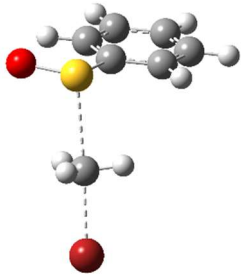
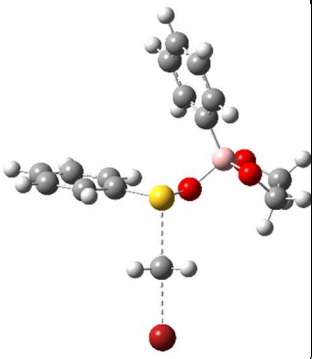
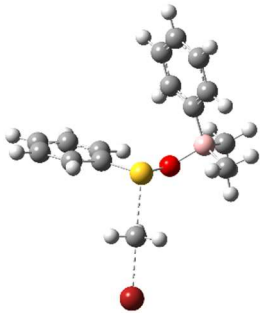
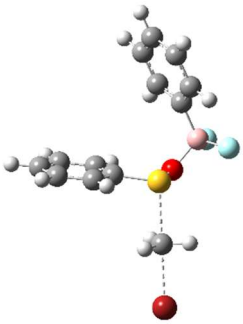
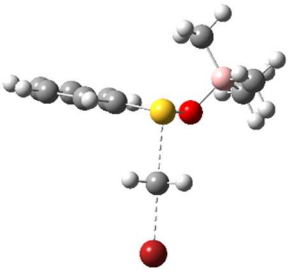
 1.4a.C.TS	 1.5a.TS	 1.5a.C.TS	 1.3a.TS2
 1.4a.TS2	 1.5a.TS2	 1.MeBr.TS	 1.6a.C.TS
 1.6b.C.TS	 1.6c.C.TS	 1.7.C.TS	

Table S2. Optimized geometric parameters for selected complexes and transition states.

Structure	r(S-O) (Å)	C-S-O (°)	r(O-B) (Å)	r(S-C) (Å)	r(C-Br) (Å)	Br-C-S (°)
1	1.608	106.82				
1.2a.C	1.660	102.87	1.556			
1.2a.C.TS	1.630	103.10	1.610	2.739	2.667	156.74
1.2a.TS	1.582	106.64	5.759	2.917	2.379	157.44
1.2b.C	1.661	102.84	1.505			
1.2b.C.TS	1.635	102.75	1.536	2.642	2.721	156.47
1.2b.TS	1.577	106.68	5.546	2.926	2.351	162.39
1.2c.C	1.652	103.68	1.585			
1.2c.C.TS	1.625	103.93	1.623	2.761	2.567	155.54
1.2c.TS	1.582	106.57	5.279	2.889	2.389	155.55
1.2Ca.C	1.653	103.73	1.550			
1.2Ca.C.TS	1.625	107.17	1.591	2.673	2.629	159.02
1.2Ca.TS	1.582	106.66	4.850	2.959	2.383	159.49
1.2C$_2$a.C	1.654	103.52	1.566			
1.2C$_2$a.C.TS	1.614	107.31	1.626	2.698	2.643	162.72
1.2C$_2$a.TS	1.582	106.57	5.799	2.974	2.393	158.16
1.3a.C	1.660	102.65	1.558			
1.3a.C.TS	1.633	101.48	1.589	2.601	2.571	156.85
1.3a.TS	1.584	106.46	5.746	2.805	2.495	161.14
1.4a.C	1.659	102.96	1.559			
1.4a.C.TS	1.635	100.86	1.595	2.621	2.516	156.24
1.4a.TS	1.583	106.43	6.024	2.805	2.477	160.27
1.5a.C	1.654	103.35	1.569			
1.5a.C.TS	1.627	105.46	1.583	2.611	2.534	157.54
1.5a.TS	1.583	106.40	4.423	2.815	2.477	162.57
1.3a.TS2	1.578	106.92	7.477	2.714	2.471	151.98
1.4a.TS2	1.580	106.73	5.422	2.722	2.438	154.440
1.5a.TS2	1.579	106.78	6.518	2.712	2.436	156.11

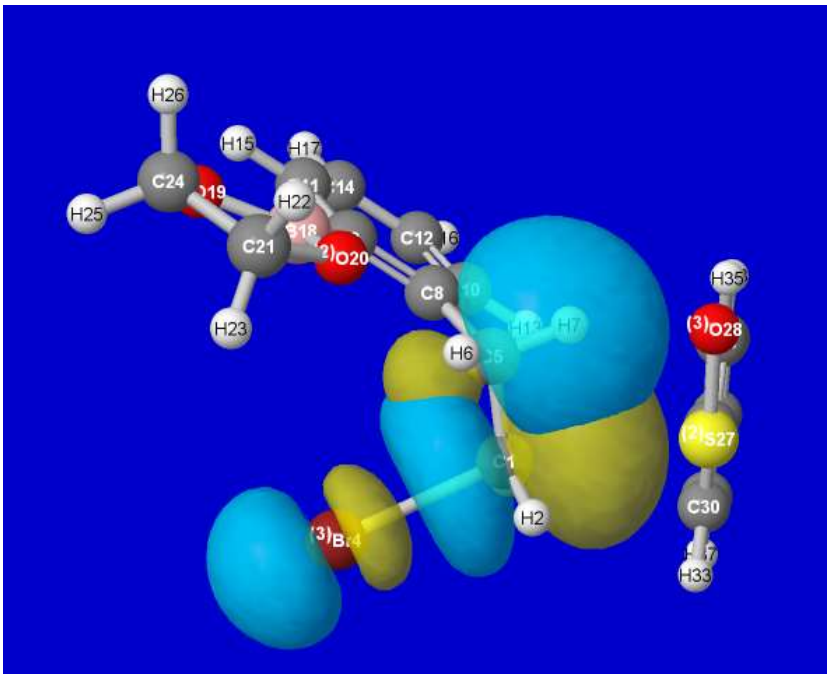


Figure S1. NBO representation of alkylation transition state hyperconjugation [$\sigma_{C\text{-}H} \rightarrow \sigma^*_{C\text{-}Br}$] of **1.3a.TS**.

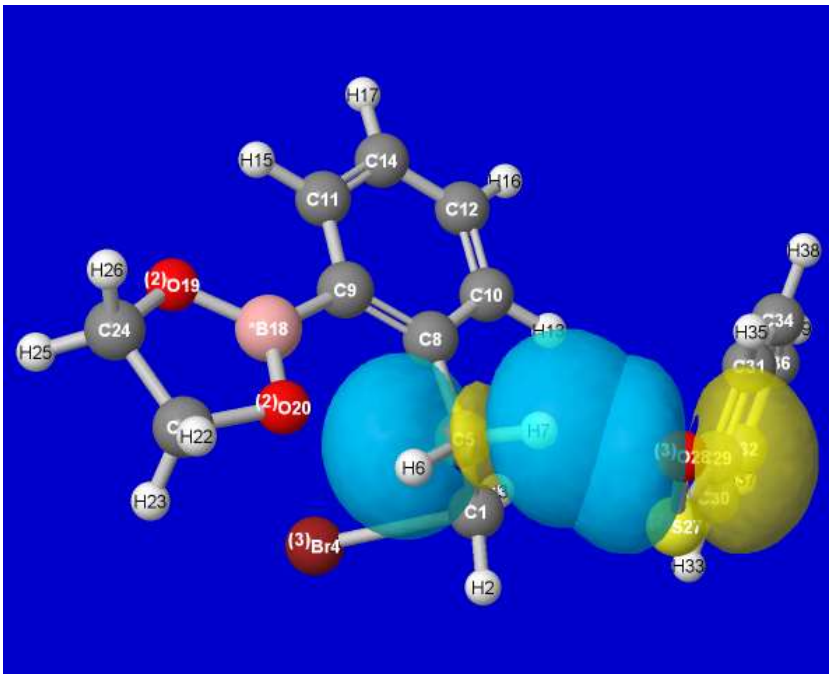


Figure S2. NBO representation H-bonding during alkylation transition state of **1.3a.TS**. [$n_O \rightarrow \sigma^*_{C\text{-}H}$]

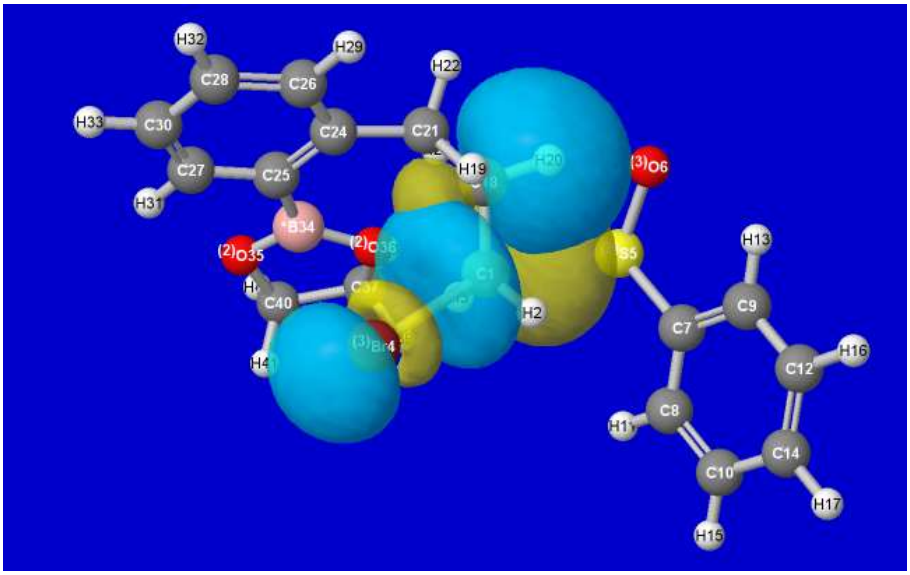


Figure S3. NBO representation of alkylation transition state hyperconjugation [$\sigma_{C\text{-}H} \rightarrow \sigma^*_{C\text{-}Br}$] of **1.4a.TS**.

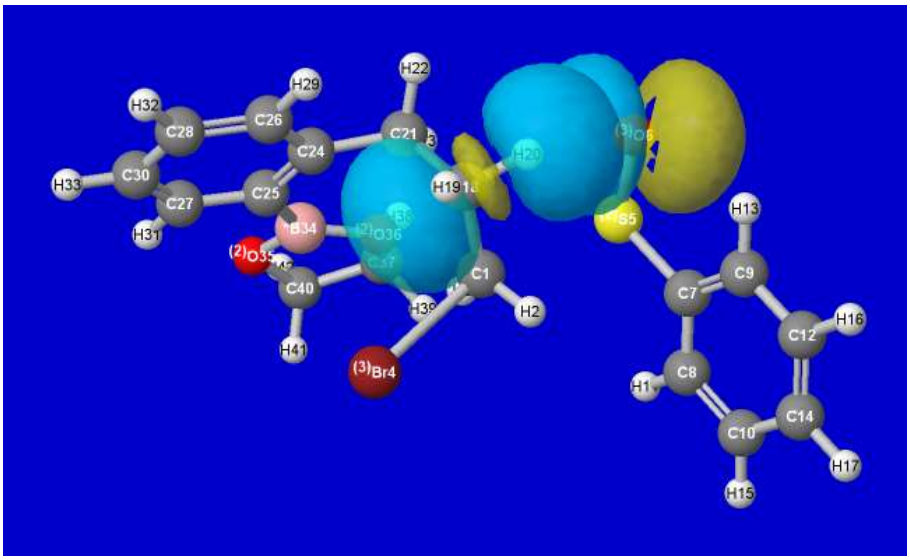


Figure S4. NBO representation H-bonding during alkylation transition state of **1.4a.TS**. [$n_O \rightarrow \sigma^*_{C\text{-}H}$]

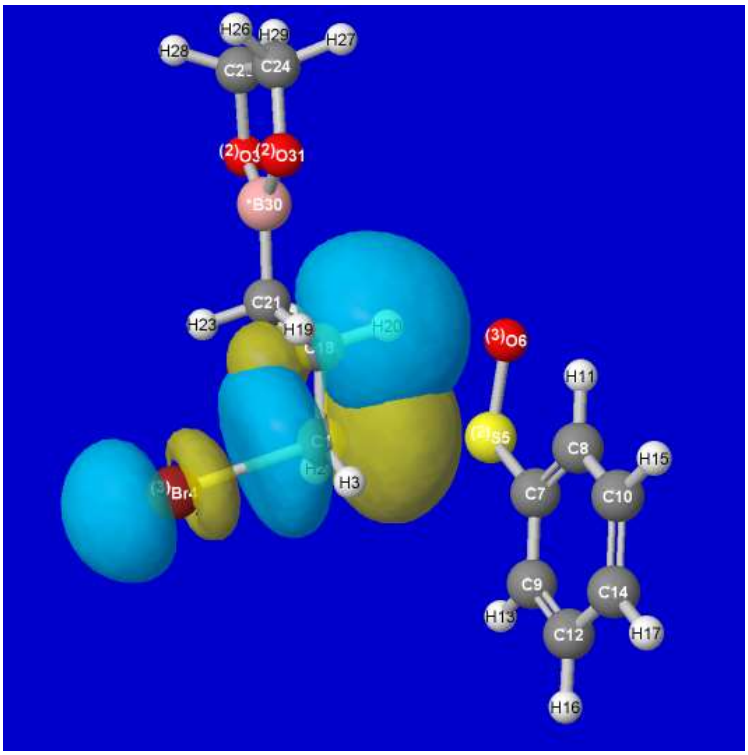


Figure S5. NBO representation of alkylation transition state hyperconjugation [$\sigma_{C\text{-}H} \rightarrow \sigma^*_{C\text{-}Br}$] of **1.5a.TS**.

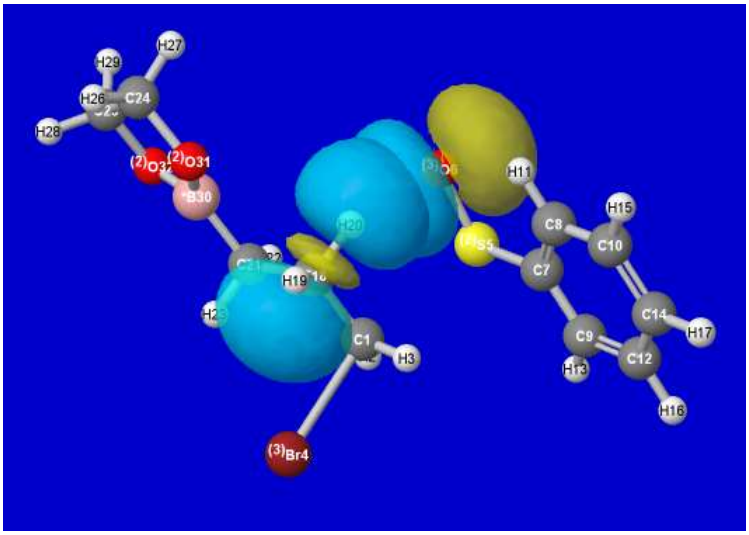
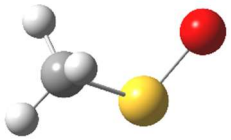
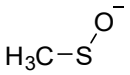


Figure S6. NBO representation H-bonding during alkylation transition state of **1.5a.TS**. [$n_O \rightarrow \sigma^*_{C\text{-}H}$]

Cartesian Coordinates and Thermochemistry Data of Structures and Transition States

Methyl sulfenate

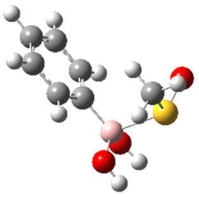


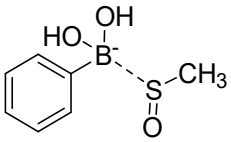



```
-1 1
 S                  0.19133800   -0.54633800    0.00000000
 C                 -1.40664400    0.35176800    0.00000000
 H                 -2.20805100   -0.39414800    0.00000000
 H                 -1.49874000    0.97862700    0.89232500
 H                 -1.49874100    0.97862700   -0.89232600
 O                  1.32299800    0.63346200    0.00000000

Zero-point correction=                           0.039081
(Hartree/Particle)
 Thermal correction to Energy=                    0.043215
 Thermal correction to Enthalpy=                  0.044159
 Thermal correction to Gibbs Free Energy=         0.012900
 Sum of electronic and zero-point Energies=           -513.432167
 Sum of electronic and thermal Energies=              -513.428033
 Sum of electronic and thermal Enthalpies=            -513.427089
 Sum of electronic and thermal Free Energies=         -513.458348
```

Methyl sulfenate S coordinated with PhB(OH)2



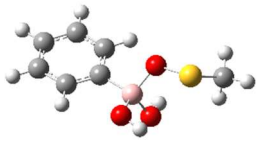


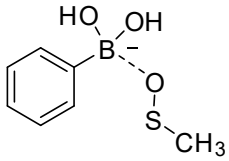

```
-1 1
 C                 -1.53050200   -1.76297700    1.08961700
 H                 -1.55329300   -1.29222800    2.07364300
 H                 -0.51219600   -2.06962500    0.84295900
 H                 -2.19972100   -2.62441900    1.07209100
```

S	-2.11593600	-0.54251600	-0.13657000
O	-1.96778500	-1.25577000	-1.54117300
B	-0.72659700	1.08197700	0.16239900
C	0.75598600	0.49918000	0.05374400
C	1.38671900	0.33236400	-1.19224500
C	1.48920200	0.12132000	1.19264300
C	2.67768500	-0.18759300	-1.29953400
H	0.85521500	0.62058600	-2.09260300
C	2.78180200	-0.39747600	1.09770800
H	1.03856500	0.24450500	2.17190400
C	3.38252700	-0.55613500	-0.15231800
H	3.13572900	-0.30350000	-2.27700200
H	3.32216100	-0.67589800	1.99734100
H	4.38682300	-0.95931200	-0.23128000
O	-1.07856000	1.49040800	1.50502700
H	-1.92288500	1.95004600	1.53323500
O	-1.04831200	1.99135300	-0.90941800
H	-1.96570200	2.28018300	-0.89034300

Zero-point correction=	0.164068
(Hartree/Particle)	
Thermal correction to Energy=	0.177391
Thermal correction to Enthalpy=	0.178335
Thermal correction to Gibbs Free Energy=	0.124159
Sum of electronic and zero-point Energies=	-921.709675
Sum of electronic and thermal Energies=	-921.696352
Sum of electronic and thermal Enthalpies=	-921.695408
Sum of electronic and thermal Free Energies=	-921.749584

Methyl sulfenate O coordinated with $PhB(OH)_2$





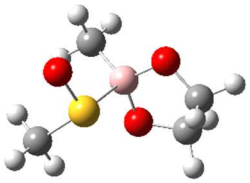
-1 1

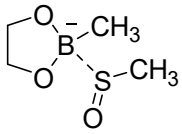
B	0.41905300	0.62545100	0.29354000
O	0.58387200	2.03414300	-0.05349600
H	1.46521000	2.31490200	0.21275100
O	0.88626200	0.44465800	1.69273700
H	0.80719900	-0.47729900	1.95289200
C	-1.13121000	0.15777200	0.07469000
C	-2.16580100	1.09006400	-0.11070700
C	-1.50863600	-1.19698900	0.11076800
C	-3.50090300	0.70005800	-0.24963700

H	-1.91529600	2.14538300	-0.14795200
C	-2.83773500	-1.60255100	-0.02634900
H	-0.74280600	-1.95671000	0.24085400
C	-3.84439900	-0.65175400	-0.20769000
H	-4.27335200	1.45017700	-0.39225900
H	-3.08968900	-2.65852700	0.00484000
H	-4.87906300	-0.96054300	-0.31627300
O	1.23083100	-0.29383900	-0.64126400
S	2.87322500	-0.00869700	-0.79785600
C	3.59866700	-1.18030400	0.39325000
H	3.28701300	-2.20127100	0.16456400
H	4.68318600	-1.10295200	0.27430000
H	3.32312700	-0.91871500	1.41450300

Zero-point correction= 0.164253
(Hartree/Particle)
Thermal correction to Energy= 0.177391
Thermal correction to Enthalpy= 0.178335
Thermal correction to Gibbs Free Energy= 0.123883
Sum of electronic and zero-point Energies= -921.735146
Sum of electronic and thermal Energies= -921.722007
Sum of electronic and thermal Enthalpies= -921.721063
Sum of electronic and thermal Free Energies= -921.775516

Methyl sulfenate S coordinated with MeB(EG)





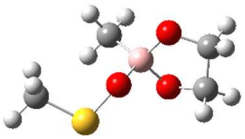
-1 1

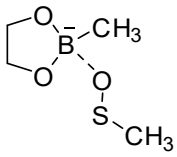
C	-2.08373600	0.82247000	1.16250700
H	-2.96139300	1.44948700	0.99792100
H	-1.38734000	1.32232200	1.83779900
H	-2.38761900	-0.13983300	1.57973900
S	-1.23305000	0.55789800	-0.43416400
B	0.44831100	-0.61025600	0.21535200
C	-0.10521100	-1.99168900	0.79195800
H	0.73547600	-2.64059100	1.07220300
H	-0.72235700	-1.85946800	1.68703700
H	-0.70653800	-2.53310600	0.05438800
O	-2.24065800	-0.30897700	-1.30290000
O	1.29519000	-0.71057700	-0.95681400
O	1.10826500	0.30453300	1.13963200
C	2.12953400	0.44444500	-0.97138500
H	1.64916000	1.25778500	-1.53171900

H	3.08245300	0.20757600	-1.45270900
C	2.28430500	0.81560300	0.51179500
H	2.36142400	1.89652000	0.66745300
H	3.17226000	0.33941200	0.94915200

Zero-point correction= 0.146315
(Hartree/Particle)
Thermal correction to Energy= 0.157604
Thermal correction to Enthalpy= 0.158548
Thermal correction to Gibbs Free Energy= 0.108980
Sum of electronic and zero-point Energies= -807.349411
Sum of electronic and thermal Energies= -807.338123
Sum of electronic and thermal Enthalpies= -807.337179
Sum of electronic and thermal Free Energies= -807.386746

Methyl sulfenate O coordinated with MeB(EG)





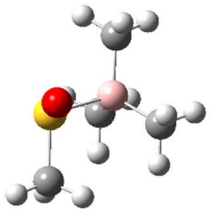
-1 1

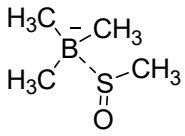
C	-3.17851500	0.30301100	0.36346000
H	-4.11501700	-0.04277500	-0.08343600
H	-2.95900200	1.31073700	0.00885800
H	-3.27868400	0.30033400	1.45059400
S	-1.89535600	-0.87657400	-0.16401400
O	-0.55313400	-0.32936200	0.66605700
B	0.51863800	0.49959200	-0.08194200
C	-0.08721900	1.86338300	-0.70525500
H	0.69891900	2.44614800	-1.20185100
H	-0.87083000	1.67647700	-1.44965500
H	-0.52324100	2.50231100	0.07301800
O	1.55882400	0.72711700	0.95517600
O	1.19160300	-0.34054100	-1.10418200
C	2.21137300	-1.05332500	-0.42503900
H	1.81300100	-1.97170200	0.03335100
H	3.00599400	-1.33717200	-1.12376000
C	2.69100300	-0.07544500	0.65899200
H	3.51282100	0.55276700	0.28032400
H	3.05035700	-0.59336500	1.55713500

Zero-point correction= 0.146814
(Hartree/Particle)
Thermal correction to Energy= 0.157573
Thermal correction to Enthalpy= 0.158517

```
 Thermal correction to Gibbs Free Energy=         0.110165
 Sum of electronic and zero-point Energies=           -807.372902
 Sum of electronic and thermal Energies=              -807.362144
 Sum of electronic and thermal Enthalpies=            -807.361199
 Sum of electronic and thermal Free Energies=         -807.409551
```

Methyl sulfenate S coordinated with Me_3B

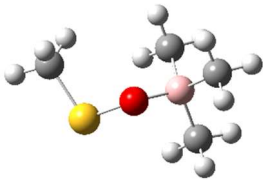


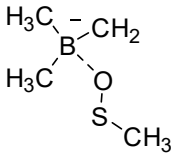


```
-1 1
 B                  0.99164000    0.04694800   -0.05899800
 S                 -0.94554300   -0.22878800    0.51836800
 C                 -1.78409500    1.25547100   -0.14563100
 H                 -1.36830500    2.14266800    0.33447200
 H                 -1.64255700    1.30789900   -1.22662500
 H                 -2.84637900    1.17383400    0.08844300
 O                 -1.61237800   -1.43443800   -0.26207700
 C                  1.05970600    0.22234600   -1.67341800
 H                  0.56007200    1.12660200   -2.04607800
 H                  2.11078300    0.29989000   -1.99017500
 H                  0.63463200   -0.63173400   -2.21651100
 C                  1.74054600   -1.30411300    0.46439100
 H                  1.38898500   -2.21670900   -0.03354100
 H                  2.81835000   -1.22965600    0.25738700
 H                  1.64190500   -1.46732800    1.54698600
 C                  1.46975900    1.37330300    0.76668700
 H                  2.55452300    1.50239500    0.63845900
 H                  1.00609700    2.30732800    0.42281900
 H                  1.29590600    1.30415100    1.84991000

Zero-point correction=                           0.154665
(Hartree/Particle)
 Thermal correction to Energy=                    0.165681
 Thermal correction to Enthalpy=                  0.166625
 Thermal correction to Gibbs Free Energy=         0.119388
 Sum of electronic and zero-point Energies=           -657.996037
 Sum of electronic and thermal Energies=              -657.985021
 Sum of electronic and thermal Enthalpies=            -657.984077
 Sum of electronic and thermal Free Energies=         -658.031314
```

Methyl sulfenate O coordinated with Me_3B

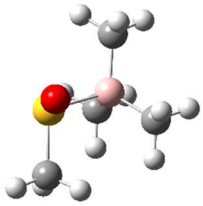


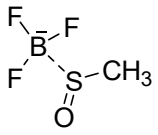



```
-1 1
 C                 -2.53731000    0.79683600    0.01334600
 H                 -3.51323900    0.51980400   -0.39613600
 H                 -2.07391600    1.54743600   -0.62779500
 H                 -2.67319000    1.19680000    1.02041000
 S                 -1.54688400   -0.73232800    0.06011700
 O                 -0.14677500   -0.23055200    0.81124600
 B                  1.15157700    0.07856000   -0.02846000
 C                  0.86170500    1.27261500   -1.11683700
 H                  1.77274400    1.51875700   -1.68213400
 H                  0.09978700    0.99802400   -1.86055000
 H                  0.52477200    2.20540800   -0.64042800
 C                  1.66200900   -1.29554200   -0.76637900
 H                  0.93369000   -1.68241600   -1.49378100
 H                  2.59947400   -1.13355500   -1.31894100
 H                  1.85581000   -2.10466800   -0.04603000
 C                  2.21195600    0.56558000    1.12223400
 H                  1.86849200    1.46420000    1.65579700
 H                  2.39136000   -0.20982000    1.88141000
 H                  3.19052000    0.81196600    0.68443500

Zero-point correction=                           0.154105
(Hartree/Particle)
 Thermal correction to Energy=                    0.165082
 Thermal correction to Enthalpy=                  0.166026
 Thermal correction to Gibbs Free Energy=         0.118642
 Sum of electronic and zero-point Energies=           -658.011229
 Sum of electronic and thermal Energies=              -658.000253
 Sum of electronic and thermal Enthalpies=            -657.999308
 Sum of electronic and thermal Free Energies=         -658.046692
```

Methyl sulfenate S coordinated with BF_3



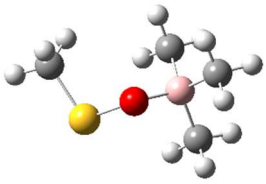


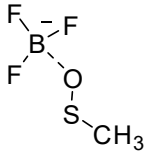
-1 1

B	-0.97097000	0.01617700	0.02965600
S	0.93423600	-0.23142200	-0.51728500
C	1.60052500	1.32336500	0.17926000
H	1.12201300	2.16094600	-0.33097100
H	1.39292000	1.35661900	1.24930500
H	2.67493900	1.33953500	-0.00265600
O	1.55327800	-1.39203700	0.33960100
F	-1.05554000	0.23375600	1.40684000
F	-1.43630700	1.13023000	-0.68758600
F	-1.65395100	-1.14611100	-0.33923000

Zero-point correction= 0.053122
(Hartree/Particle)
Thermal correction to Energy= 0.061327
Thermal correction to Enthalpy= 0.062271
Thermal correction to Gibbs Free Energy= 0.019912
Sum of electronic and zero-point Energies= -838.131926
Sum of electronic and thermal Energies= -838.123721
Sum of electronic and thermal Enthalpies= -838.122777
Sum of electronic and thermal Free Energies= -838.165136

Methyl sulfenate O coordinated with BF_3





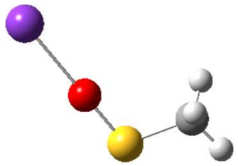
-1 1

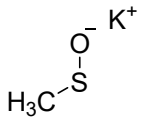
B	1.10131300	0.06332200	-0.01010000
F	0.83872300	1.19690300	0.80914000
F	1.54982400	-0.99289400	0.82880800
O	-0.06579900	-0.32294200	-0.80326600
S	-1.48156000	-0.72882600	0.00953600
F	2.12489800	0.38614700	-0.93395000
C	-2.36782900	0.85757300	-0.00375400
H	-3.33443700	0.66427900	0.46952000
H	-1.82363600	1.60819800	0.56821800
H	-2.53118300	1.19881600	-1.02714900

Zero-point correction= 0.053582
(Hartree/Particle)

```
 Thermal correction to Energy=                    0.061656
 Thermal correction to Enthalpy=                  0.062601
 Thermal correction to Gibbs Free Energy=         0.019961
 Sum of electronic and zero-point Energies=           -838.171672
 Sum of electronic and thermal Energies=              -838.163597
 Sum of electronic and thermal Enthalpies=            -838.162653
 Sum of electronic and thermal Free Energies=         -838.205293
```

Methyl sulfenate with K^+ counterion

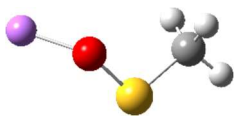


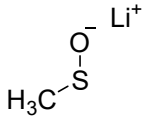



```
0 1
 C                  2.33213600    1.00184300    0.00022500
 H                  3.41586300    0.85342900   -0.02705000
 H                  2.06924400    1.55777700    0.90467400
 H                  2.02700100    1.57285100   -0.88124300
 S                  1.55440200   -0.65091100   -0.00009200
 O                 -0.05087800   -0.32415400    0.00078600
 K                 -2.41938600    0.15856300   -0.00013400

Zero-point correction=                           0.040027
(Hartree/Particle)
 Thermal correction to Energy=                    0.046378
 Thermal correction to Enthalpy=                  0.047322
 Thermal correction to Gibbs Free Energy=         0.007745
 Sum of electronic and zero-point Energies=          -1113.339599
 Sum of electronic and thermal Energies=             -1113.333248
 Sum of electronic and thermal Enthalpies=           -1113.332304
 Sum of electronic and thermal Free Energies=        -1113.371880
```

Methyl sulfenate with Li^+ counterion



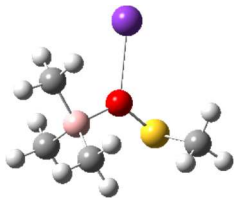


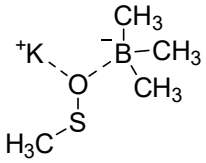

```
0 1
 C                  1.49125000    0.63386700   -0.02974200
```

H	2.43459000	0.13474900	-0.26969400
H	1.56491400	1.08040000	0.96506100
H	1.29906500	1.41416000	-0.77065300
S	0.18650100	-0.63882300	-0.06718200
O	-1.16197000	0.20223400	0.34799400
Li	-2.64477200	0.72359500	-0.48510100

Zero-point correction=	0.041091
(Hartree/Particle)	
Thermal correction to Energy=	0.046931
Thermal correction to Enthalpy=	0.047875
Thermal correction to Gibbs Free Energy=	0.011835
Sum of electronic and zero-point Energies=	-520.939104
Sum of electronic and thermal Energies=	-520.933264
Sum of electronic and thermal Enthalpies=	-520.932320
Sum of electronic and thermal Free Energies=	-520.968361

Methyl sulfenate O coordinated with Me_3B, with K^+



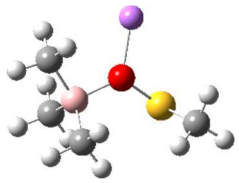


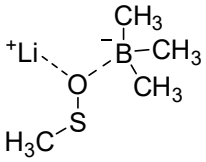
0 1

C	-0.61730200	-2.61159700	0.77736000
H	-0.83841700	-3.62447700	0.42896500
H	-1.45770900	-2.23702900	1.36120500
H	0.28708200	-2.63460000	1.38822200
S	-0.36197700	-1.61011100	-0.72291000
O	0.08795200	-0.12557100	-0.09799700
B	-0.95350000	1.06878700	0.05550400
C	-2.13079800	0.64650300	1.10850800
H	-2.82879000	1.48057100	1.26915000
H	-2.73740700	-0.19901300	0.75455900
H	-1.73798100	0.37005400	2.09787900
C	-0.00968100	2.26974600	0.65519300
H	0.48522100	1.99690700	1.60002800
H	0.77199900	2.59818300	-0.04853600
H	-0.60998200	3.16359600	0.87172700
C	-1.55047900	1.45680300	-1.41591200
H	-2.21899700	2.32763400	-1.35674600
H	-0.75835400	1.71681200	-2.13395500
H	-2.13722800	0.64387600	-1.86558600
K	2.60450700	0.27637700	0.05027400

Zero-point correction=	0.155217
(Hartree/Particle)	
Thermal correction to Energy=	0.168432
Thermal correction to Enthalpy=	0.169376
Thermal correction to Gibbs Free Energy=	0.114426
Sum of electronic and zero-point Energies=	-1257.911184
Sum of electronic and thermal Energies=	-1257.897969
Sum of electronic and thermal Enthalpies=	-1257.897025
Sum of electronic and thermal Free Energies=	-1257.951975

Methyl sulfenate O coordinated with Me_3B, with Li^+





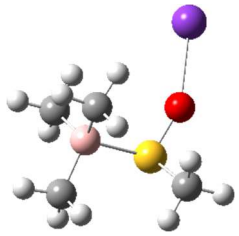
0 1

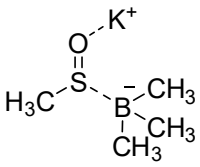
C	2.52180900	-0.53300500	0.65552100
H	3.49437800	-0.76038400	0.21008700
H	2.03678100	-1.45957900	0.96064500
H	2.66906600	0.12134200	1.51635300
S	1.56692500	0.30798900	-0.64582800
O	0.14643000	0.70915700	0.15723100
B	-1.18743000	-0.18191500	0.00785000
C	-0.89275800	-1.68546300	0.56777600
H	-1.80187700	-2.30102300	0.51691400
H	-0.12797800	-2.21802500	-0.01439600
H	-0.56559000	-1.69400400	1.61754100
Li	0.13605200	2.40677300	0.91730800
C	-2.24276900	0.63124500	0.95892900
H	-1.90104100	0.72240100	2.00139300
H	-2.46650900	1.64622900	0.59515900
H	-3.20684900	0.10659100	0.99658700
C	-1.64306600	-0.17186800	-1.55828200
H	-2.58666900	-0.71800800	-1.69831000
H	-1.80910400	0.84584200	-1.94131100
H	-0.90715600	-0.64864800	-2.22011100

Zero-point correction=	0.156867
(Hartree/Particle)	
Thermal correction to Energy=	0.169150
Thermal correction to Enthalpy=	0.170094
Thermal correction to Gibbs Free Energy=	0.120161
Sum of electronic and zero-point Energies=	-665.505721

```
 Sum of electronic and thermal Energies=             -665.493437
 Sum of electronic and thermal Enthalpies=           -665.492493
 Sum of electronic and thermal Free Energies=        -665.542427
```

Methyl sulfenate S coordinated with Me_3B, with K^+

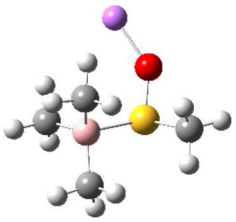


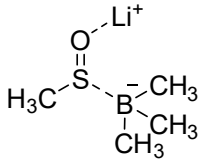



```
0 1
 C                 -1.09987000   -2.24620100    0.37735100
 H                 -0.57117900   -3.15589200    0.09099400
 H                 -2.16430100   -2.35781900    0.16597100
 H                 -0.94473900   -2.03600000    1.43644900
 S                 -0.45136100   -0.87048400   -0.62909400
 B                 -1.45636700    0.76341300    0.07956700
 C                 -1.22537100    0.87356000    1.68292400
 H                 -1.67855100    1.80429600    2.05459400
 H                 -1.68427000    0.05852500    2.25761700
 H                 -0.16438400    0.91187300    1.96263900
 O                  1.07988500   -0.78394200   -0.20492400
 K                  3.25592400    0.32306000    0.09391800
 C                 -3.00536100    0.49283100   -0.35121500
 H                 -3.59725500    1.39345600   -0.13319900
 H                 -3.48563600   -0.32907400    0.19540500
 H                 -3.13753400    0.29219000   -1.42345500
 C                 -0.78386400    1.99551400   -0.74905700
 H                  0.28041100    2.14253700   -0.52230500
 H                 -0.87253600    1.89196300   -1.83940700
 H                 -1.29124900    2.93380300   -0.48270900

Zero-point correction=                           0.155537
(Hartree/Particle)
 Thermal correction to Energy=                    0.168876
 Thermal correction to Enthalpy=                  0.169820
 Thermal correction to Gibbs Free Energy=         0.113929
 Sum of electronic and zero-point Energies=          -1257.899088
 Sum of electronic and thermal Energies=             -1257.885749
 Sum of electronic and thermal Enthalpies=           -1257.884805
 Sum of electronic and thermal Free Energies=        -1257.940696
```

Methyl sulfenate S coordinated with Me_3B, with Li^+

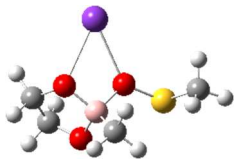


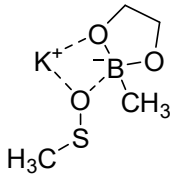



```
0 1
 C                  1.40602600   -1.70251400    0.29778200
 H                  2.45076900   -1.87969700    0.04188200
 H                  0.80008000   -2.55037100   -0.02398000
 H                  1.29839700   -1.54520200    1.37145800
 S                  0.84461100   -0.22679000   -0.60613400
 B                 -1.06550100    0.07866100    0.07071600
 C                 -1.02874200    0.23331300    1.68531900
 H                 -2.03693000    0.47933700    2.04896800
 H                 -0.72614000   -0.67884900    2.21547200
 H                 -0.37106600    1.04276900    2.02922400
 O                  1.80337600    0.91672600   -0.03880500
 C                 -1.87605800   -1.23272500   -0.45790300
 H                 -2.94831500   -1.08334200   -0.26763100
 H                 -1.60083400   -2.16536200    0.05067000
 H                 -1.77910400   -1.40837300   -1.53808600
 C                 -1.51749100    1.44168100   -0.69917100
 H                 -0.94889400    2.33241900   -0.39967600
 H                 -1.45502700    1.36982600   -1.79344700
 H                 -2.56896500    1.65623900   -0.46117900
 Li                 1.79011500    2.63120200    0.47505900

Zero-point correction=                           0.157226
(Hartree/Particle)
 Thermal correction to Energy=                    0.169643
 Thermal correction to Enthalpy=                  0.170587
 Thermal correction to Gibbs Free Energy=         0.120392
 Sum of electronic and zero-point Energies=           -665.496431
 Sum of electronic and thermal Energies=              -665.484014
 Sum of electronic and thermal Enthalpies=            -665.483070
 Sum of electronic and thermal Free Energies=         -665.533265
```

Methyl sulfenate O coordinated with MeB(EG), with K^+



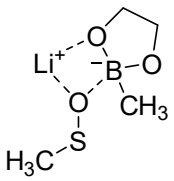


0 1

C	3.24709400	-0.05792500	0.35213500
H	4.20962300	-0.42165600	-0.01817400
H	3.03628600	-0.51609500	1.31849200
H	3.29123200	1.02851000	0.44817000
S	2.01729400	-0.54950900	-0.89623600
O	0.60965800	0.13553900	-0.30124500
B	-0.41546400	-0.74399800	0.47244000
C	0.21144600	-1.34273900	1.83205800
H	-0.55011100	-1.89160900	2.39951400
H	1.03421600	-2.04182600	1.63986900
H	0.60080000	-0.55407800	2.48767200
O	-1.53658500	0.23344200	0.68475100
O	-0.98697000	-1.78132800	-0.39985600
C	-2.11669300	-1.22097400	-1.05021200
H	-1.82298400	-0.69217500	-1.97013900
H	-2.82617700	-2.00916200	-1.32084700
C	-2.68231200	-0.23790700	-0.02022600
H	-3.36779100	-0.74826200	0.67147000
H	-3.22234100	0.59731000	-0.48109100
K	-0.38043100	2.53774900	0.01320600

Zero-point correction= 0.147929
(Hartree/Particle)
Thermal correction to Energy= 0.160843
Thermal correction to Enthalpy= 0.161787
Thermal correction to Gibbs Free Energy= 0.107104
Sum of electronic and zero-point Energies= -1407.278018
Sum of electronic and thermal Energies= -1407.265104
Sum of electronic and thermal Enthalpies= -1407.264160
Sum of electronic and thermal Free Energies= -1407.318843

Methyl sulfenate O coordinated with MeB(EG), with Li^+

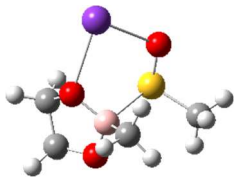


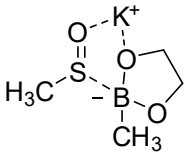
0 1

C	-3.19153100	0.33742300	0.32720100
H	-4.14888000	0.05282000	-0.11801200
H	-2.94506800	1.35695500	0.03173100
H	-3.26810600	0.26096100	1.41307500
S	-1.97808800	-0.85257800	-0.31936900
O	-0.58129500	-0.40870200	0.49324100
B	0.51433100	0.49402900	-0.16274900
C	-0.06164400	1.92534800	-0.60725400
H	0.74793100	2.56978900	-0.96974200
H	-0.79334500	1.84190500	-1.41951000
H	-0.55134800	2.44989200	0.22145100
O	1.48272900	0.52100300	1.00350200
O	1.23137300	-0.20706100	-1.22288100
C	2.29995800	-0.93393900	-0.63119000
H	1.96615300	-1.92882300	-0.30090400
H	3.10925000	-1.06586400	-1.35492400
C	2.70963100	-0.07475900	0.56816200
H	3.41435400	0.71065600	0.26685800
H	3.16042400	-0.65445500	1.37936700
Li	0.26181500	-0.39636500	2.21394800

Zero-point correction=	0.149948
(Hartree/Particle)	
Thermal correction to Energy=	0.161809
Thermal correction to Enthalpy=	0.162754
Thermal correction to Gibbs Free Energy=	0.112453
Sum of electronic and zero-point Energies=	-814.876154
Sum of electronic and thermal Energies=	-814.864293
Sum of electronic and thermal Enthalpies=	-814.863349
Sum of electronic and thermal Free Energies=	-814.913650

Methyl sulfenate S coordinated with MeB(EG), with K^+



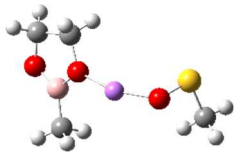


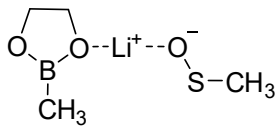
0 1

C	0.29398400	2.93624200	-0.05551300
H	-0.16950100	3.71312500	-0.66485500
H	1.37939700	3.05892100	-0.06657700
H	-0.07937900	2.98854500	0.96811500
S	-0.08931000	1.30545600	-0.77446700
B	0.83967300	-0.08344600	0.63029200
C	0.42522400	0.38177400	2.09682700
H	0.70311600	-0.39558300	2.82052000
H	0.93945000	1.29949100	2.39853700
H	-0.65031600	0.55978500	2.20518000
O	-1.66729600	1.12361900	-0.58571200
O	0.28568000	-1.34945000	0.17614100
O	2.23596500	-0.07025200	0.27943200
C	1.16579800	-1.84927200	-0.83728000
H	0.82747000	-1.51869500	-1.82710800
H	1.16702400	-2.94148200	-0.81526800
C	2.53424100	-1.24155500	-0.48498300
H	3.11158000	-0.97831700	-1.37593200
H	3.13188200	-1.92976000	0.12493200
K	-2.44633700	-1.22739900	0.11575100

Zero-point correction= 0.147639
(Hartree/Particle)
Thermal correction to Energy= 0.160978
Thermal correction to Enthalpy= 0.161922
Thermal correction to Gibbs Free Energy= 0.106805
Sum of electronic and zero-point Energies= -1407.257096
Sum of electronic and thermal Energies= -1407.243756
Sum of electronic and thermal Enthalpies= -1407.242812
Sum of electronic and thermal Free Energies= -1407.297929

Optimized attempt at methyl sulfenate S coordinated with MeB(EG), with Li^+





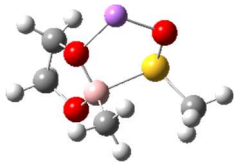
0 1

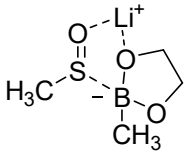
C	-3.64189200	0.97205600	-0.80803200
H	-4.37840100	1.36305300	-0.10157200
H	-4.11850800	0.83120000	-1.78255500
H	-2.81780900	1.68268100	-0.91070800
S	-3.03495600	-0.65977500	-0.26332100
B	2.06881900	0.80184300	0.07564100
C	1.68011900	2.29615500	0.28282100
H	2.55757600	2.94527700	0.30962700

H	1.04709700	2.63330300	-0.54624800
H	1.10479300	2.44510500	1.20057500
O	-2.36580400	-0.34091600	1.20995200
O	1.23223000	-0.25736300	0.41233600
O	3.24407200	0.36675800	-0.46910800
C	1.84532700	-1.49552800	-0.04936500
H	1.26625300	-1.86490100	-0.89657400
H	1.81724800	-2.22503600	0.75897100
C	3.27582100	-1.07954300	-0.44012900
H	3.56705000	-1.44856200	-1.42292300
H	4.01672900	-1.39227100	0.29763900
Li	-0.56235200	-0.24311100	1.26383000

Zero-point correction= 0.149586
(Hartree/Particle)
Thermal correction to Energy= 0.163157
Thermal correction to Enthalpy= 0.164101
Thermal correction to Gibbs Free Energy= 0.105035
Sum of electronic and zero-point Energies= -814.865780
Sum of electronic and thermal Energies= -814.852210
Sum of electronic and thermal Enthalpies= -814.851265
Sum of electronic and thermal Free Energies= -814.910331

Constrained (frozen S-B) methyl sulfenate S coordinated with MeB(EG), with Li^+





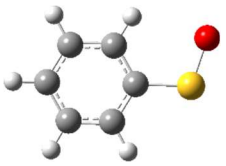
0 1

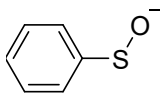
C	2.57276000	-0.85834200	-0.57917800
H	3.47358200	-0.40472800	-0.99342900
H	2.29616300	-1.73251000	-1.17297000
H	2.73578300	-1.14558800	0.45958200
S	1.20738700	0.33760200	-0.69263800
B	-0.44902700	-0.57131500	0.40078300
C	0.16804900	-1.46853000	1.55973500
H	-0.64122200	-1.80377600	2.22107900
H	0.65933100	-2.36641600	1.17263200
H	0.89381000	-0.93345100	2.18145800
O	1.63203200	1.53016800	0.30279100
O	-1.12118700	0.65873900	0.82647700
O	-1.28332700	-1.19961100	-0.57693700
C	-2.08616800	0.98789500	-0.18907500
H	-1.65040200	1.69996700	-0.89953200

H	-2.95915800	1.44731500	0.27803700
C	-2.40316300	-0.35769100	-0.86331100
H	-2.53330900	-0.25233900	-1.94381700
H	-3.31000100	-0.81031400	-0.44653400
Li	0.21111500	2.00747200	1.41137400

Zero-point correction= 0.149626
(Hartree/Particle)
Thermal correction to Energy= 0.161910
Thermal correction to Enthalpy= 0.162854
Thermal correction to Gibbs Free Energy= 0.111814
Sum of electronic and zero-point Energies= -814.857687
Sum of electronic and thermal Energies= -814.845403
Sum of electronic and thermal Enthalpies= -814.844459
Sum of electronic and thermal Free Energies= -814.895499

Benzenesulfenate (**1**)





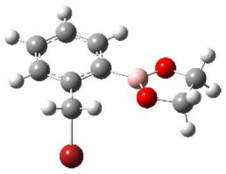
-1 1

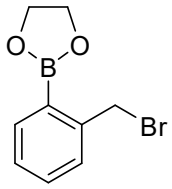
C	-0.30517900	1.10259700	0.00000300
C	-1.67874300	1.34727100	0.00000500
C	-2.59482900	0.29411500	0.00000100
C	-2.11323000	-1.02254900	-0.00000600
C	-0.74774200	-1.27905100	-0.00000700
C	0.17913500	-0.21611800	-0.00000100
H	0.41171400	1.91531600	0.00000500
H	-2.03557500	2.37297000	0.00000900
H	-2.81134100	-1.85397600	-0.00000900
H	-0.39149100	-2.30539600	-0.00001400
S	1.91814100	-0.55616900	0.00001200
O	2.67014700	0.86534700	-0.00001900
H	-3.66120500	0.48941600	0.00000200

Zero-point correction= 0.092252
(Hartree/Particle)
Thermal correction to Energy= 0.099145
Thermal correction to Enthalpy= 0.100089
Thermal correction to Gibbs Free Energy= 0.060555
Sum of electronic and zero-point Energies= -705.173031
Sum of electronic and thermal Energies= -705.166138
Sum of electronic and thermal Enthalpies= -705.165194

```
 Sum of electronic and thermal Free Energies=          -705.204729
```

Ethylene glycol ester of 2-bromomethylphenyl boronic acid (reactant **2a**)

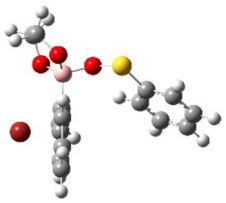


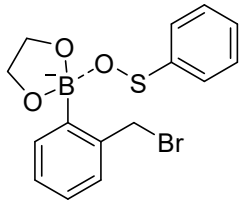



```
0 1
 C                  0.65788400    2.45150600   -0.37606200
 C                  0.43465800    1.14576800    0.09570200
 C                 -0.86544300    0.81812900    0.55009600
 C                 -1.87455400    1.78926700    0.52640800
 C                 -1.62560200    3.07637100    0.05952500
 C                 -0.35198200    3.40969700   -0.39790600
 H                  1.64848500    2.71699900   -0.72669500
 H                 -2.86746800    1.52955300    0.87825100
 H                 -2.42061300    3.81344700    0.05443200
 H                 -0.14648600    4.40881700   -0.76498700
 C                 -1.21499000   -0.53741500    1.07015600
 H                 -2.05570300   -0.51442600    1.75626600
 H                 -0.37634700   -1.07924300    1.48790800
 B                  1.65684500    0.17396200    0.08624200
 O                  2.82895800    0.50247600   -0.55266700
 O                  1.71633700   -1.05204800    0.70328700
 C                  2.98803500   -1.66304900    0.37816600
 C                  3.80406200   -0.52706500   -0.27015200
 H                  3.44114800   -2.04588400    1.29235900
 H                  2.80472600   -2.49178700   -0.30854900
 H                  4.55571100   -0.11459500    0.40620900
 H                  4.28442600   -0.82711300   -1.20134600
 Br                -1.86362500   -1.76137900   -0.40930300

Zero-point correction=                           0.179299
(Hartree/Particle)
 Thermal correction to Energy=                    0.191138
 Thermal correction to Enthalpy=                  0.192082
 Thermal correction to Gibbs Free Energy=         0.138264
 Sum of electronic and zero-point Energies=          -3098.500935
 Sum of electronic and thermal Energies=             -3098.489097
 Sum of electronic and thermal Enthalpies=           -3098.488153
 Sum of electronic and thermal Free Energies=        -3098.541971
```

Complex of **1** with **2a** – **1.2a.C**



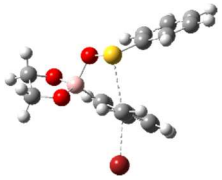


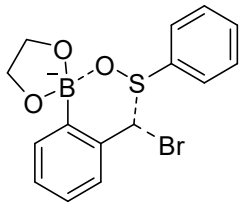
-1 1

C	-0.50078900	0.84383400	2.43196300
C	-0.70694100	0.48814600	1.08708700
C	-0.99962300	-0.87171500	0.83028100
C	-1.05597500	-1.80614500	1.87701300
C	-0.84153600	-1.42074600	3.19511500
C	-0.56551200	-0.08087000	3.47323900
H	-0.28591200	1.88249600	2.65743000
H	-1.28029900	-2.84462800	1.65114400
H	-0.88809800	-2.15335400	3.99374600
H	-0.39795800	0.23892800	4.49704800
C	-1.21706600	-1.36086000	-0.56269200
H	-0.72622300	-2.30767000	-0.76961700
H	-0.99969400	-0.61805200	-1.31902800
B	-0.56062800	1.62798600	-0.06983400
O	-0.50755200	2.99974600	0.47505700
O	-1.65949100	1.63076000	-1.03902600
C	-1.84484900	2.98100800	-1.44533000
C	-1.47322600	3.79497300	-0.19912300
H	-1.18058800	3.22913200	-2.28569600
H	-2.88000300	3.13521900	-1.76523900
H	-1.05732200	4.77767100	-0.44862700
H	-2.35287500	3.94927700	0.44393100
Br	-3.17287700	-1.82548400	-0.93261300
C	4.34436600	0.05298700	0.16708100
C	5.08693200	-1.11292700	0.00911300
C	4.56607200	-2.19604300	-0.70516000
C	3.29164800	-2.09373600	-1.26224200
C	2.53928300	-0.92792800	-1.11520000
C	3.06063600	0.15186000	-0.39469400
H	4.75840500	0.88437100	0.72910700
H	6.07560700	-1.17778800	0.45079700
H	2.87582900	-2.92600800	-1.82057200
H	1.55330400	-0.84229000	-1.55142200
S	2.18492300	1.68534200	-0.19631000
O	0.72131100	1.37102100	-0.91438800
H	5.14623100	-3.10398500	-0.82327200

Zero-point correction=	0.271959
(Hartree/Particle)	
Thermal correction to Energy=	0.291783
Thermal correction to Enthalpy=	0.292727
Thermal correction to Gibbs Free Energy=	0.218797
Sum of electronic and zero-point Energies=	-3803.692634
Sum of electronic and thermal Energies=	-3803.672811
Sum of electronic and thermal Enthalpies=	-3803.671867
Sum of electronic and thermal Free Energies=	-3803.745797

Transition state for internal alkylation of **1.2a.C** – **1.2a.C.TS**





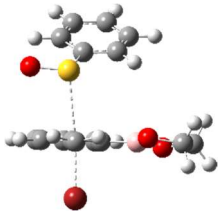
-1 1

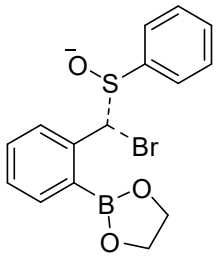
C	0.21400700	0.89755200	2.50748700
C	0.51874900	0.66781500	1.15740100
C	0.52902000	-0.68577900	0.71867600
C	0.17468000	-1.73274600	1.60044500
C	-0.10621800	-1.46779600	2.92894500
C	-0.06851900	-0.14390400	3.38779300
H	0.19684400	1.92007800	2.86843100
H	0.16736900	-2.75333700	1.23312700
H	-0.34875800	-2.27645700	3.60918700
H	-0.27590300	0.06976600	4.43145100
C	0.86978100	-0.99365500	-0.64113800
H	1.38068800	-0.27059800	-1.25049100
H	0.53142400	-1.90845000	-1.10279000
Br	3.21368500	-2.26336700	-0.57335600
B	0.61942700	1.90081600	0.12399900
O	1.71530700	1.87525900	-0.84537600
O	0.63819300	3.20696100	0.74418900
C	1.33519200	4.07768900	-0.14383100
H	0.63794100	4.53236400	-0.86049000
H	1.81869600	4.87668400	0.42510400
C	2.33618400	3.15885900	-0.85762600
H	3.29059200	3.11553600	-0.31543500
H	2.53813000	3.47529200	-1.88587700
O	-0.77260100	1.85115300	-0.68394800
S	-1.09794100	0.60293100	-1.68045700
C	-2.57564100	-0.10178500	-0.97588600

C	-3.12801700	0.37895200	0.21300300
C	-3.18883100	-1.15748200	-1.66515300
C	-4.29335700	-0.20353100	0.71245100
H	-2.64526200	1.19839200	0.72874900
C	-4.34881700	-1.73142200	-1.15405500
H	-2.76400400	-1.52739300	-2.59275700
C	-4.90678200	-1.25747200	0.03651100
H	-4.72118000	0.17128000	1.63589200
H	-4.81948000	-2.54936000	-1.68813400
H	-5.81192300	-1.70567800	0.42977000

Zero-point correction= 0.271126
(Hartree/Particle)
Thermal correction to Energy= 0.290538
Thermal correction to Enthalpy= 0.291482
Thermal correction to Gibbs Free Energy= 0.219826
Sum of electronic and zero-point Energies= -3803.680657
Sum of electronic and thermal Energies= -3803.661245
Sum of electronic and thermal Enthalpies= -3803.660301
Sum of electronic and thermal Free Energies= -3803.731957

Transition state for reaction of **1** and **2a** w/o precomplexation – **1.2a.TS**





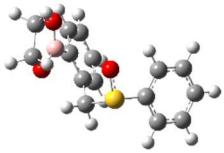
-1 1

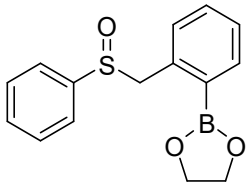
C	-1.25187100	-1.06492000	-0.56076100
H	-1.21569700	-2.10225800	-0.84865600
H	-1.30085600	-0.33520000	-1.34843700
C	-0.69077100	-0.69812700	0.73178300
C	-0.39476500	-1.73258100	1.63910100
C	-0.46726500	0.65241600	1.11692600
C	0.11549000	-1.46029500	2.90127500
H	-0.57414800	-2.75919000	1.33999800
C	0.04258400	0.89575100	2.40239400
C	0.33287400	-0.13739500	3.29057900
H	0.33993700	-2.27478200	3.58108200
H	0.21663100	1.92098700	2.70862500
H	0.72534700	0.08570800	4.27632600

Br	-3.61356100	-1.09183100	-0.27343300
B	-0.74659700	1.89571800	0.22045200
O	-0.68143700	3.17592700	0.72730800
O	-1.06493200	1.87817600	-1.11713700
C	-1.34577900	3.23251400	-1.53702800
H	-2.42028400	3.32381400	-1.71010000
H	-0.81357300	3.43436900	-2.46672700
C	-0.86117900	4.10564200	-0.36303600
H	-1.58753900	4.86397100	-0.06983700
H	0.09732300	4.58733700	-0.56991400
S	1.31590900	-1.64480200	-1.81840000
O	1.54393900	-3.14428700	-1.36734600
C	2.52218600	-0.66493100	-0.95601400
C	3.43077700	-1.26039700	-0.07058500
C	2.57879300	0.72281500	-1.17545700
C	4.38231200	-0.47697000	0.58171000
H	3.37727400	-2.33117900	0.08644200
C	3.53309300	1.49371000	-0.52041000
H	1.87961000	1.19210700	-1.86030600
C	4.44209300	0.90048100	0.36334400
H	5.08300700	-0.94688000	1.26455500
H	3.56950500	2.56355600	-0.69802700
H	5.18454400	1.50516200	0.87173900

Zero-point correction= 0.271297
(Hartree/Particle)
Thermal correction to Energy= 0.291776
Thermal correction to Enthalpy= 0.292720
Thermal correction to Gibbs Free Energy= 0.216480
Sum of electronic and zero-point Energies= -3803.670124
Sum of electronic and thermal Energies= -3803.649645
Sum of electronic and thermal Enthalpies= -3803.648700
Sum of electronic and thermal Free Energies= -3803.724941

Sulfoxide product formed from **1** and **2a**.





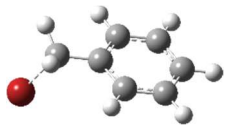
0 1

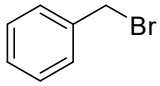
C	1.49438600	2.41946100	-0.42701200
C	1.38452200	1.16082600	0.18866300
C	0.25303700	0.91175900	1.00060300
C	-0.70875300	1.91552400	1.17622600

C	-0.56515600	3.16238900	0.57405600
C	0.54019000	3.41571700	-0.23648900
H	2.35211000	2.61984100	-1.05951000
H	-1.57490600	1.71876800	1.79868400
H	-1.31403100	3.92981600	0.73508100
H	0.65873000	4.38215900	-0.71353000
C	0.03036100	-0.41906000	1.64385600
H	0.94437900	-0.86000200	2.03758300
H	-0.72951400	-0.39215000	2.42566000
B	2.53210300	0.13076900	-0.05316700
O	2.97050100	-0.79329700	0.86791700
O	3.29838100	0.14762000	-1.19490900
C	4.38132700	-0.79437400	-1.02298500
H	4.45529900	-1.42045400	-1.91224600
H	5.31129100	-0.23454300	-0.89838200
C	4.00050700	-1.59016500	0.24015700
H	4.83128100	-1.71115000	0.93542000
H	3.58201200	-2.57064600	0.00209800
O	0.36513000	-1.68541900	-0.76746800
S	-0.56026600	-1.75426000	0.44652500
C	-2.14617400	-1.02034200	-0.06544200
C	-2.24984600	-0.43611800	-1.32301700
C	-3.24947800	-1.12680200	0.78139400
C	-3.48180100	0.07542900	-1.73205700
H	-1.37792100	-0.39412700	-1.96456500
C	-4.47416300	-0.60757500	0.36577200
H	-3.16260600	-1.61028300	1.74872200
C	-4.58999000	-0.00626800	-0.88924700
H	-3.57453900	0.53501300	-2.70941600
H	-5.33776600	-0.68140300	1.01651200
H	-5.54599300	0.38982200	-1.21186200

Zero-point correction= 0.273803
(Hartree/Particle)
Thermal correction to Energy= 0.291573
Thermal correction to Enthalpy= 0.292517
Thermal correction to Gibbs Free Energy= 0.225313
Sum of electronic and zero-point Energies= -1229.386398
Sum of electronic and thermal Energies= -1229.368629
Sum of electronic and thermal Enthalpies= -1229.367684
Sum of electronic and thermal Free Energies= -1229.434888

BnBr (reactant – **2**)



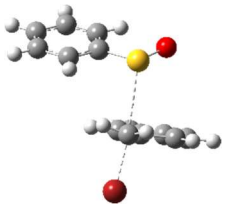


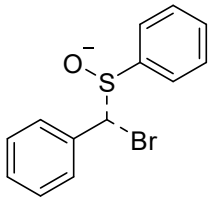
0 1

C	-2.59093500	1.20752200	-0.22213900
C	-1.29840500	1.20714800	0.29682900
C	-0.63816800	-0.00001400	0.56017100
C	-1.29842200	-1.20716100	0.29680400
C	-2.59095200	-1.20750500	-0.22216500
C	-3.23945600	0.00001600	-0.48437900
H	-3.09288700	2.14804800	-0.41853100
H	-0.79746100	-2.14766400	0.50047700
H	-3.09291700	-2.14802000	-0.41857700
H	-4.24585300	0.00002700	-0.88725700
C	0.73713600	-0.00002900	1.13175200
H	0.96206000	-0.89322100	1.70611100
H	0.96206200	0.89313400	1.70615600
Br	2.16050400	0.00000600	-0.30943200
H	-0.79742900	2.14763900	0.50051700

Zero-point correction= 0.118656
(Hartree/Particle)
Thermal correction to Energy= 0.125768
Thermal correction to Enthalpy= 0.126712
Thermal correction to Gibbs Free Energy= 0.085051
Sum of electronic and zero-point Energies= -2845.069493
Sum of electronic and thermal Energies= -2845.062381
Sum of electronic and thermal Enthalpies= -2845.061436
Sum of electronic and thermal Free Energies= -2845.103097

Transition state for reaction of **1** and **2a** – **1.2.TS**





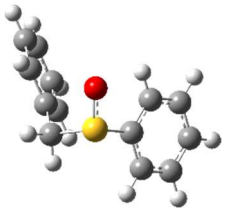
-1 1

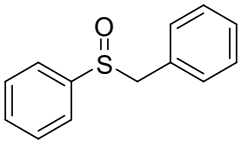
C	1.15192900	0.59621800	-0.56308400
H	1.40280900	0.72110100	-1.60287600
H	0.47085500	1.31757900	-0.14273000
C	1.20693700	-0.73594500	0.01634300
C	0.65143300	-0.99164400	1.28317300
C	1.83407700	-1.79114500	-0.66965000
C	0.72433500	-2.26079100	1.84556800
H	0.16616000	-0.18633900	1.82328300
C	1.90702900	-3.05975500	-0.10465500
H	2.26490800	-1.60746100	-1.64781100

C	1.35635600	-3.29881800	1.15617200
H	0.29036100	-2.44339300	2.82226900
H	2.39178500	-3.86407500	-0.64651200
H	1.41474500	-4.28778300	1.59656600
Br	3.06817100	1.75237200	0.19228900
S	-1.38397400	0.02769900	-1.97910500
C	-2.42101200	0.40628300	-0.58369500
C	-2.53679500	1.73491200	-0.13634500
C	-3.13308800	-0.60540900	0.07436500
C	-3.34927100	2.03674900	0.95104200
H	-1.99767400	2.52905800	-0.64447200
C	-3.94763000	-0.29026400	1.16224600
H	-3.03822800	-1.62351500	-0.28462000
C	-4.06186800	1.02679000	1.60898400
H	-3.43160200	3.06528500	1.28676400
H	-4.49666500	-1.08084200	1.66390400
H	-4.69614800	1.26718800	2.45463000
O	-1.53479100	-1.52326100	-2.24820300

Zero-point correction=	0.210771
(Hartree/Particle)	
Thermal correction to Energy=	0.226430
Thermal correction to Enthalpy=	0.227374
Thermal correction to Gibbs Free Energy=	0.162793
Sum of electronic and zero-point Energies=	-3550.239116
Sum of electronic and thermal Energies=	-3550.223457
Sum of electronic and thermal Enthalpies=	-3550.222513
Sum of electronic and thermal Free Energies=	-3550.287095

Sulfoxide product formed from **1** and **2a**.





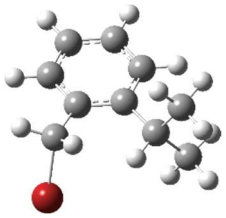
0 1

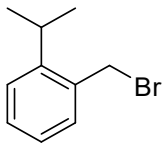
C	0.77404300	-1.42434000	1.20919500
H	0.26348400	-1.17486100	2.14060000
H	1.34532100	-2.34242400	1.35610900
C	1.61508700	-0.30882800	0.68092000
C	2.66119200	-0.57136400	-0.21419100
C	1.37436000	1.01661500	1.06790400
C	3.44545400	0.46747600	-0.71213100
H	2.86150800	-1.59249100	-0.51687000
C	2.16245100	2.05442000	0.57509900

H	0.57310200	1.23467600	1.76541300
C	3.19860700	1.78293100	-0.31897900
H	4.25244300	0.24888300	-1.40242200
H	1.96962700	3.07348000	0.89109400
H	3.81318100	2.59007300	-0.70138300
S	-0.60359100	-2.00397800	0.05732200
C	-1.55953200	-0.45875000	-0.06411400
C	-2.41529100	-0.10276200	0.97835100
C	-1.47891900	0.29827300	-1.22773800
C	-3.18242200	1.05455000	0.85898800
H	-2.49125700	-0.71696200	1.86933300
C	-2.25555900	1.45194200	-1.33983300
H	-0.82308000	-0.02267300	-2.02805600
C	-3.10199000	1.83161800	-0.29846500
H	-3.84856400	1.34282400	1.66388600
H	-2.19999900	2.05113700	-2.24144400
H	-3.70594000	2.72696300	-0.39055600
O	0.02784200	-2.23820900	-1.31160900

Zero-point correction= 0.213296
(Hartree/Particle)
Thermal correction to Energy= 0.226375
Thermal correction to Enthalpy= 0.227319
Thermal correction to Gibbs Free Energy= 0.171501
Sum of electronic and zero-point Energies= -975.954175
Sum of electronic and thermal Energies= -975.941096
Sum of electronic and thermal Enthalpies= -975.940152
Sum of electronic and thermal Free Energies= -975.995970

2-Isopropylbenzyl bromide (reactant – **2iP**)





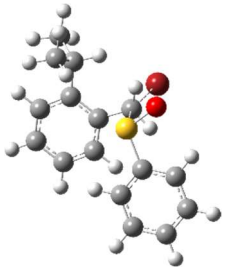
0 1

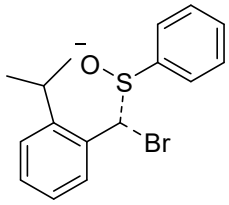
C	2.41681100	0.32225800	-0.45315700
C	1.20831300	-0.15893600	0.06783400
C	0.25207600	0.78573000	0.50063900
C	0.52549500	2.15772000	0.38010800
C	1.72757200	2.61275500	-0.14722700
C	2.68093500	1.68462700	-0.56400100
H	3.17121300	-0.38382000	-0.78153100
H	-0.21974300	2.87305400	0.71216700

H	1.92036200	3.67625400	-0.22789300
H	3.62727700	2.01920000	-0.97423900
C	-1.04658200	0.39474100	1.12093200
H	-1.48848100	1.20488400	1.69165600
H	-1.00943000	-0.50736000	1.72112700
Br	-2.47609600	-0.02404400	-0.25893400
C	0.98200800	-1.66435900	0.16264600
H	-0.04965400	-1.83877200	0.47315000
C	1.15059500	-2.36310500	-1.19954700
H	0.90602000	-3.42517300	-1.10811900
H	0.48911500	-1.92627000	-1.95195900
H	2.17746700	-2.29032900	-1.56809200
C	1.89581300	-2.29944900	1.22894700
H	2.95105100	-2.18422700	0.96457400
H	1.74275100	-1.83842400	2.20843400
H	1.68721000	-3.36935700	1.32036100

Zero-point correction= 0.202654
(Hartree/Particle)
Thermal correction to Energy= 0.214062
Thermal correction to Enthalpy= 0.215006
Thermal correction to Gibbs Free Energy= 0.163473
Sum of electronic and zero-point Energies= -2962.957185
Sum of electronic and thermal Energies= -2962.945778
Sum of electronic and thermal Enthalpies= -2962.944833
Sum of electronic and thermal Free Energies= -2962.996366

One transition state for reaction of **1** and **2iP** – **1.2iP.TSa**





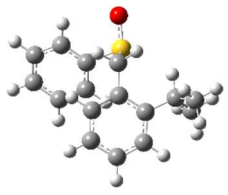
-1 1

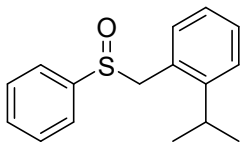
C	0.45692200	-0.82339300	0.05618200
H	0.68882100	-1.07920800	1.07347400
H	-0.46500600	-1.22735400	-0.32801500
C	0.98029600	0.38531400	-0.56450300
C	0.37648700	0.81421900	-1.76440700
C	2.05694300	1.13379200	-0.02344400
C	0.79440000	1.96402500	-2.41701100

H	-0.43544500	0.22556400	-2.17662200
C	2.45393600	2.29424200	-0.69641200
C	1.84008500	2.71311600	-1.87520600
H	0.31190800	2.27587100	-3.33632500
H	3.26705900	2.88799500	-0.29391200
H	2.17962800	3.61685400	-2.36917400
Br	1.76065100	-2.62931000	-0.81508200
S	-1.51203800	0.38738600	1.77889100
C	-2.87810800	0.28954000	0.64088700
C	-3.03695000	1.27877600	-0.34570500
C	-3.80189200	-0.76158800	0.71860100
C	-4.10208500	1.20821500	-1.23768900
H	-2.33183300	2.10140600	-0.40786200
C	-4.86678900	-0.82054200	-0.17997500
H	-3.66949500	-1.51353600	1.48780100
C	-5.02497400	0.15881700	-1.16217300
H	-4.21670000	1.97742600	-1.99439700
H	-5.57814000	-1.63740300	-0.11138200
H	-5.85526400	0.10972700	-1.85749300
O	-1.68673200	-0.81000000	2.79961700
C	2.77537600	0.73217800	1.25913600
H	2.42204200	-0.25630600	1.55534300
C	4.29762000	0.60879200	1.05896800
H	4.75500700	1.57205400	0.81613100
H	4.76646300	0.24209400	1.97673600
H	4.53409900	-0.09187800	0.25424200
C	2.44478100	1.70217700	2.41073500
H	2.92302900	1.36948600	3.33683700
H	2.80377700	2.71223700	2.19078200
H	1.36742100	1.75657100	2.58461100

Zero-point correction= (Hartree/Particle)	0.294612
Thermal correction to Energy=	0.314759
Thermal correction to Enthalpy=	0.315703
Thermal correction to Gibbs Free Energy=	0.240125
Sum of electronic and zero-point Energies=	-3668.126670
Sum of electronic and thermal Energies=	-3668.106523
Sum of electronic and thermal Enthalpies=	-3668.105578
Sum of electronic and thermal Free Energies=	-3668.181157

Sulfoxide product formed from first T.S. of **1** and **2iP**.



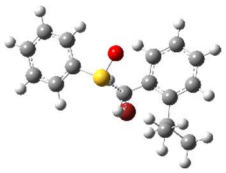


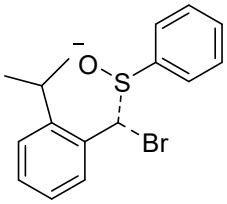
0 1

C	-0.28034800	-0.91753700	1.27381400
H	-0.97038600	-1.70975100	1.56489500
H	0.42941500	-0.75554400	2.08517600
C	-0.96428200	0.35243800	0.85704600
C	-0.39486700	1.56711400	1.27084200
C	-2.14715100	0.36654500	0.08591000
C	-0.97367600	2.78845600	0.94731300
H	0.51240400	1.54608200	1.86473100
C	-2.71469800	1.60935100	-0.22841400
C	-2.14392300	2.80756100	0.19029500
H	-0.51895100	3.71294400	1.28419900
H	-3.62759500	1.64226500	-0.81255200
H	-2.61228500	3.74992800	-0.07130900
S	0.72515400	-1.75599300	-0.07714600
C	2.04190800	-0.51380500	-0.26475700
C	1.92281000	0.45423600	-1.26030300
C	3.17352500	-0.58884000	0.54359100
C	2.94927800	1.38388100	-1.42787100
H	1.04759400	0.48335000	-1.89924800
C	4.19475600	0.34277200	0.36637400
H	3.25316800	-1.37437200	1.28592800
C	4.08158400	1.32930700	-0.61521800
H	2.86669800	2.14227100	-2.19770000
H	5.08031700	0.29490600	0.98968900
H	4.88050600	2.04882500	-0.75286500
O	1.35341900	-2.96622900	0.61581800
C	-2.84079600	-0.90735600	-0.38838800
H	-2.21626800	-1.76219300	-0.12252600
C	-4.19485900	-1.10260500	0.32146500
H	-4.89124000	-0.29576000	0.07552300
H	-4.65282600	-2.04696100	0.01340300
H	-4.07327500	-1.12228600	1.40777400
C	-3.00653700	-0.94539200	-1.91901100
H	-3.44558000	-1.89903400	-2.22563300
H	-3.66489600	-0.14778200	-2.27406500
H	-2.04297200	-0.83793500	-2.42376300

Zero-point correction= 0.297310
(Hartree/Particle)
Thermal correction to Energy= 0.314747
Thermal correction to Enthalpy= 0.315692
Thermal correction to Gibbs Free Energy= 0.249809
Sum of electronic and zero-point Energies= -1093.841983
Sum of electronic and thermal Energies= -1093.824546
Sum of electronic and thermal Enthalpies= -1093.823601
Sum of electronic and thermal Free Energies= -1093.889484

Other transition state for reaction of **1** and **2iP** – **1.2iP.TSb**





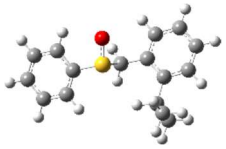
-1 1

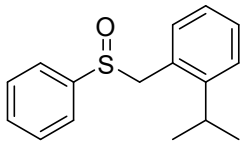
C	-0.28840500	0.64555700	0.01349300
H	-0.28396100	0.78827700	1.07883100
H	0.64866500	0.82547500	-0.48636000
C	-1.23056400	-0.26411600	-0.61757000
C	-0.94608600	-0.68760800	-1.93180900
C	-2.40704900	-0.73165500	0.02339500
C	-1.78172000	-1.56270900	-2.60918000
H	-0.04815300	-0.31764900	-2.41456300
C	-3.22737300	-1.62147400	-0.67719200
C	-2.93082900	-2.03551000	-1.97466900
H	-1.53980700	-1.87779100	-3.61772300
H	-4.12522000	-2.00130600	-0.20275100
H	-3.59450000	-2.72392900	-2.48614800
Br	-1.08637900	2.85856100	-0.38669100
S	1.47018200	-1.51986400	1.01321200
C	2.94147000	-0.65241500	0.50761800
C	3.31116200	0.53763300	1.15966000
C	3.74240700	-1.14442500	-0.53181200
C	4.45985200	1.21841300	0.77107900
H	2.70123700	0.92563300	1.96997900
C	4.89298300	-0.45356800	-0.91231600
H	3.44774600	-2.06448000	-1.02283700
C	5.26031100	0.72857700	-0.26778500
H	4.73493400	2.13576300	1.28110200
H	5.50708200	-0.84343800	-1.71790700
H	6.15542700	1.26209900	-0.56660700
O	1.37470700	-2.81254600	0.10616400
C	-2.78733300	-0.31725900	1.43995000
C	-4.23115000	0.21046600	1.53108300
H	-4.96525200	-0.56943100	1.31083600
H	-4.43137000	0.57540900	2.54268800
H	-4.39409900	1.03667100	0.83438700
C	-2.55585300	-1.47105400	2.43607100
H	-2.77823300	-1.14344700	3.45618700
H	-3.20276400	-2.32337100	2.20712500
H	-1.51986300	-1.81727600	2.40740400

H	-2.14008300	0.50822000	1.73973800

Zero-point correction=	0.294661
(Hartree/Particle)	
Thermal correction to Energy=	0.314780
Thermal correction to Enthalpy=	0.315724
Thermal correction to Gibbs Free Energy=	0.240450
Sum of electronic and zero-point Energies=	-3668.126678
Sum of electronic and thermal Energies=	-3668.106559
Sum of electronic and thermal Enthalpies=	-3668.105615
Sum of electronic and thermal Free Energies=	-3668.180889

Sulfoxide product formed from second T.S. of **1** and **2iP**.





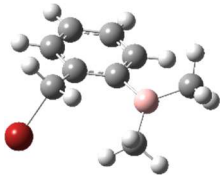
0 1

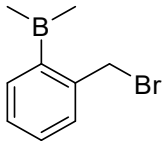
C	0.05394400	0.39940300	-0.69964300
H	-0.16008500	-0.56162200	-1.16660100
H	-0.43768400	1.18928100	-1.26866100
C	1.51871900	0.68011200	-0.52091100
C	1.95422900	2.00034100	-0.71548400
C	2.45500600	-0.31565000	-0.16573800
C	3.29196800	2.35184400	-0.57683800
H	1.22691700	2.75768200	-0.98641700
C	3.79960000	0.05930600	-0.03844300
C	4.22151600	1.37078400	-0.23696100
H	3.60460600	3.37757800	-0.73512700
H	4.53657400	-0.69163200	0.22370000
H	5.27033900	1.62351200	-0.12773300
S	-0.85412300	0.36979200	0.94662400
C	-2.51516300	0.03971300	0.27003800
C	-2.88809100	-1.27309000	-0.01751700
C	-3.39929400	1.10016400	0.09865900
C	-4.16760700	-1.51974300	-0.51306300
H	-2.20002500	-2.09530800	0.14734400
C	-4.67819400	0.84193300	-0.39481800
H	-3.08579800	2.10444400	0.35853400
C	-5.06077000	-0.46384800	-0.70280900
H	-4.46848700	-2.53563700	-0.74138600
H	-5.37562700	1.66008400	-0.53355200
H	-6.05666300	-0.66068000	-1.08262100
O	-0.86169400	1.81097300	1.45059100
C	2.06764500	-1.77420500	0.06142900

C	2.64902400	-2.68546300	-1.03709500
H	3.74267500	-2.67752800	-1.02044500
H	2.31879500	-3.71784000	-0.88938200
H	2.32592100	-2.36394900	-2.03088200
C	2.46930600	-2.26987500	1.46328300
H	2.11487700	-3.29329900	1.61621800
H	3.55482100	-2.27187900	1.59450500
H	2.03625100	-1.64017000	2.24469500
H	0.98107500	-1.85784600	0.00257100

Zero-point correction= 0.297409
(Hartree/Particle)
Thermal correction to Energy= 0.314806
Thermal correction to Enthalpy= 0.315751
Thermal correction to Gibbs Free Energy= 0.250214
Sum of electronic and zero-point Energies= -1093.842055
Sum of electronic and thermal Energies= -1093.824658
Sum of electronic and thermal Enthalpies= -1093.823713
Sum of electronic and thermal Free Energies= -1093.889250

2-Bromomethylphenyl dimethyl brorane (reactant – **2b**)





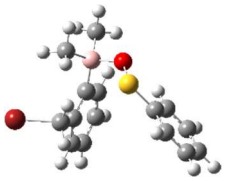
0 1

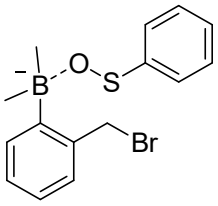
C	2.50384600	0.67166300	-0.41513600
C	1.40554500	-0.08331600	0.04838600
C	0.26217200	0.63874300	0.47415100
C	0.25567100	2.03999100	0.42782300
C	1.34145200	2.75085500	-0.06958100
C	2.47292500	2.05993500	-0.50207700
H	3.40452000	0.15427600	-0.72657900
H	-0.61809800	2.57711500	0.78243000
H	1.31068900	3.83387800	-0.10666600
H	3.33115400	2.60042600	-0.88550000
C	-0.93758000	-0.03406100	1.06083500
H	-1.34471600	0.51008500	1.90786800
H	-0.78598400	-1.07389900	1.32187800
B	1.56337800	-1.65448400	0.01751900
Br	-2.50281200	-0.08039300	-0.22408100
C	2.97047900	-2.29158000	0.34048100
H	2.87614600	-3.28851800	0.78332900
H	3.49821900	-2.44423000	-0.61376800

H	3.62342100	-1.68250100	0.97046900
C	0.40710600	-2.63847700	-0.40250900
H	0.06269100	-3.18338500	0.48950100
H	-0.46649900	-2.18440400	-0.87228100
H	0.80029100	-3.41517700	-1.06968200

Zero-point correction= 0.185630
(Hartree/Particle)
Thermal correction to Energy= 0.197778
Thermal correction to Enthalpy= 0.198722
Thermal correction to Gibbs Free Energy= 0.145746
Sum of electronic and zero-point Energies= -2949.123874
Sum of electronic and thermal Energies= -2949.111726
Sum of electronic and thermal Enthalpies= -2949.110782
Sum of electronic and thermal Free Energies= -2949.163758

Complex of **1** with **2b** – **1.2b.C**





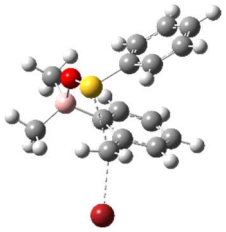
-1 1

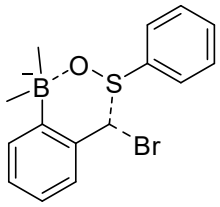
C	-0.18659700	0.16713300	-2.52380100
C	-0.61152500	0.40552000	-1.19691800
C	-1.06486400	-0.75116100	-0.50540900
C	-1.06602600	-2.02014700	-1.11777100
C	-0.64457800	-2.19869700	-2.42651200
C	-0.20202500	-1.08261400	-3.13724900
H	0.17577900	1.00368300	-3.10826700
H	-1.41204000	-2.87703000	-0.54648700
H	-0.65564500	-3.18353000	-2.88101800
H	0.13573300	-1.18686900	-4.16400100
C	-1.52347100	-0.72823400	0.91179900
H	-1.25188500	0.15881000	1.46114800
H	-1.25197100	-1.62625800	1.45862800
Br	-3.57443900	-0.77008800	1.08121300
B	-0.47201700	1.96923700	-0.62500500
O	0.97710400	2.14842700	-0.00971600
S	1.39975400	1.40389300	1.40352600
C	2.65905900	0.24813000	0.91008400
C	3.08148200	0.11985200	-0.41715300
C	3.26407600	-0.53369200	1.90791900
C	4.09148500	-0.78696000	-0.73958000

H	2.60850600	0.72485100	-1.17922100
C	4.27118200	-1.43398900	1.57379100
H	2.94652600	-0.43889600	2.94182600
C	4.69249400	-1.56823100	0.24755200
H	4.40902600	-0.88149300	-1.77287600
H	4.72833200	-2.03456300	2.35306600
H	5.47670400	-2.27107100	-0.00945000
C	-0.44312200	3.06024100	-1.84801900
H	-1.35998200	3.01868100	-2.45237300
H	-0.37963800	4.07633400	-1.43810300
H	0.40183600	2.94922400	-2.53907700
C	-1.59559200	2.46532700	0.46120600
H	-1.53259700	3.55607600	0.57630400
H	-2.61836900	2.24202700	0.13169200
H	-1.49963700	2.05234200	1.47246000

Zero-point correction= 0.280497
(Hartree/Particle)
Thermal correction to Energy= 0.300153
Thermal correction to Enthalpy= 0.301097
Thermal correction to Gibbs Free Energy= 0.229124
Sum of electronic and zero-point Energies= -3654.325069
Sum of electronic and thermal Energies= -3654.305413
Sum of electronic and thermal Enthalpies= -3654.304469
Sum of electronic and thermal Free Energies= -3654.376443

Transition state for internal alkylation of **1.2b.C** – **1.2b.C.TS**





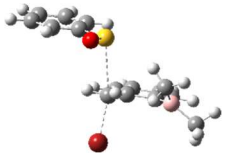
-1 1

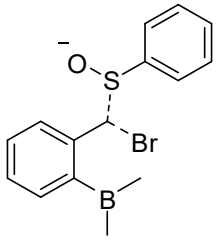
C	0.10203000	1.67306800	2.08531100
C	0.43622900	1.23666200	0.78846300
C	0.76757700	-0.14830200	0.67746700
C	0.65958300	-1.01997500	1.78701300
C	0.32779200	-0.54010500	3.04017600
C	0.07084400	0.82752400	3.19109600
H	-0.15181600	2.71572900	2.23539300
H	0.88726900	-2.07207400	1.65077900
H	0.27470400	-1.21037000	3.89077400

H	-0.17495400	1.22690400	4.17012800
C	1.20713900	-0.72359900	-0.56658700
H	1.50374600	-0.11167400	-1.39319500
H	1.05793500	-1.77449600	-0.76159000
Br	3.69416000	-1.30176900	-0.29980700
B	0.27254300	2.25463000	-0.48725800
O	-0.89929200	1.65138900	-1.43464800
S	-1.04788700	0.10912300	-1.92492000
C	-2.38870000	-0.52737900	-0.93807000
C	-3.02125700	0.25075400	0.03404400
C	-2.81698800	-1.84111600	-1.17792000
C	-4.07801800	-0.29006100	0.76728500
H	-2.68207400	1.26430000	0.20260500
C	-3.87111200	-2.36897700	-0.43875000
H	-2.33007900	-2.44629100	-1.93604000
C	-4.50715000	-1.59678900	0.53755800
H	-4.56674400	0.31647400	1.52215500
H	-4.19765500	-3.38601900	-0.62606800
H	-5.32875700	-2.01132100	1.11029900
C	1.61587700	2.51074000	-1.38204800
H	2.38359300	3.01102200	-0.77587100
H	2.10335500	1.63313000	-1.82009300
H	1.38468000	3.18775600	-2.21544600
C	-0.37984200	3.69193000	-0.08256500
H	0.30060300	4.28763700	0.54078500
H	-0.57600700	4.28432400	-0.98500600
H	-1.32959600	3.61039400	0.46099400

Zero-point correction=	0.279321
(Hartree/Particle)	
Thermal correction to Energy=	0.298714
Thermal correction to Enthalpy=	0.299658
Thermal correction to Gibbs Free Energy=	0.229139
Sum of electronic and zero-point Energies=	-3654.316877
Sum of electronic and thermal Energies=	-3654.297484
Sum of electronic and thermal Enthalpies=	-3654.296540
Sum of electronic and thermal Free Energies=	-3654.367059

Transition state for reaction of **1** and **2b** w/o precomplexation – **1.2b.TS**

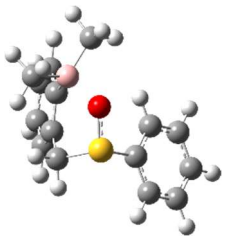


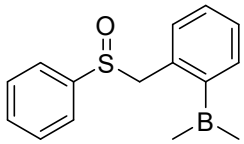


```
-1 1
 C                 -0.54857200   -0.76076600    0.15786200
 H                  0.35180100   -1.10175900    0.64114400
 H                 -0.86351700   -1.32129000   -0.70227100
 C                 -0.93567500    0.63364200    0.32629500
 C                 -0.21757100    1.39625500    1.26597400
 C                 -2.03530900    1.21728400   -0.36726000
 C                 -0.52314000    2.73070500    1.49955900
 H                  0.59507100    0.92789000    1.80981600
 C                 -2.33533000    2.56091800   -0.08016100
 C                 -1.58566900    3.32191800    0.81629800
 H                  0.05610200    3.30305600    2.21552000
 H                 -3.17707600    3.03130500   -0.57726400
 H                 -1.84095500    4.36088600    0.99355000
 Br                -1.97258900   -2.00608400    1.61720500
 B                 -2.94174700    0.49851500   -1.43819800
 S                  1.52707500   -0.40652400   -1.82046200
 O                  1.67961300   -1.92800500   -2.22434500
 C                  2.86481300   -0.04108100   -0.70354100
 C                  3.74501300   -1.04906000   -0.28666300
 C                  3.04816600    1.27339600   -0.23975900
 C                  4.78993500   -0.74403300    0.58476700
 H                  3.59588200   -2.05589600   -0.65894300
 C                  4.09331800    1.56518800    0.63097200
 H                  2.37837100    2.06237200   -0.56577000
 C                  4.97168500    0.55975200    1.04996000
 H                  5.46752900   -1.53051400    0.90136200
 H                  4.22728400    2.58305600    0.98222000
 H                  5.78664300    0.79249400    1.72593400
 C                 -4.49054700    0.80573500   -1.46177500
 H                 -4.66499600    1.59613700   -2.20839600
 H                 -5.06999100   -0.05609900   -1.80947100
 H                 -4.90974900    1.15862600   -0.51644000
 C                 -2.37980700   -0.45600500   -2.55888300
 H                 -1.30665900   -0.38846000   -2.74565500
 H                 -2.60028600   -1.49558100   -2.27285100
 H                 -2.91405900   -0.30050000   -3.50336900

Zero-point correction=                           0.277632
(Hartree/Particle)
 Thermal correction to Energy=                    0.298481
 Thermal correction to Enthalpy=                  0.299426
 Thermal correction to Gibbs Free Energy=         0.222713
 Sum of electronic and zero-point Energies=          -3654.294129
 Sum of electronic and thermal Energies=             -3654.273280
 Sum of electronic and thermal Enthalpies=           -3654.272335
 Sum of electronic and thermal Free Energies=        -3654.349048
```

Sulfoxide product formed from **1** and **2b**.





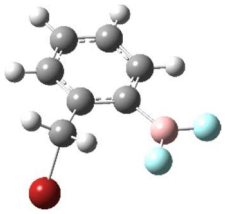
0 1

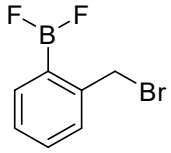
C	-2.22405500	1.51058700	0.85944400
C	-1.71648700	0.43826000	0.10547000
C	-0.95213200	0.77920000	-1.03319700
C	-0.69127200	2.11354300	-1.36994500
C	-1.22736400	3.14912200	-0.60993300
C	-2.00304700	2.84195500	0.50814200
H	-2.81073200	1.29903200	1.74744100
H	-0.07993000	2.34079700	-2.23790800
H	-1.03820200	4.18099200	-0.88410200
H	-2.42596000	3.63933700	1.11058400
C	-0.39126900	-0.30482300	-1.90307100
H	-1.15415900	-0.88560900	-2.42535900
H	0.33701600	0.05135000	-2.63279500
B	-1.99688800	-1.09831900	0.52983300
O	-0.55647600	-1.94965000	0.21823600
S	0.47853500	-1.61120500	-0.91305800
C	1.79178700	-0.65132900	-0.12050400
C	1.63364700	-0.15266200	1.16872100
C	2.98289600	-0.49267100	-0.82992900
C	2.69044000	0.54758300	1.74956000
H	0.70953100	-0.31774500	1.70589900
C	4.02639500	0.21799900	-0.24072200
H	3.10277200	-0.91626600	-1.82115900
C	3.87959100	0.73763800	1.04619100
H	2.58200600	0.94263500	2.75275900
H	4.95521100	0.35332300	-0.78195400
H	4.69702600	1.28208000	1.50430400
C	-3.12321300	-1.83609600	-0.37449400
H	-2.98834300	-1.73240600	-1.45793900
H	-3.17398000	-2.90965300	-0.15372100
H	-4.11142500	-1.41611500	-0.14483400
C	-2.18707700	-1.35759800	2.11146200
H	-3.15419100	-0.96947500	2.45612300
H	-2.18428200	-2.43034600	2.33930100
H	-1.41570300	-0.88807800	2.73408300

Zero-point correction= 0.281442
(Hartree/Particle)
Thermal correction to Energy= 0.298426

```
 Thermal correction to Enthalpy=                  0.299370
 Thermal correction to Gibbs Free Energy=         0.237073
 Sum of electronic and zero-point Energies=          -1080.020291
 Sum of electronic and thermal Energies=             -1080.003307
 Sum of electronic and thermal Enthalpies=           -1080.002362
 Sum of electronic and thermal Free Energies=        -1080.064659
```

2-bromomethylphenyl difluoro borane (reactant – **2c**)

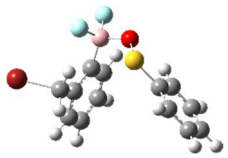


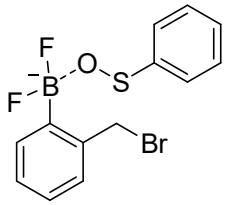



```
0 1
 C                  2.54669600    0.09457300   -0.39026300
 C                  1.29419900   -0.32164200    0.09827000
 C                  0.38039700    0.66850200    0.54022100
 C                  0.75053500    2.01581000    0.48253100
 C                  1.99719400    2.40242200   -0.00341900
 C                  2.90104900    1.43866300   -0.44468100
 H                  3.25387000   -0.65336700   -0.72873800
 H                  0.05164400    2.77189400    0.82308100
 H                  2.26035000    3.45351600   -0.03459300
 H                  3.87284700    1.73101500   -0.82443400
 C                 -0.97423000    0.34452300    1.08426500
 H                 -1.35528500    1.13490700    1.72274600
 H                 -1.03946500   -0.61462400    1.58170300
 B                  1.03088500   -1.84411900    0.11495100
 Br                -2.35345100    0.21778100   -0.38306900
 F                 -0.07672700   -2.41995300    0.58958600
 F                  1.94310000   -2.70029000   -0.35721400

Zero-point correction=                           0.118761
(Hartree/Particle)
 Thermal correction to Energy=                    0.128780
 Thermal correction to Enthalpy=                  0.129724
 Thermal correction to Gibbs Free Energy=         0.080560
 Sum of electronic and zero-point Energies=          -3069.208509
 Sum of electronic and thermal Energies=             -3069.198491
 Sum of electronic and thermal Enthalpies=           -3069.197547
 Sum of electronic and thermal Free Energies=        -3069.246710
```

Complex of **1** with **2c** – **1.2c.C**



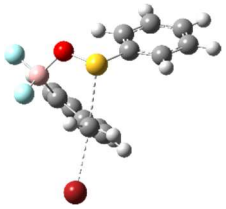


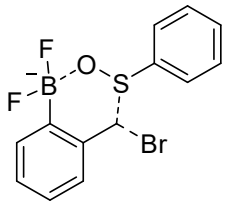
-1 1

C	0.11569100	-1.62035000	1.79738200
C	0.59854400	-0.54318500	1.02978700
C	1.17068000	-0.86517500	-0.22219900
C	1.22345400	-2.20016100	-0.66178900
C	0.73781200	-3.23803600	0.12188300
C	0.18322300	-2.94288600	1.36890000
H	-0.32359300	-1.40648200	2.76588900
H	1.66075400	-2.41960700	-1.63133900
H	0.78888900	-4.26178700	-0.23261100
H	-0.19818300	-3.74002400	1.99890500
C	1.71605900	0.17602600	-1.14155000
H	1.41912100	1.18467400	-0.89419300
H	1.54222300	-0.04995700	-2.18944100
Br	3.75796800	0.27447800	-1.06741400
B	0.39059400	0.94561600	1.66050800
O	-0.98370600	1.51327900	1.42691600
S	-1.43304600	1.92327000	-0.11891100
C	-2.75605600	0.78252800	-0.46189900
C	-3.20955900	-0.15142400	0.47372200
C	-3.37494300	0.86750300	-1.71855200
C	-4.27055200	-0.99683900	0.14759800
H	-2.72809200	-0.21083400	1.44051600
C	-4.43333100	0.01945400	-2.03052300
H	-3.02994000	1.59162600	-2.44995800
C	-4.88819600	-0.91896500	-1.10024500
H	-4.61450900	-1.72092200	0.87856000
H	-4.90295100	0.09125100	-3.00558100
H	-5.71186400	-1.57888200	-1.34701500
F	0.47722900	0.89224500	3.08494300
F	1.36029500	1.89627000	1.20343500

Zero-point correction= 0.212647
(Hartree/Particle)
Thermal correction to Energy= 0.230545
Thermal correction to Enthalpy= 0.231489
Thermal correction to Gibbs Free Energy= 0.162436
Sum of electronic and zero-point Energies= -3774.435785
Sum of electronic and thermal Energies= -3774.417887
Sum of electronic and thermal Enthalpies= -3774.416943
Sum of electronic and thermal Free Energies= -3774.485996

Transition state for internal alkylation of **1.2c.C** – **1.2c.C.TS**





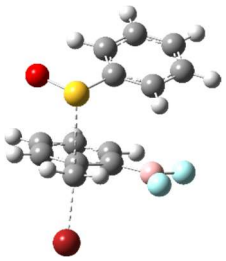
-1 1

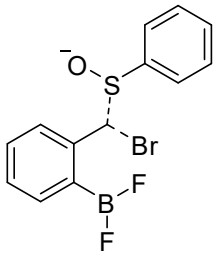
C	0.12194800	2.08216600	1.82326400
C	0.43801000	1.44109400	0.61828700
C	0.75133900	0.05575900	0.68136600
C	0.66950200	-0.64539200	1.90422300
C	0.37192500	0.02545800	3.07842200
C	0.11496700	1.40118200	3.03911100
H	-0.13047300	3.13660600	1.80297300
H	0.88840300	-1.70723200	1.92124500
H	0.34169300	-0.51017400	4.02043300
H	-0.10926100	1.93400600	3.95726000
C	1.11812500	-0.65214500	-0.51573500
H	1.51583900	-0.12974200	-1.36575600
H	0.99196900	-1.72099400	-0.59066800
Br	3.71627500	-1.38717900	-0.17773600
B	0.20346200	2.18467800	-0.79244500
O	-1.02090500	1.57165800	-1.48802500
S	-1.06495500	-0.01908500	-1.86315500
C	-2.37738200	-0.63226000	-0.82402500
C	-3.02136200	0.17802200	0.11185600
C	-2.75711300	-1.97050500	-0.99094700
C	-4.04933900	-0.36001400	0.88668700
H	-2.72211700	1.21160900	0.22168200
C	-3.78082700	-2.49441000	-0.20765700
H	-2.25988700	-2.59659100	-1.72448600
C	-4.43104700	-1.69192500	0.73334500
H	-4.55167900	0.26899800	1.61309400
H	-4.07319500	-3.53050800	-0.33524100
H	-5.23022300	-2.10328500	1.33890400
F	-0.14784300	3.54280600	-0.64424500
F	1.30851200	2.08887200	-1.68808500

Zero-point correction= 0.211672
(Hartree/Particle)
Thermal correction to Energy= 0.229152
Thermal correction to Enthalpy= 0.230096

```
 Thermal correction to Gibbs Free Energy=          0.163035
 Sum of electronic and zero-point Energies=         -3774.420201
 Sum of electronic and thermal Energies=            -3774.402721
 Sum of electronic and thermal Enthalpies=          -3774.401777
 Sum of electronic and thermal Free Energies=       -3774.468838
```

Transition state for reaction of **1** and **2c** w/o precomplexation – **1.2c.TS**



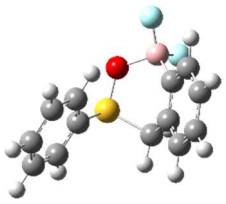


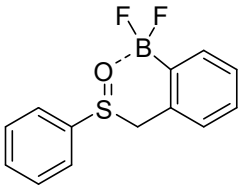

```
-1 1
 C                 -1.45006800   -0.80860900   -0.47956900
 H                 -1.67715800   -1.86042700   -0.43121600
 H                 -1.23132800   -0.41267000   -1.45451200
 C                 -0.88166300   -0.19041200    0.71186300
 C                 -0.92094000   -0.92417000    1.91086900
 C                 -0.33526500    1.12538300    0.72733000
 C                 -0.43339700   -0.39513200    3.09855600
 H                 -1.34162600   -1.92277100    1.90040500
 C                  0.14800900    1.63481600    1.94630000
 C                  0.10028800    0.89501200    3.12294800
 H                 -0.47315800   -0.98617400    4.00673700
 H                  0.56764800    2.63386500    1.96730700
 H                  0.47681000    1.31570800    4.04803100
 Br                -3.70701100   -0.15524200   -0.54741500
 B                 -0.22875500    2.05256000   -0.49742500
 S                  1.06117700   -2.22170000   -0.98992400
 O                  1.22545900   -3.25439800    0.19115000
 C                  2.26685600   -0.94327200   -0.72144300
 C                  3.12481000   -0.98723800    0.38521800
 C                  2.36648200    0.12246200   -1.63302200
 C                  4.06898900    0.02103700    0.57346400
 H                  3.03839200   -1.81612800    1.07774300
 C                  3.31287100    1.12348500   -1.43433100
 H                  1.71549500    0.15842500   -2.50095000
 C                  4.17003200    1.08098200   -0.32967100
 H                  4.73100500   -0.02180300    1.43238500
 H                  3.38286800    1.94052500   -2.14467000
```

H	4.90586100	1.86250000	-0.17848900
F	0.30070000	3.28106900	-0.38501700
F	-0.65738700	1.75625800	-1.73027300

Zero-point correction= 0.210814
(Hartree/Particle)
Thermal correction to Energy= 0.229406
Thermal correction to Enthalpy= 0.230350
Thermal correction to Gibbs Free Energy= 0.159082
Sum of electronic and zero-point Energies= -3774.381000
Sum of electronic and thermal Energies= -3774.362408
Sum of electronic and thermal Enthalpies= -3774.361464
Sum of electronic and thermal Free Energies= -3774.432732

Sulfoxide product formed from **1** and **2c**.





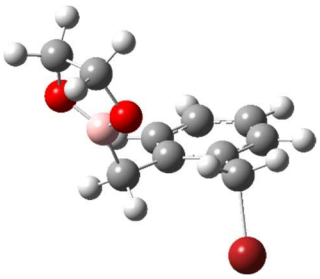
0 1

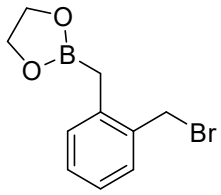
C	-2.33448600	1.41768200	0.84404000
C	-1.78141900	0.36416900	0.10688700
C	-1.02587800	0.69000700	-1.03701100
C	-0.82353400	2.01992300	-1.41736400
C	-1.40538600	3.04863500	-0.67897100
C	-2.16349100	2.74608200	0.45229000
H	-2.90743100	1.19460700	1.73784800
H	-0.22356600	2.25097100	-2.29145100
H	-1.26237800	4.07965500	-0.98217500
H	-2.61427700	3.54506000	1.03094600
C	-0.43189600	-0.42665600	-1.83861300
H	-1.17861000	-1.07207200	-2.30588200
H	0.28586900	-0.10498800	-2.59373500
B	-1.92195200	-1.16987100	0.54186700
O	-0.49638600	-1.86389500	0.45808600
S	0.49983400	-1.62718900	-0.75769100
C	1.80774500	-0.59579000	-0.06609700
C	1.64350700	0.05801000	1.15170700
C	3.00143700	-0.53182800	-0.78612100
C	2.70228700	0.81782000	1.64629300
H	0.71900500	-0.03536500	1.70493100
C	4.04540100	0.24075700	-0.28268300

H	3.12248600	-1.07314000	-1.71791500
C	3.89525800	0.91391300	0.93025900
H	2.59216300	1.33194600	2.59356800
H	4.97718000	0.30389000	-0.83159000
H	4.71379900	1.50560900	1.32287200
F	-2.75061300	-1.92336000	-0.32188200
F	-2.29583100	-1.37741300	1.87009500

Zero-point correction= 0.213589
(Hartree/Particle)
Thermal correction to Energy= 0.228691
Thermal correction to Enthalpy= 0.229635
Thermal correction to Gibbs Free Energy= 0.170346
Sum of electronic and zero-point Energies= -1200.113270
Sum of electronic and thermal Energies= -1200.098168
Sum of electronic and thermal Enthalpies= -1200.097224
Sum of electronic and thermal Free Energies= -1200.156513

Ethylene glycol ester of (2-bromoethyl)phenylmethyl boronic acid (reactant – **2Ca**)





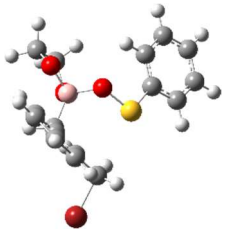
0 1

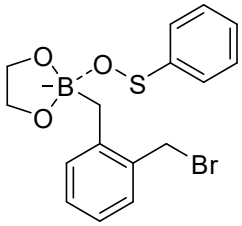
C	0.24701700	2.41615300	0.86319400
C	-0.44274400	3.43982000	0.21768300
C	-1.36665700	3.13394600	-0.78060400
C	-1.58581100	1.80295000	-1.11810300
C	-0.89269500	0.76469900	-0.47901900
C	0.03961100	1.07046000	0.53634800
H	0.96010300	2.66280300	1.64278800
H	-0.26070200	4.47163200	0.49681000
H	-1.90965100	3.92198800	-1.28925700
H	-2.30446200	1.55593400	-1.89268200
C	-1.15666900	-0.63591200	-0.91195300
H	-0.29646900	-1.29295700	-0.85087500
H	-1.60519500	-0.68764700	-1.89868900
C	0.82829200	-0.00300800	1.26665800
H	0.20524600	-0.88432600	1.43910400
H	1.11788400	0.38181800	2.24762800

Br	-2.53621900	-1.55959400	0.26312400
B	2.13241800	-0.41814900	0.48541200
O	3.36221700	0.14006900	0.72102200
O	2.15193500	-1.35735900	-0.51566900
C	4.29712400	-0.38886900	-0.25008900
H	4.58823700	0.41913800	-0.92370500
H	5.18003900	-0.75604800	0.27308800
C	3.51790100	-1.51011200	-0.97258300
H	3.54125400	-1.41094100	-2.05778300
H	3.86384300	-2.50729700	-0.69482200

Zero-point correction= 0.207076
(Hartree/Particle)
Thermal correction to Energy= 0.220326
Thermal correction to Enthalpy= 0.221270
Thermal correction to Gibbs Free Energy= 0.163111
Sum of electronic and zero-point Energies= -3137.796916
Sum of electronic and thermal Energies= -3137.783666
Sum of electronic and thermal Enthalpies= -3137.782722
Sum of electronic and thermal Free Energies= -3137.840882

Complex of **1** with **2Ca** – **1.2Ca.C**





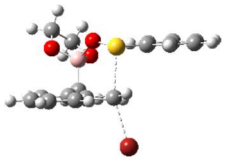
-1 1

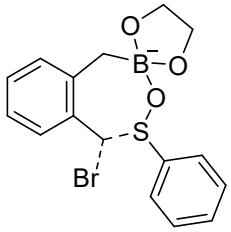
S	1.37073100	-0.93640300	0.58187300
O	1.08379800	0.69035600	0.63664900
B	0.52512600	1.41375300	-0.61492500
O	1.38956300	1.22424400	-1.79235000
O	0.63464000	2.84237900	-0.26723800
C	2.26094500	2.34311700	-1.87087100
H	3.19036100	2.15740500	-1.31310900
H	2.52367300	2.54290000	-2.91508300
C	1.46002100	3.48207100	-1.22897300
H	0.84221400	3.99625100	-1.98211600
H	2.10012200	4.23020700	-0.74760800
C	-1.00813800	0.91984800	-0.96727900
H	-0.97951700	-0.10213300	-1.35472400

H	-1.31946900	1.54810200	-1.81132100
C	3.14597600	-1.05087100	0.53931500
C	3.97197800	0.06640500	0.69657800
C	3.72041800	-2.32318200	0.39139900
C	5.35809900	-0.09046300	0.69868600
H	3.52068700	1.04269100	0.81478100
C	5.10470100	-2.46766700	0.40149100
H	3.08749800	-3.19599000	0.26501400
C	5.93384300	-1.35271600	0.55285800
H	5.99055900	0.78306800	0.81793500
H	5.53757400	-3.45527600	0.28331500
H	7.01159800	-1.46835200	0.55550900
C	-2.03018400	1.06158800	0.12640700
C	-2.43170500	2.35244800	0.51714200
C	-2.62125400	-0.03089200	0.80528100
C	-3.36134500	2.56652700	1.52805900
H	-1.98124400	3.19963100	0.01375100
C	-3.55829400	0.19614600	1.82890400
C	-3.93137500	1.48083200	2.19847600
H	-3.64119700	3.57992600	1.79684000
H	-3.99801700	-0.65783400	2.33507700
H	-4.65336800	1.63626600	2.99216100
C	-2.29168400	-1.44135200	0.47713800
H	-1.29220300	-1.60312800	0.09385600
H	-2.50550300	-2.12606900	1.29135600
Br	-3.46248900	-2.18631000	-1.03300400

Zero-point correction=	0.300085
(Hartree/Particle)	
Thermal correction to Energy=	0.321011
Thermal correction to Enthalpy=	0.321955
Thermal correction to Gibbs Free Energy=	0.245745
Sum of electronic and zero-point Energies=	-3842.988127
Sum of electronic and thermal Energies=	-3842.967201
Sum of electronic and thermal Enthalpies=	-3842.966257
Sum of electronic and thermal Free Energies=	-3843.042468

Transition state for internal alkylation of **1.2Ca.C** – **1.2Ca.C.TS**



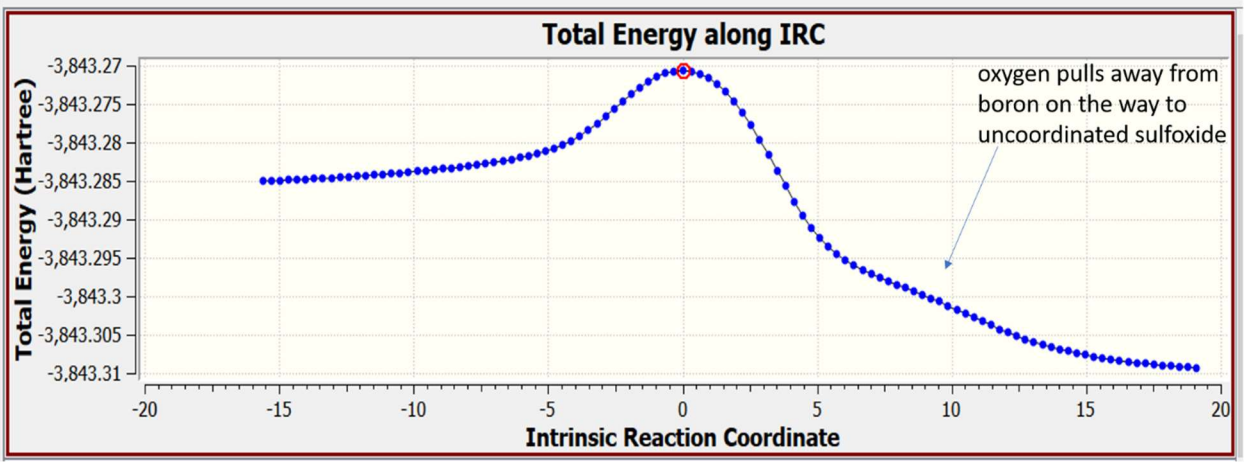


-1 1

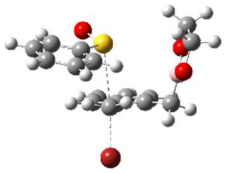
C	1.30770000	0.96479700	0.31384600
H	1.41512900	1.74273100	1.05240300
H	0.62344600	1.14442900	-0.49225200
Br	2.97688400	2.41077200	-1.11289500
S	-0.97349700	0.22466800	1.49414200
O	-1.36125000	-1.25492700	0.94404300
B	-1.01470900	-1.98308800	-0.42755900
O	-2.17781200	-1.84227400	-1.31667700
O	-0.96267500	-3.39634100	-0.06557400
C	-2.81253000	-3.10910000	-1.45086200
H	-3.90160500	-2.99825900	-1.40992000
H	-2.54927500	-3.56128100	-2.41815200
C	-2.25832900	-3.94000800	-0.28727500
H	-2.18140700	-5.00592400	-0.52222400
H	-2.88587900	-3.82695100	0.60847800
C	0.36328100	-1.44676900	-1.13258300
H	0.18725500	-0.46355400	-1.57680400
H	0.53371700	-2.13312000	-1.96880900
C	-2.16606000	1.36890900	0.81537900
C	-3.06946900	1.01959000	-0.19213700
C	-2.16614700	2.66617500	1.34953800
C	-3.97355600	1.97625500	-0.65671300
H	-3.05053100	0.01781000	-0.60607600
C	-3.06686100	3.61115700	0.86742400
H	-1.47232200	2.93448300	2.13985400
C	-3.97715400	3.27005900	-0.13615900
H	-4.67642600	1.70520900	-1.43732500
H	-3.06262800	4.61297300	1.28243200
H	-4.68113700	4.00665000	-0.50605200
C	1.56797600	-1.44736300	-0.24237900
C	2.29163600	-2.63094600	-0.03723600
C	1.96959100	-0.30044900	0.49437500
C	3.34403200	-2.69975500	0.87008300
H	2.00722700	-3.51679700	-0.59352800
C	3.01733700	-0.39170400	1.43542600
C	3.70678300	-1.57683300	1.62368700
H	3.88065200	-3.63369300	0.99898300
H	3.29732200	0.49564700	1.99272600
H	4.51953000	-1.63240100	2.33830000

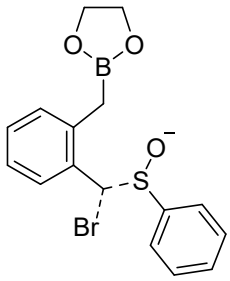
Zero-point correction=	0.298959
(Hartree/Particle)	
Thermal correction to Energy=	0.319597
Thermal correction to Enthalpy=	0.320541
Thermal correction to Gibbs Free Energy=	0.245767
Sum of electronic and zero-point Energies=	-3842.971673
Sum of electronic and thermal Energies=	-3842.951035
Sum of electronic and thermal Enthalpies=	-3842.950091
Sum of electronic and thermal Free Energies=	-3843.024865

Intrinsic Reaction Coordinate for **1.2Ca.C.TS**



Transition state for reaction of **1** and **2Ca** w/o precomplexation – **1.2Ca.TS**



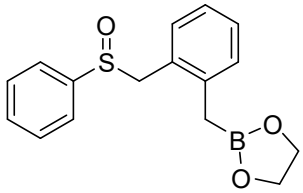



```
-1 1
 C                 -0.26742200   -1.07112100   -0.16331500
 H                  0.60881900   -1.52479800    0.26882900
 H                 -0.09409700   -0.42027700   -1.00242800
 Br                -0.72036400   -2.93762600   -1.57307400
 S                  1.20854600    1.17975600    1.06685500
 O                  1.12915600    1.05592400    2.64235100
 B                 -1.79863600    1.94646800   -1.12025800
 O                 -0.89575500    2.27089700   -2.10175100
 O                 -1.98402200    2.95209200   -0.20651100
 C                 -0.45207200    3.63082700   -1.88036600
 H                  0.63796700    3.64859600   -1.87077200
 H                 -0.81566400    4.25072000   -2.70234600
 C                 -1.06746700    4.02659900   -0.51989400
 H                 -1.62251000    4.96420000   -0.56274900
 H                 -0.31978300    4.08267800    0.27290400
 C                 -2.57613000    0.57566900   -1.07935500
```

H	-2.19477500	-0.08286600	-1.86425100
H	-3.61843100	0.79338000	-1.34076400
C	2.77304700	0.48122800	0.57779900
C	3.14173900	0.47380500	-0.77930900
C	3.64775300	-0.05715100	1.53096600
C	4.36304700	-0.06618200	-1.16758800
H	2.47431700	0.89185600	-1.52682400
C	4.87071400	-0.59534200	1.12996000
H	3.35300800	-0.04201400	2.57365800
C	5.23761200	-0.60488800	-0.21643900
H	4.63655000	-0.06737600	-2.21759500
H	5.54139400	-1.00935100	1.87618600
H	6.18882100	-1.02431500	-0.52378100
C	-2.55127600	-0.12049700	0.26326300
C	-3.63803400	-0.00272000	1.13258300
C	-1.43669100	-0.89275200	0.67914400
C	-3.64836500	-0.62534600	2.38087600
H	-4.49662300	0.58455000	0.82379400
C	-1.46404500	-1.52165400	1.93837400
C	-2.55435000	-1.39015400	2.78726300
H	-4.50978900	-0.51573600	3.03040700
H	-0.60987900	-2.11613600	2.24322900
H	-2.55354400	-1.87785000	3.75524200

Zero-point correction=	0.299040
(Hartree/Particle)	
Thermal correction to Energy=	0.320884
Thermal correction to Enthalpy=	0.321828
Thermal correction to Gibbs Free Energy=	0.241314
Sum of electronic and zero-point Energies=	-3842.967120
Sum of electronic and thermal Energies=	-3842.945276
Sum of electronic and thermal Enthalpies=	-3842.944332
Sum of electronic and thermal Free Energies=	-3843.024845

Sulfoxide product formed from **1** and **2Ca**.



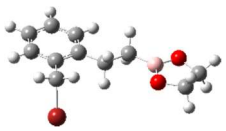
0 1

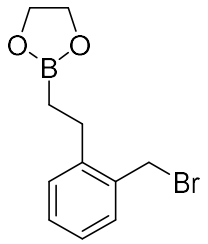
C	-0.43420100	-1.37614200	0.56283900
H	-1.10202200	-2.23470400	0.64955200
H	-0.59825400	-0.70846000	1.40757500
S	-1.05886000	-0.43888700	-0.93656300

O	-0.34994000	0.91428300	-0.92008500
B	2.05480900	1.58746200	0.52600500
O	1.55679000	2.81869200	0.88186000
O	2.77530600	1.61652800	-0.64134700
C	1.99447700	3.78190200	-0.10264900
H	1.13502300	4.35904600	-0.44507200
H	2.71484200	4.45581800	0.36695000
C	2.62715600	2.93060400	-1.22348000
H	3.60665500	3.29654600	-1.53307300
H	1.97913200	2.85004800	-2.09845300
C	1.93316500	0.33257600	1.47168000
H	0.99637900	0.41372600	2.02718600
H	2.72531700	0.44198600	2.22438200
C	-2.75421300	-0.15287300	-0.32831200
C	-3.07424200	1.07966900	0.23191900
C	-3.71196300	-1.15543800	-0.47883900
C	-4.37865000	1.30446900	0.67223900
H	-2.31133000	1.84532300	0.30929700
C	-5.01148500	-0.92209300	-0.03131400
H	-3.45633900	-2.10238200	-0.94227000
C	-5.34405400	0.30553700	0.54415100
H	-4.64027200	2.26048700	1.11113100
H	-5.76411600	-1.69424200	-0.14092400
H	-6.35719600	0.48526500	0.88482700
C	2.08586600	-1.01919800	0.80966800
C	3.37901200	-1.52361600	0.60485600
C	0.99366600	-1.80535600	0.38458100
C	3.60407400	-2.74999300	-0.01122400
H	4.22653700	-0.93495300	0.94032800
C	1.23204700	-3.04507000	-0.23060600
C	2.52148700	-3.52010100	-0.43584600
H	4.61861100	-3.10586700	-0.15237500
H	0.38491100	-3.64636100	-0.54512300
H	2.67974100	-4.48168500	-0.91035200

Zero-point correction=	0.301457
(Hartree/Particle)	
Thermal correction to Energy=	0.320577
Thermal correction to Enthalpy=	0.321521
Thermal correction to Gibbs Free Energy=	0.250826
Sum of electronic and zero-point Energies=	-1268.681530
Sum of electronic and thermal Energies=	-1268.662410
Sum of electronic and thermal Enthalpies=	-1268.661466
Sum of electronic and thermal Free Energies=	-1268.732161

Ethylene glycol ester of 2-(2-bromoethyl)phenylethyl boronic acid (reactant – **2C$_2$a**)



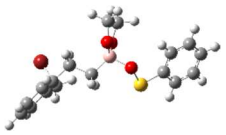


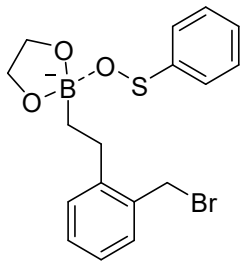
0 1

C	-0.92127400	2.52635800	-0.28961500
C	-0.83067100	1.21197900	0.17810500
C	-2.02975600	0.55649500	0.54711800
C	-3.25487400	1.22597700	0.43793600
C	-3.32263300	2.53492300	-0.02978300
C	-2.14739400	3.18467800	-0.39578400
H	-0.02170300	3.05431600	-0.57847300
H	-4.16494000	0.70978300	0.72579500
H	-4.27927100	3.03873300	-0.10530400
H	-2.17858200	4.20458100	-0.76284700
C	-2.03385600	-0.83534000	1.07729900
H	-2.92985000	-1.06241400	1.64554800
H	-1.14870500	-1.10444400	1.64310400
Br	-2.06976000	-2.22992000	-0.40223900
C	0.50267000	0.49218800	0.29996300
H	0.65014500	0.21282500	1.34999400
H	0.43233100	-0.45808400	-0.23944000
C	1.74487900	1.25057100	-0.18566800
H	1.62947600	1.54265500	-1.23748200
H	1.86230600	2.19478100	0.36079300
C	4.59109100	-1.19593000	0.44892500
C	5.31886400	-0.02835900	-0.25080600
H	4.87677100	-1.29840000	1.49773300
H	4.73585400	-2.15065500	-0.05692800
H	6.14953300	0.36526500	0.33536600
H	5.67845900	-0.29748200	-1.24617500
B	3.09006000	0.45569800	-0.05678500
O	4.30972600	0.99848000	-0.38922900
O	3.18992400	-0.83897900	0.38978700

Zero-point correction= 0.235085
(Hartree/Particle)
Thermal correction to Energy= 0.249760
Thermal correction to Enthalpy= 0.250704
Thermal correction to Gibbs Free Energy= 0.189060
Sum of electronic and zero-point Energies= -3177.090747
Sum of electronic and thermal Energies= -3177.076072
Sum of electronic and thermal Enthalpies= -3177.075127
Sum of electronic and thermal Free Energies= -3177.136772

Complex of **1** with **$2C_2a$** – **$2C_2a$.C**





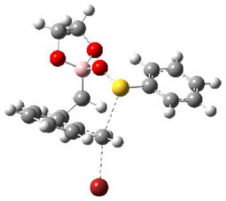
-1 1

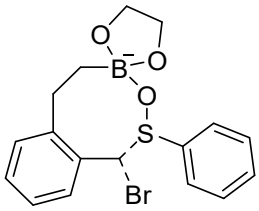
O	2.22548400	-1.51914500	-0.32072100
B	0.99106100	-1.25118500	0.60433100
O	1.17532500	-0.02486500	1.39867700
O	1.05177300	-2.36029900	1.57880600
C	1.81016600	-0.39809000	2.61205600
H	2.90462900	-0.37617700	2.50548500
H	1.53242600	0.29635200	3.41214500
C	1.31782500	-1.83001700	2.86884500
H	0.39776200	-1.82498300	3.47335500
H	2.06326300	-2.44006300	3.39284800
C	-0.36093400	-1.22922100	-0.29347600
H	-0.42605800	-2.16411700	-0.86720400
H	-0.31041800	-0.42590700	-1.04173500
C	4.12703600	0.25970900	-1.02383100
C	4.68328900	1.27230600	-1.82258300
C	4.82266100	-0.18807600	0.10420000
C	5.91575300	1.82578600	-1.48934500
H	4.15136300	1.62813300	-2.69952400
C	6.05540300	0.37774300	0.43054100
H	4.38975200	-0.97228000	0.71116800
C	6.61083700	1.38429000	-0.35955300
H	6.33303200	2.60960300	-2.11253900
H	6.58474000	0.02495200	1.30960600
H	7.56913200	1.82002500	-0.10116700
C	-3.46770500	0.06708000	-0.88589800
C	-2.92016300	-1.09286300	-0.29467400
C	-4.61801800	-0.03019200	-1.68358500
C	-3.56296600	-2.31524600	-0.53406900
C	-5.23812800	-1.25381200	-1.90915700
H	-5.02729200	0.87063400	-2.13003700
C	-4.70470000	-2.40416600	-1.32647700
H	-3.15337500	-3.21492800	-0.08556800
H	-6.12460300	-1.31057800	-2.53051600
H	-5.17696200	-3.36712200	-1.48842000
C	-1.65580300	-1.06883300	0.53594100
H	-1.70552800	-1.88483800	1.26363100
H	-1.60023300	-0.14622000	1.11939900
S	2.57397600	-0.44389000	-1.52883300
C	-2.84567600	1.40687100	-0.70181900

```
 H                -3.07882000    2.09398700   -1.50880500
 H                -1.77871200    1.38509600   -0.51465300
 Br               -3.57477000    2.37975600    0.93472600

Zero-point correction=                           0.328330
(Hartree/Particle)
 Thermal correction to Energy=                    0.350678
 Thermal correction to Enthalpy=                  0.351622
 Thermal correction to Gibbs Free Energy=         0.270846
 Sum of electronic and zero-point Energies=          -3882.282099
 Sum of electronic and thermal Energies=             -3882.259751
 Sum of electronic and thermal Enthalpies=           -3882.258807
 Sum of electronic and thermal Free Energies=        -3882.339583
```

Transition state for internal alkylation of **1.2C$_2$a.C** – **1.2C$_2$a.C.TS**



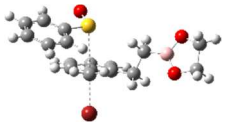


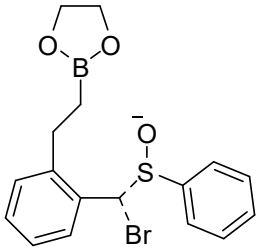

```
-1 1
 C                -1.46560300   -0.90580900    0.22834200
 H                -1.55349200   -1.70410300    0.94656900
 H                -0.92084400   -1.10755200   -0.67354400
 Br               -3.47463500   -2.09625900   -1.00942400
 S                 0.93138100   -0.41190400    1.36300400
 O                 1.48554800    1.02723900    0.88549300
 B                 1.49412800    1.73470800   -0.57840800
 O                 2.90647300    1.70709700   -1.00384000
 O                 1.19415100    3.13524100   -0.31681600
 C                 3.43206000    3.02701200   -0.95121600
 H                 4.44096700    3.02338100   -0.52393000
 H                 3.49096200    3.45096400   -1.96485000
 C                 2.42900000    3.80444500   -0.09048200
 H                 2.34261200    4.85650500   -0.37879900
 H                 2.70582400    3.75774100    0.97250400
 C                 0.49205100    0.99534900   -1.60777400
 H                 0.58653900   -0.09199100   -1.51308100
 H                 0.86963500    1.21090300   -2.61577200
 C                 2.08004800   -1.64775300    0.77055100
 C                 1.83715600   -2.97454600    1.15765100
 C                 3.19060900   -1.33565700   -0.01902900
 C                 2.70384100   -3.98338300    0.74903400
```

H	0.98013500	-3.21853900	1.77723500
C	4.05289600	-2.35908900	-0.41651500
H	3.36924300	-0.30895600	-0.31679600
C	3.81705400	-3.68070600	-0.03964000
H	2.51098000	-5.00711800	1.05018900
H	4.91514300	-2.11648000	-1.02852200
H	4.49155900	-4.46852000	-0.35489500
C	-1.96657600	0.40131600	0.54941500
C	-1.73680300	1.51703600	-0.29672000
C	-2.67316000	0.56791100	1.76060900
C	-2.24873900	2.75340600	0.10924200
C	-3.16596100	1.80497400	2.13798800
H	-2.83539700	-0.29838800	2.39287200
C	-2.95251500	2.90500700	1.30161500
H	-2.08368500	3.61850200	-0.52304300
H	-3.71036900	1.91817300	3.06818100
H	-3.33187000	3.88171400	1.58154300
C	-1.00484100	1.41338600	-1.61717300
H	-1.07551700	2.39331300	-2.09534000
H	-1.56540900	0.72241500	-2.26081300

Zero-point correction=	0.327493
(Hartree/Particle)	
Thermal correction to Energy=	0.349390
Thermal correction to Enthalpy=	0.350334
Thermal correction to Gibbs Free Energy=	0.273256
Sum of electronic and zero-point Energies=	-3882.259473
Sum of electronic and thermal Energies=	-3882.237576
Sum of electronic and thermal Enthalpies=	-3882.236632
Sum of electronic and thermal Free Energies=	-3882.313710

Transition state for reaction of **1** and **2C$_2$a** w/o precomplexation – **1.2C$_2$a.TS**





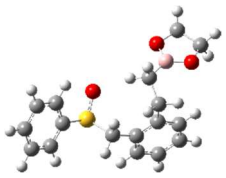
-1 1

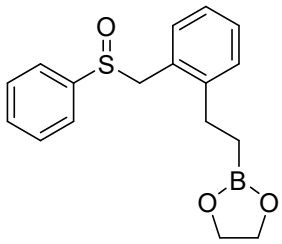
C	-0.59041900	-0.71704700	-0.35905700
H	0.32604300	-1.27736000	-0.28252500
H	-0.64405000	-0.00789000	-1.16618400
Br	-1.67156000	-2.41658100	-1.65076400
S	1.48031100	1.28124400	0.39312300
O	1.50032000	1.55960300	1.94996700

C	-2.95147500	1.14966500	-0.30885000
H	-2.77821500	0.59323900	-1.23243300
H	-4.03382600	1.29486700	-0.24292400
C	2.79819200	0.12828600	0.06630200
C	3.04628500	-0.29608400	-1.25144600
C	3.59834000	-0.35962400	1.10828100
C	4.07591200	-1.19354000	-1.51318100
H	2.43571400	0.07868100	-2.06748900
C	4.62881700	-1.25877200	0.83351400
H	3.39875900	-0.02145600	2.11834600
C	4.87553600	-1.68227000	-0.47322500
H	4.25795600	-1.51421700	-2.53364300
H	5.24350300	-1.63010500	1.64736300
H	5.67754000	-2.38105300	-0.68218700
C	-2.50866500	0.33190600	0.88508600
C	-3.22016100	0.43499000	2.08303800
C	-1.38608100	-0.53360700	0.84159900
C	-2.85552700	-0.28609200	3.21967400
H	-4.08440000	1.09062400	2.12365600
C	-1.03235900	-1.26052200	1.99527200
C	-1.75220700	-1.13940100	3.17556400
H	-3.43206100	-0.18461400	4.13249400
H	-0.17684400	-1.92564400	1.95078300
H	-1.45928700	-1.70495400	4.05267600
C	-2.26480200	2.53308000	-0.39571200
H	-1.17489600	2.40306300	-0.42057700
H	-2.45822400	3.10465100	0.51921300
B	-2.66809600	3.39805500	-1.63760800
O	-2.47212100	4.75925700	-1.70318300
O	-3.23263000	2.89085300	-2.78385700
C	-3.52034600	3.99047800	-3.67776300
H	-4.60395000	4.11334800	-3.73711200
H	-3.13191600	3.75487600	-4.66881300
C	-2.82302100	5.20613500	-3.03261100
H	-1.90736200	5.48790600	-3.55714700
H	-3.47398000	6.07743800	-2.95597900

Zero-point correction= 0.327208
(Hartree/Particle)
Thermal correction to Energy= 0.350540
Thermal correction to Enthalpy= 0.351484
Thermal correction to Gibbs Free Energy= 0.266405
Sum of electronic and zero-point Energies= -3882.261066
Sum of electronic and thermal Energies= -3882.237734
Sum of electronic and thermal Enthalpies= -3882.236790
Sum of electronic and thermal Free Energies= -3882.321869

Sulfoxide product formed from **1** and **2C$_2$a**.





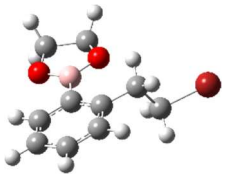
0 1

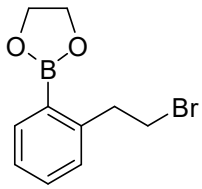
C	-1.14627800	-1.08198000	0.54465500
H	-1.92617500	-1.79982900	0.80750300
H	-1.12851900	-0.28626400	1.28628900
S	-1.77715000	-0.28731700	-1.03542400
O	-0.91931800	0.94952200	-1.28765200
B	3.00980300	1.49768500	0.30188000
O	3.16832100	2.18914000	-0.87679000
O	4.20826700	1.06849800	0.82553400
C	4.58343900	2.33738600	-1.13338100
H	4.79070600	2.05022900	-2.16447900
H	4.85395300	3.38614400	-0.99226500
C	5.26215200	1.41060400	-0.10354700
H	6.07153200	1.89961000	0.43918700
H	5.63850100	0.48984800	-0.55476400
C	1.62081200	1.28176700	0.99407300
H	0.81881000	1.38858300	0.25770400
H	1.49363200	2.11436500	1.70188100
C	-3.36415000	0.30627000	-0.35956800
C	-4.43325300	-0.58139900	-0.24012500
C	-3.49524500	1.65035700	-0.02630300
C	-5.65074900	-0.11201100	0.25019400
H	-4.32648200	-1.62150300	-0.52900200
C	-4.71913700	2.11062500	0.46021400
H	-2.65130500	2.31733300	-0.15729500
C	-5.79315000	1.23176600	0.60116000
H	-6.48811200	-0.79288800	0.34957400
H	-4.83327400	3.15573300	0.72428700
H	-6.74328200	1.59398800	0.97645900
C	0.18041100	-1.75879200	0.33274800
C	1.38104000	-1.27907100	0.89886900
C	0.20388800	-2.92479000	-0.44874500
C	2.56224900	-1.99367400	0.64697800
C	1.38669000	-3.61186600	-0.69462600
H	-0.72564000	-3.29955200	-0.86570100
C	2.57666000	-3.13951400	-0.14230900
H	3.48688100	-1.63604000	1.08638400
H	1.37819900	-4.51004200	-1.30149400
H	3.50835600	-3.66662400	-0.31539700

C	1.45349400	-0.04378800	1.77785100
H	2.29514700	-0.16360300	2.46506400
H	0.56106100	0.02055100	2.40589200

Zero-point correction= 0.330000
(Hartree/Particle)
Thermal correction to Energy= 0.350513
Thermal correction to Enthalpy= 0.351457
Thermal correction to Gibbs Free Energy= 0.276165
Sum of electronic and zero-point Energies= -1307.973885
Sum of electronic and thermal Energies= -1307.953372
Sum of electronic and thermal Enthalpies= -1307.952428
Sum of electronic and thermal Free Energies= -1308.027720

Ethylene glycol ester of 2-(2-bromoethyl)phenyl boronic acid (reactant – **3a**)





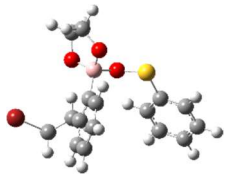
0 1

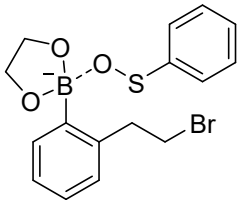
C	-2.95996200	-1.03040100	-0.27903500
C	-1.71222700	-0.46917100	0.05432800
C	-0.64432100	-1.34646900	0.36128300
C	-0.86087800	-2.72925100	0.31697000
C	-2.10309200	-3.26092600	-0.02091800
C	-3.16194600	-2.40627000	-0.32163800
H	-3.78547600	-0.36577200	-0.50708100
H	-0.04251800	-3.39978300	0.55901400
H	-2.24269600	-4.33611300	-0.04373100
H	-4.13469200	-2.80790600	-0.58210300
C	0.74778400	-0.85580300	0.72534400
H	1.25309500	-1.62061200	1.31924700
H	0.69458400	0.05374200	1.32207100
B	-1.62381300	1.08818800	0.06025800
O	-2.72807700	1.87339200	-0.18113700
O	-0.48878400	1.82981800	0.28494500
C	-0.81123700	3.22777600	0.09605200
C	-2.34941700	3.25782700	-0.01397100
H	-0.43357800	3.79649300	0.94572400
H	-0.31939100	3.57382500	-0.81529600
H	-2.82492700	3.63954600	0.89199500
H	-2.70227100	3.82979800	-0.87229600
C	1.55860700	-0.58239400	-0.53661200

```
 H                  1.70101600   -1.47205800   -1.14489300
 H                  1.13948700    0.22332500   -1.13177500
 Br                 3.40947000    0.02826800   -0.09609900

Zero-point correction=                           0.207738
(Hartree/Particle)
 Thermal correction to Energy=                    0.220948
 Thermal correction to Enthalpy=                  0.221892
 Thermal correction to Gibbs Free Energy=         0.164856
 Sum of electronic and zero-point Energies=          -3137.797351
 Sum of electronic and thermal Energies=             -3137.784142
 Sum of electronic and thermal Enthalpies=           -3137.783197
 Sum of electronic and thermal Free Energies=        -3137.840234
```

Complex of **1** with **3a** – **1.3a.C**



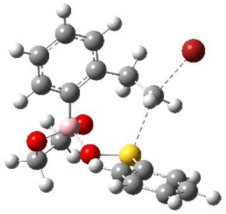


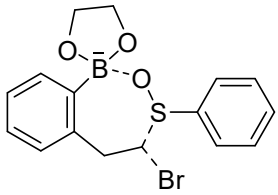

```
-1 1
 C                 -0.24344500    0.85282900    2.40461700
 C                 -0.43478100    0.53688000    1.04705900
 C                 -0.87992300   -0.77380300    0.75022700
 C                 -1.08724400   -1.69640200    1.78568100
 C                 -0.88040000   -1.35466700    3.12051400
 C                 -0.45772700   -0.06444700    3.43315200
 H                  0.08135400    1.85762000    2.65133300
 H                 -1.41545900   -2.70530100    1.55480300
 H                 -1.04912100   -2.08782700    3.90263100
 H                 -0.29530500    0.22405800    4.46717700
 C                 -1.09596700   -1.21988100   -0.68885200
 H                 -0.24300500   -1.84205500   -1.00009400
 H                 -1.10123700   -0.35289200   -1.34639300
 B                 -0.10469600    1.68363000   -0.06567600
 O                  0.08505600    3.02497600    0.53216600
 O                 -1.14564300    1.85939300   -1.08593800
 C                 -1.14173200    3.23408800   -1.44833100
 C                 -0.73925900    3.95444000   -0.15541900
 H                 -0.40850900    3.42467600   -2.24535200
 H                 -2.13175800    3.52656500   -1.81203500
 H                 -0.19477600    4.88631800   -0.34663700
 H                 -1.62656500    4.19574600    0.44973600
 C                  4.65367100   -0.34333300    0.23668900
```

C	5.31060300	-1.55049500	0.02069700
C	4.73423200	-2.53992700	-0.78171200
C	3.49146400	-2.30133600	-1.36802700
C	2.82490500	-1.09279000	-1.16315300
C	3.40107800	-0.10722400	-0.35426000
H	5.11003700	0.41400900	0.86649300
H	6.27563400	-1.72150800	0.48577600
H	3.03360300	-3.05974300	-1.99464000
H	1.86374900	-0.89971500	-1.62039200
S	2.63593300	1.47140300	-0.07740200
O	1.18225600	1.31333600	-0.86246300
H	5.24767800	-3.48047800	-0.94501600
C	-2.31644800	-2.07882100	-0.97239900
H	-2.36514600	-2.36724900	-2.01937900
H	-2.39307200	-2.96415100	-0.34777100
Br	-4.05277300	-1.12345600	-0.65721300

Zero-point correction= 0.300513
(Hartree/Particle)
Thermal correction to Energy= 0.321471
Thermal correction to Enthalpy= 0.322415
Thermal correction to Gibbs Free Energy= 0.246210
Sum of electronic and zero-point Energies= -3842.983647
Sum of electronic and thermal Energies= -3842.962688
Sum of electronic and thermal Enthalpies= -3842.961744
Sum of electronic and thermal Free Energies= -3843.037950

Transition state for internal alkylation of **1.3a.C** – **1.3a.C.TS**





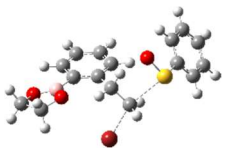
-1 1

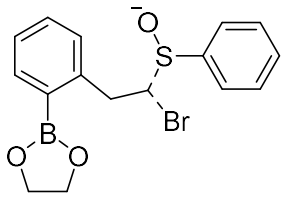
C	1.09367500	0.79743100	-0.91909400
H	1.58680700	0.47618700	-1.82177500
H	1.45508300	0.41420000	0.01880000
C	-0.12908000	1.66723700	-0.99806700
H	-0.79037800	1.26034900	-1.76674200
H	0.18388600	2.64914400	-1.36332500
C	-0.88165300	1.80603500	0.31342800
C	-0.53227100	2.86077500	1.16809500
C	-1.90348300	0.89950900	0.67691100

C	-1.16571900	3.03600200	2.39672700
H	0.24908400	3.55031600	0.86454900
C	-2.52408000	1.10292800	1.92277700
C	-2.16851700	2.14582200	2.77762500
H	-0.88181200	3.85929500	3.04392000
H	-3.31823100	0.42573600	2.21846000
H	-2.67577600	2.26811400	3.72960100
C	-4.30066400	-1.45759400	-0.94562500
C	-3.84966500	-0.54296400	-2.09333500
H	-3.95897600	-2.48895700	-1.10984800
H	-5.38589300	-1.46881400	-0.80943300
H	-3.75672100	-1.07727400	-3.04482800
H	-4.55144500	0.29092700	-2.23326300
S	-0.04982600	-1.53435700	-1.06011200
O	-1.37732300	-1.53424600	-0.10835500
O	-3.67506400	-0.90051400	0.20480100
O	-2.58212600	-0.04087200	-1.67637900
B	-2.41244800	-0.33576700	-0.24239600
C	1.13516300	-2.36246200	-0.01634000
C	2.35469100	-2.74467400	-0.59049800
C	0.87343300	-2.62977700	1.32938300
C	3.31459400	-3.38015100	0.19220400
H	2.55252000	-2.55116900	-1.63958500
C	1.84073700	-3.27548800	2.09955400
H	-0.07749300	-2.33597800	1.75360200
C	3.06187200	-3.64939200	1.53927800
H	4.25881300	-3.67151200	-0.25391100
H	1.63596600	-3.48414400	3.14386400
H	3.80950900	-4.14969500	2.14381500
Br	3.03675500	2.46935500	-0.71939400

Zero-point correction=	0.299546
(Hartree/Particle)	
Thermal correction to Energy=	0.320068
Thermal correction to Enthalpy=	0.321012
Thermal correction to Gibbs Free Energy=	0.246734
Sum of electronic and zero-point Energies=	-3842.962024
Sum of electronic and thermal Energies=	-3842.941503
Sum of electronic and thermal Enthalpies=	-3842.940559
Sum of electronic and thermal Free Energies=	-3843.014836

Transition state for reaction of **1** and **3a** w/o precomplexation – **1.3a.TS**





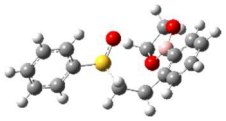
-1 1

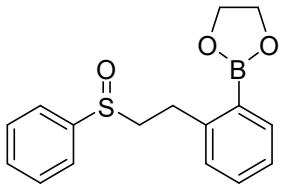
C	0.30593000	-1.42699800	0.12510500
H	0.36256000	-2.39730500	0.58713300
H	1.01320500	-1.22218600	-0.66161500
Br	-1.28675300	-2.36450300	-1.55165400
C	-0.42128100	-0.33772600	0.81637600
H	-1.31931800	-0.73271800	1.28492800
H	0.24654200	-0.02680400	1.66275900
C	-0.72340700	0.89131400	-0.01858200
C	-2.03153000	1.40578200	-0.17827300
C	0.34571200	1.54788300	-0.64279900
C	-2.20518100	2.55390200	-0.97896300
C	0.14998600	2.68255900	-1.42405600
H	1.35300800	1.16920700	-0.50796200
C	-1.13656200	3.19175900	-1.59785600
H	-3.20650300	2.94798300	-1.11134400
H	0.99975800	3.16872500	-1.89128700
H	-1.30220200	4.07487500	-2.20496400
B	-3.32746800	0.81290900	0.45555400
O	-4.57687500	1.19356800	0.01081300
O	-3.39982300	-0.08011400	1.50043200
C	-4.78644600	-0.43489700	1.70283600
H	-5.01279400	-0.39310000	2.76831800
H	-4.93764500	-1.45471700	1.34187200
C	-5.56903300	0.60364900	0.87778000
H	-6.35637400	0.15784400	0.26955900
H	-5.99907200	1.39162100	1.50091000
S	2.54810700	-1.14183300	1.78607400
O	1.87915600	-0.05574200	2.72465600
C	3.68686300	-0.26200000	0.72489800
C	4.39723500	-0.96853500	-0.25864900
C	3.89758900	1.11236600	0.87970900
C	5.30277300	-0.30022300	-1.07657600
H	4.24049700	-2.03576700	-0.38273100
C	4.80937800	1.77237800	0.05506900
H	3.34396200	1.64229200	1.64582500
C	5.51507600	1.07448000	-0.92543600
H	5.84560100	-0.85290100	-1.83605300
H	4.96846000	2.83832400	0.18138400
H	6.22202400	1.59114400	-1.56451300

Zero-point correction= 0.299186
(Hartree/Particle)
Thermal correction to Energy= 0.320778
Thermal correction to Enthalpy= 0.321722
Thermal correction to Gibbs Free Energy= 0.242037

```
 Sum of electronic and zero-point Energies=          -3842.961092
 Sum of electronic and thermal Energies=             -3842.939500
 Sum of electronic and thermal Enthalpies=           -3842.938556
 Sum of electronic and thermal Free Energies=        -3843.018241
```

Sulfoxide product formed from **1** and **3a**.



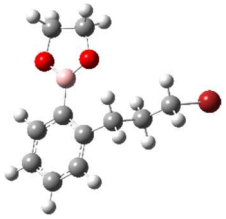


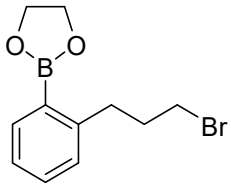

```
0 1
 C                 -0.79105200    0.83821300    1.21303700
 H                 -1.50142000    0.73823100    2.03691400
 H                 -1.02315400    1.74513500    0.64996600
 C                  0.65038800    0.82582600    1.75191000
 H                  0.90733100   -0.17869800    2.08513100
 H                  0.63958500    1.45916200    2.64466000
 C                  1.70370000    1.37576100    0.80453800
 C                  1.81494100    2.76913400    0.70775300
 C                  2.56313800    0.56269200    0.03114000
 C                  2.74458900    3.37166500   -0.13524400
 H                  1.16263400    3.39435300    1.30990600
 C                  3.49626400    1.19393100   -0.81481700
 C                  3.59453500    2.57833000   -0.90408900
 H                  2.80823500    4.45320200   -0.18564900
 H                  4.15693500    0.57623700   -1.41251700
 H                  4.32565100    3.03374800   -1.56259200
 C                  3.16541000   -3.11207600   -0.61208800
 C                  2.07375900   -3.18594000    0.47297200
 H                  2.90540700   -3.66638700   -1.51401700
 H                  4.13772200   -3.45252800   -0.24855800
 H                  1.11795000   -3.53975200    0.08029500
 H                  2.36124400   -3.79938500    1.32686000
 S                 -1.18300200   -0.58961300    0.09841300
 O                 -0.52860400   -0.31811300   -1.25608300
 O                  3.26095900   -1.70685100   -0.93159100
 O                  1.90851000   -1.81698600    0.90973200
 B                  2.55623600   -0.99659900    0.01449000
 C                 -2.96040700   -0.22181300   -0.10218000
 C                 -3.85558800   -0.58084400    0.90545000
 C                 -3.39822000    0.35743200   -1.28826900
 C                 -5.21420800   -0.32569000    0.72708300
 H                 -3.50563400   -1.05785100    1.81483700
 C                 -4.76074600    0.60607700   -1.45845300
 H                 -2.67732900    0.59913100   -2.06044300
```

C	-5.66635300	0.26840800	-0.45287100
H	-5.91861000	-0.59835100	1.50442900
H	-5.11318400	1.05958000	-2.37784300
H	-6.72433500	0.45993800	-0.59014100

Zero-point correction= 0.302248
(Hartree/Particle)
Thermal correction to Energy= 0.321392
Thermal correction to Enthalpy= 0.322336
Thermal correction to Gibbs Free Energy= 0.250749
Sum of electronic and zero-point Energies= -1268.677897
Sum of electronic and thermal Energies= -1268.658753
Sum of electronic and thermal Enthalpies= -1268.657809
Sum of electronic and thermal Free Energies= -1268.729396

Ethylene glycol ester of 2-(3-bromoproyl)phenyl boronic acid (reactant – **4a**)





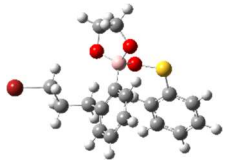
0 1

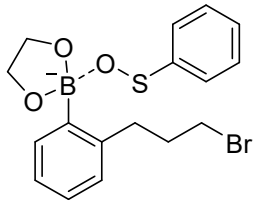
C	-3.32160500	-0.90947800	-0.61609700
C	-2.15298200	-0.41657700	-0.00259800
C	-1.22678700	-1.34955300	0.52387400
C	-1.50481400	-2.71814400	0.41636800
C	-2.66561400	-3.18211700	-0.19779100
C	-3.58295700	-2.27180600	-0.71965900
H	-4.03799300	-0.20071300	-1.01577300
H	-0.79805600	-3.43271600	0.82650900
H	-2.85329400	-4.24835600	-0.26355900
H	-4.49211500	-2.61977900	-1.19699100
C	0.07529000	-0.93671600	1.18125100
H	0.38236800	-1.72339700	1.87723200
H	-0.06498300	-0.02365900	1.76097700
B	-1.99266700	1.13402100	0.04472500
O	-2.94393300	1.97069200	-0.49713000
O	-0.94243800	1.82646800	0.60082800
C	-1.13245800	3.23553800	0.33369900
C	-2.57561100	3.33496000	-0.19818000
H	-0.97798600	3.79617700	1.25564000
H	-0.39209000	3.54852500	-0.40566900
H	-3.26942600	3.72540900	0.54973000

H	-2.65350000	3.93324400	-1.10613000
C	1.20578600	-0.71024800	0.15109200
H	1.37696300	-1.63068900	-0.41401300
H	0.90133700	0.06146000	-0.55929700
C	2.48408800	-0.28813500	0.85057200
H	2.86462000	-1.04748600	1.52993000
H	2.38270700	0.66015100	1.37309000
Br	3.97347800	0.01223200	-0.44571600

Zero-point correction= 0.236017
(Hartree/Particle)
Thermal correction to Energy= 0.250626
Thermal correction to Enthalpy= 0.251571
Thermal correction to Gibbs Free Energy= 0.190470
Sum of electronic and zero-point Energies= -3177.093447
Sum of electronic and thermal Energies= -3177.078837
Sum of electronic and thermal Enthalpies= -3177.077893
Sum of electronic and thermal Free Energies= -3177.138994

Complex of **1** with **4a** – **1.4a.C**





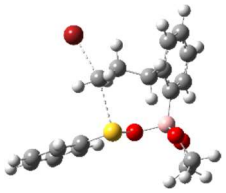
-1 1

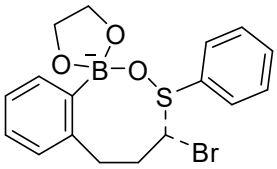
C	0.42211700	0.88789600	2.50192100
C	0.10092600	0.53034000	1.17917000
C	-0.36262700	-0.78955600	0.96589200
C	-0.46836200	-1.68028300	2.04520600
C	-0.13634700	-1.29846900	3.34316000
C	0.31113000	0.00169400	3.57349400
H	0.76773400	1.89942600	2.68589300
H	-0.81412000	-2.69504800	1.86551500
H	-0.22337700	-2.00736700	4.16040000
H	0.57430300	0.32084600	4.57741500
C	-0.75948100	-1.29731300	-0.41182600
H	-0.19596600	-2.21128300	-0.63310700
H	-0.48944800	-0.56170900	-1.16761000
B	0.29612800	1.63839300	-0.00015400
O	0.56526900	2.99700900	0.52349700
O	-0.86876300	1.78890900	-0.88307400
C	-0.89946000	3.14897400	-1.29518500
C	-0.32791400	3.91228200	-0.09329900

H	-0.27400200	3.30047300	-2.18696400
H	-1.92556000	3.44190200	-1.53988900
H	0.19856500	4.82687000	-0.38985200
H	-1.12873200	4.19255200	0.60817000
C	5.04156300	-0.40976400	-0.20318100
C	5.64768300	-1.64742400	-0.39371900
C	4.94413900	-2.69935700	-0.98827700
C	3.62495900	-2.49296800	-1.39113300
C	3.00678100	-1.25540600	-1.20851100
C	3.71186800	-0.20638700	-0.60885000
H	5.59834600	0.39758300	0.26242700
H	6.67387500	-1.79221700	-0.07307100
H	3.06749000	-3.30049600	-1.85439000
H	1.98434400	-1.09076300	-1.52021200
S	3.01193900	1.40951300	-0.37255300
O	1.46598600	1.23275500	-0.94689300
H	5.41896100	-3.66292300	-1.13332200
C	-2.25946200	-1.65115200	-0.56273400
H	-2.42415300	-2.04827200	-1.56890100
H	-2.53161000	-2.44162900	0.14287100
C	-3.14875800	-0.44302900	-0.34237000
H	-3.11422600	-0.07183500	0.67788000
H	-2.93967700	0.36731700	-1.03306300
Br	-5.08248200	-0.89764200	-0.63215300

Zero-point correction=	0.328871
(Hartree/Particle)	
Thermal correction to Energy=	0.351314
Thermal correction to Enthalpy=	0.352258
Thermal correction to Gibbs Free Energy=	0.271993
Sum of electronic and zero-point Energies=	-3882.281756
Sum of electronic and thermal Energies=	-3882.259313
Sum of electronic and thermal Enthalpies=	-3882.258369
Sum of electronic and thermal Free Energies=	-3882.338634

Transition state for internal alkylation of **1.4a.C** – **1.4a.C.TS**





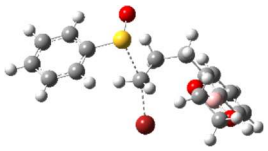
-1 1

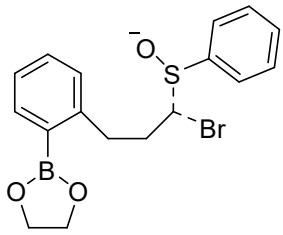
C	0.80346500	1.34457600	-0.74887300
H	1.85237800	1.21394000	-0.94367300

H	0.44097000	1.09319600	0.23433000
Br	1.47612700	3.58338400	0.18019600
S	0.76488500	-1.27145200	-0.91347200
C	2.33408400	-1.50929500	-0.11106200
C	3.48849100	-1.41727400	-0.90135000
C	2.43525900	-1.77094700	1.25758800
C	4.73965600	-1.58063500	-0.31443900
H	3.41089200	-1.22404500	-1.96635700
C	3.69616800	-1.93986000	1.83065200
H	1.53464500	-1.84200900	1.85246500
C	4.84967800	-1.84371400	1.05338200
H	5.63023100	-1.50763400	-0.92853400
H	3.77308000	-2.14485600	2.89281900
H	5.82585500	-1.97390500	1.50596800
O	-0.26259300	-1.59439800	0.31722400
C	-0.15446600	1.67360300	-1.86060000
H	-0.34835200	2.74791200	-1.82306300
H	0.33556800	1.48981400	-2.82136700
C	-1.51475000	0.93232400	-1.82587400
H	-2.12897300	1.37663000	-2.61728500
H	-1.37802600	-0.11208300	-2.09920700
C	-2.25897100	1.02940100	-0.50430000
C	-2.39997100	-0.07801200	0.36423300
C	-2.81718900	2.26946900	-0.15869600
C	-3.10008600	0.13710500	1.56647700
C	-3.50321300	2.45245200	1.03895400
H	-2.71440100	3.10680100	-0.84373100
C	-3.64129500	1.37443000	1.91233500
H	-3.22794300	-0.70143800	2.24229900
H	-3.92646700	3.42115400	1.28363400
H	-4.17319500	1.49492300	2.85101200
B	-1.83799700	-1.57548600	0.07023800
O	-2.35265700	-2.56355000	1.00755800
O	-2.10719600	-2.11101500	-1.27188100
C	-2.58545500	-3.44722500	-1.13922300
H	-3.65962900	-3.48001400	-1.36850600
H	-2.06561100	-4.11322600	-1.83668500
C	-2.32098100	-3.81313200	0.32940500
H	-3.07973000	-4.48174300	0.74639600
H	-1.33690600	-4.28907300	0.44212200

Zero-point correction= 0.328070
(Hartree/Particle)
Thermal correction to Energy= 0.349888
Thermal correction to Enthalpy= 0.350833
Thermal correction to Gibbs Free Energy= 0.273432
Sum of electronic and zero-point Energies= -3882.252700
Sum of electronic and thermal Energies= -3882.230882
Sum of electronic and thermal Enthalpies= -3882.229938
Sum of electronic and thermal Free Energies= -3882.307339

Transition state for reaction of **1** and **4a** w/o precomplexation – **1.4a.TS**





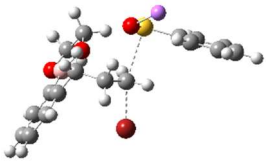
-1 1

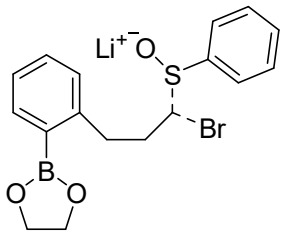
C	0.60887600	-0.51260300	-0.02735300
H	1.53794100	-0.89075300	-0.41774900
H	0.26406100	0.43674300	-0.40205100
Br	-0.52538900	-1.71263100	-1.87336800
S	2.45267800	1.11057800	1.32760300
O	2.43483400	0.32924200	2.70403500
C	3.85355700	0.48619100	0.40990100
C	4.13132400	1.00462500	-0.86511000
C	4.68191000	-0.50351400	0.95037600
C	5.22418700	0.53259600	-1.58520800
H	3.49422200	1.77438500	-1.29004000
C	5.77552300	-0.96957800	0.21976400
H	4.45616600	-0.89092100	1.93690000
C	6.05413200	-0.45746200	-1.04788400
H	5.43062600	0.93791300	-2.57015700
H	6.41376200	-1.73707200	0.64554000
H	6.90499000	-0.82218000	-1.61194900
C	0.10076100	-1.05001100	1.26125200
H	-0.04162000	-2.13256800	1.18993800
H	0.92705200	-0.90575700	1.98797200
C	-1.14152500	-0.35559700	1.86149600
H	-1.17984600	-0.64126100	2.91799900
H	-0.98374600	0.72151400	1.83488800
C	-2.48179900	-0.71371600	1.24553700
C	-3.22212900	0.15226300	0.40676900
C	-3.02213800	-1.96748800	1.56674400
C	-4.47129000	-0.28943900	-0.07709300
C	-4.25223800	-2.38636500	1.07107100
H	-2.46323200	-2.62697500	2.22377200
C	-4.98651500	-1.54073200	0.23927600
H	-5.04244800	0.37112200	-0.71968900
H	-4.63883900	-3.36438700	1.33754100
H	-5.94866200	-1.85252900	-0.15187300
B	-2.77391400	1.57216400	-0.05497100
O	-3.63233400	2.40364000	-0.74541800
O	-1.53782300	2.14668500	0.13458100
C	-1.57706500	3.50020000	-0.37067500
H	-1.55404100	4.18659300	0.47874800
H	-0.69969000	3.67240400	-0.99421000

C	-2.90023400	3.57772500	-1.15653800
H	-2.74574500	3.53034400	-2.23705400
H	-3.48507000	4.46630200	-0.91696200

Zero-point correction= 0.327819
(Hartree/Particle)
Thermal correction to Energy= 0.350731
Thermal correction to Enthalpy= 0.351676
Thermal correction to Gibbs Free Energy= 0.268968
Sum of electronic and zero-point Energies= -3882.253203
Sum of electronic and thermal Energies= -3882.230291
Sum of electronic and thermal Enthalpies= -3882.229346
Sum of electronic and thermal Free Energies= -3882.312054

Transition state for reaction of **1** and **4a** w/o precomplexation – **1.4a.TS** with Li counterion





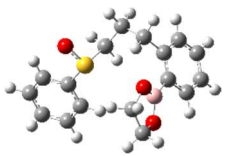
0 1

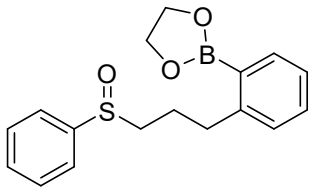
C	0.60887600	-0.51260300	-0.02735300
H	1.53794100	-0.89075300	-0.41774900
H	0.26406100	0.43674300	-0.40205100
Br	-0.52538900	-1.71263100	-1.87336800
S	2.45267800	1.11057800	1.32760300
O	2.43483400	0.32924200	2.70403500
C	3.85355700	0.48619100	0.40990100
C	4.13132400	1.00462500	-0.86511000
C	4.68191000	-0.50351400	0.95037600
C	5.22418700	0.53259600	-1.58520800
H	3.49422200	1.77438500	-1.29004000
C	5.77552300	-0.96957800	0.21976400
H	4.45616600	-0.89092100	1.93690000
C	6.05413200	-0.45746200	-1.04788400
H	5.43062600	0.93791300	-2.57015700
H	6.41376200	-1.73707200	0.64554000
H	6.90499000	-0.82218000	-1.61194900
C	0.10076100	-1.05001100	1.26125200
H	-0.04162000	-2.13256800	1.18993800
H	0.92705200	-0.90575700	1.98797200

C	-1.14152500	-0.35559700	1.86149600
H	-1.17984600	-0.64126100	2.91799900
H	-0.98374600	0.72151400	1.83488800
C	-2.48179900	-0.71371600	1.24553700
C	-3.22212900	0.15226300	0.40676900
C	-3.02213800	-1.96748800	1.56674400
C	-4.47129000	-0.28943900	-0.07709300
C	-4.25223800	-2.38636500	1.07107100
H	-2.46323200	-2.62697500	2.22377200
C	-4.98651500	-1.54073200	0.23927600
H	-5.04244800	0.37112200	-0.71968900
H	-4.63883900	-3.36438700	1.33754100
H	-5.94866200	-1.85252900	-0.15187300
B	-2.77391400	1.57216400	-0.05497100
O	-3.63233400	2.40364000	-0.74541800
O	-1.53782300	2.14668500	0.13458100
C	-1.57706500	3.50020000	-0.37067500
H	-1.55404100	4.18659300	0.47874800
H	-0.69969000	3.67240400	-0.99421000
C	-2.90023400	3.57772500	-1.15653800
H	-2.74574500	3.53034400	-2.23705400
H	-3.48507000	4.46630200	-0.91696200
Li	4.20952759	0.00833801	3.26935199

Zero-point correction= 0.330215
(Hartree/Particle)
Thermal correction to Energy= 0.354678
Thermal correction to Enthalpy= 0.355623
Thermal correction to Gibbs Free Energy= 0.269902
Sum of electronic and zero-point Energies= -3889.746665
Sum of electronic and thermal Energies= -3889.722202
Sum of electronic and thermal Enthalpies= -3889.721258
Sum of electronic and thermal Free Energies= -3889.806978

Sulfoxide product formed from **1** and **4a**.





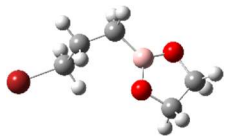
0 1

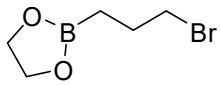
C	0.69915500	-1.75180800	0.61666200
H	1.50367500	-2.48718300	0.54803300
H	0.33154600	-1.52752400	-0.38735800

S	1.50536400	-0.19786000	1.22652300
O	2.24441400	-0.58219300	2.51071800
C	2.75860000	-0.07056700	-0.09203200
C	2.39867200	0.45551300	-1.33259800
C	4.06743600	-0.45177700	0.18318300
C	3.37086800	0.57441000	-2.32439200
H	1.37994700	0.77297800	-1.52739600
C	5.03366900	-0.32485600	-0.81553400
H	4.31618300	-0.83355900	1.16640100
C	4.68642900	0.18400500	-2.06687500
H	3.10233200	0.97871300	-3.29352100
H	6.05690300	-0.62010200	-0.61319500
H	5.44041000	0.28389700	-2.83912700
C	-0.41189400	-2.22659300	1.55128700
H	-0.68629800	-3.23579100	1.22837500
H	-0.00878600	-2.33298500	2.56291200
C	-1.67102900	-1.33363400	1.60199400
H	-2.35917600	-1.78295400	2.32623500
H	-1.41382600	-0.35108400	1.99388200
C	-2.38737200	-1.19719200	0.26866800
C	-2.50887600	0.02966200	-0.42566400
C	-2.93573700	-2.35482700	-0.30253400
C	-3.15415100	0.02980400	-1.68020300
C	-3.58197700	-2.32857000	-1.53438700
H	-2.85870100	-3.29636000	0.23204100
C	-3.68779400	-1.12731000	-2.23522100
H	-3.24212700	0.96605600	-2.21997300
H	-4.00139900	-3.24088600	-1.94457100
H	-4.18515600	-1.09416500	-3.19806800
B	-2.02564800	1.42053500	0.09354600
O	-1.79647500	2.46837000	-0.77072300
O	-1.83224600	1.77409200	1.40805500
C	-1.31890900	3.12640700	1.44430900
H	-1.86604400	3.69420500	2.19664000
H	-0.26284500	3.08596100	1.72008200
C	-1.53522100	3.65440600	0.01354600
H	-0.65955700	4.16331100	-0.38933400
H	-2.40143500	4.31598200	-0.05980400

Zero-point correction= (Hartree/Particle)	0.330758
Thermal correction to Energy=	0.351181
Thermal correction to Enthalpy=	0.352125
Thermal correction to Gibbs Free Energy=	0.277190
Sum of electronic and zero-point Energies=	-1307.975738
Sum of electronic and thermal Energies=	-1307.955314
Sum of electronic and thermal Enthalpies=	-1307.954370
Sum of electronic and thermal Free Energies=	-1308.029306

Ethylene glycol ester of 3-bromopropyl boronic acid (reactant – **5a**)



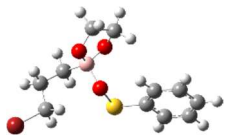


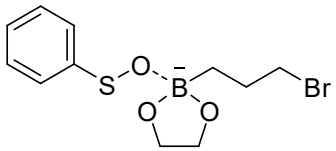
0 1

B	2.00749500	0.53117300	0.08352600
O	1.91739000	-0.73395000	0.61065300
O	3.20393600	0.75807700	-0.55394800
C	4.04745700	-0.40230600	-0.36409100
C	3.11074700	-1.46694900	0.24494400
H	4.46140600	-0.70219100	-1.32690600
H	4.86364500	-0.13083000	0.30859600
H	2.83354500	-2.24080400	-0.47369300
H	3.52556300	-1.93760200	1.13633400
C	0.88865000	1.62244600	0.21896300
H	0.84693000	2.22011100	-0.69925400
H	1.22279700	2.32485500	0.99472200
C	-0.52059200	1.12031300	0.59901700
H	-1.17060200	1.97182800	0.81711200
H	-0.46736000	0.51380200	1.50673400
C	-1.13068100	0.30012900	-0.52373700
H	-0.56905600	-0.60585500	-0.73727400
H	-1.27113100	0.87675500	-1.43538100
Br	-2.96163700	-0.34802100	-0.05751000

Zero-point correction=	0.154596
(Hartree/Particle)	
Thermal correction to Energy=	0.164617
Thermal correction to Enthalpy=	0.165561
Thermal correction to Gibbs Free Energy=	0.115611
Sum of electronic and zero-point Energies=	-2946.063827
Sum of electronic and thermal Energies=	-2946.053806
Sum of electronic and thermal Enthalpies=	-2946.052862
Sum of electronic and thermal Free Energies=	-2946.102813

Complex of **1** with **5a** – **1.5a.C**





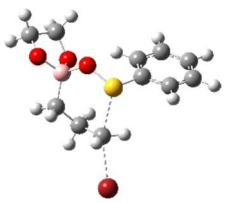
-1 1

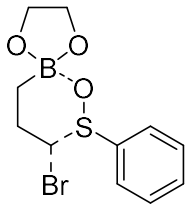
C	-1.34737900	1.18347800	-1.46269800

H	-1.04301800	0.45626700	-2.22985500
H	-1.53091300	2.11915100	-2.00815000
C	-2.70388100	0.74662000	-0.85985900
H	-3.48383200	0.75261800	-1.62958400
H	-3.00488200	1.46456300	-0.09106900
C	-2.63495800	-0.63861200	-0.24838600
H	-1.95904300	-0.70011200	0.59774700
H	-2.39597400	-1.41199300	-0.97523000
Br	-4.41801600	-1.21881800	0.49198300
B	-0.13839900	1.46327200	-0.41214200
O	-0.53034800	2.27788500	0.75556600
O	0.97729500	2.19238900	-1.04143100
O	0.36544700	0.12648300	0.23613000
S	1.06004900	-1.01946100	-0.73406400
C	2.74445700	-1.07103300	-0.16716500
C	3.18279900	-0.34538100	0.94560700
C	3.64461200	-1.90900800	-0.84535400
C	4.50824100	-0.45331500	1.36726300
H	2.48099800	0.29341900	1.46555900
C	4.96306900	-2.01196900	-0.41217300
H	3.31539800	-2.47474500	-1.71142800
C	5.40577000	-1.28390100	0.69612700
H	4.83836900	0.11633900	2.22976400
H	5.64973600	-2.65982600	-0.94659800
H	6.43440600	-1.36379100	1.02849900
C	1.53107900	3.04647200	-0.05165200
H	1.98004000	3.92729200	-0.52282300
H	2.31402600	2.52853500	0.52107100
C	0.33939200	3.39676200	0.85054600
H	-0.17039400	4.30402100	0.49121400
H	0.63852300	3.56718500	1.89156500

Zero-point correction= 0.247825
(Hartree/Particle)
Thermal correction to Energy= 0.265511
Thermal correction to Enthalpy= 0.266455
Thermal correction to Gibbs Free Energy= 0.198039
Sum of electronic and zero-point Energies= -3651.252899
Sum of electronic and thermal Energies= -3651.235213
Sum of electronic and thermal Enthalpies= -3651.234269
Sum of electronic and thermal Free Energies= -3651.302686

Transition state for internal alkylation of **1.5a.C** – **1.5a.C.TS**



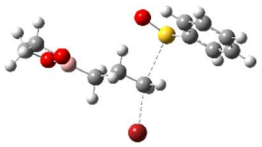


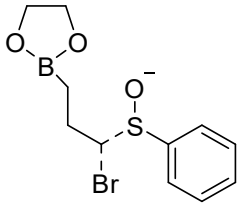
-1 1

C	-1.61354800	-0.55689800	-0.31979400
H	-1.88050500	-0.93831400	-1.29181400
H	-1.80800900	0.48337700	-0.12711900
S	0.43667100	0.47851000	-1.56148600
O	1.74826200	-0.42387100	-1.22696100
Br	-4.04431400	-0.88860100	0.31371300
C	-0.84663500	-1.41987000	0.63794300
H	-1.57345100	-2.08122200	1.11656200
H	-0.43229700	-0.79679300	1.43605100
C	0.26310900	-2.27535600	-0.02700400
H	0.40760100	-3.16322900	0.60061400
H	-0.10413300	-2.65557000	-0.99022100
C	3.67705100	-1.34206000	1.06630400
C	3.83813800	-2.59111900	0.19243800
H	4.19205900	-0.48134900	0.61309000
H	4.06175400	-1.47697400	2.08202300
H	4.78927700	-2.60687300	-0.35118100
H	3.77748500	-3.50447100	0.80351100
B	1.72909200	-1.61300400	-0.18287600
C	0.60883400	1.95744900	-0.56797100
C	-0.15157100	3.07380000	-0.94001900
C	1.45357100	2.01459500	0.54367900
C	-0.07355200	4.24324200	-0.18702600
H	-0.79292700	3.03380300	-1.81441000
C	1.53354700	3.19764100	1.27827700
H	2.01885300	1.13483100	0.82776000
C	0.77241400	4.31152300	0.92153200
H	-0.66442400	5.10522500	-0.47615200
H	2.19010000	3.24418800	2.14044900
H	0.83812600	5.22570100	1.50030100
O	2.27183100	-1.12949300	1.09928000
O	2.74630100	-2.53289900	-0.71499700

Zero-point correction= (Hartree/Particle)	0.246739
Thermal correction to Energy=	0.264006
Thermal correction to Enthalpy=	0.264950
Thermal correction to Gibbs Free Energy=	0.197723
Sum of electronic and zero-point Energies=	-3651.229083
Sum of electronic and thermal Energies=	-3651.211815
Sum of electronic and thermal Enthalpies=	-3651.210871
Sum of electronic and thermal Free Energies=	-3651.278099

Transition state for reaction of **1** and **5a** w/o precomplexation – **1.5a.TS**





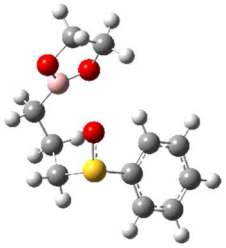
-1 1

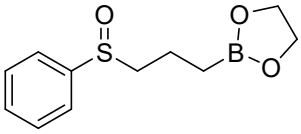
C	0.18159500	-1.01075400	-0.45707000
H	0.18652500	-1.30970700	-1.49282100
H	1.11201500	-1.10686700	0.07773400
Br	-0.45066700	-3.30716900	0.22298200
S	1.57797700	1.18215300	-1.53708700
O	0.64000100	2.30814300	-0.93842000
C	2.97099100	1.04193500	-0.42531900
C	3.06529100	1.84927300	0.71358600
C	3.98755800	0.11494700	-0.70610500
C	4.16545600	1.72662200	1.56292300
H	2.27443400	2.56215500	0.91517600
C	5.07987600	0.00028100	0.14808500
H	3.92280700	-0.51268400	-1.58981000
C	5.17662300	0.80516900	1.28837500
H	4.23179700	2.35623400	2.44431600
H	5.86010900	-0.71951300	-0.07585000
H	6.02956700	0.71318500	1.95108000
C	-0.88854300	-0.13285900	0.06977300
H	-0.99203500	-0.28405600	1.14763900
H	-0.51658100	0.90943700	-0.05202900
C	-2.24282300	-0.25988700	-0.64268000
H	-2.12209500	-0.06823200	-1.71589600
H	-2.59288800	-1.29895100	-0.57202000
C	-4.54990800	2.05805000	1.29835200
C	-5.39918500	1.72883000	0.05341100
H	-5.05839800	1.82183400	2.23352300
H	-4.22698000	3.10122000	1.31932100
H	-6.25870500	1.09778700	0.29100900
H	-5.74401800	2.61955400	-0.47257000
B	-3.37706600	0.66351200	-0.08765900
O	-3.38002300	1.21908900	1.17064600
O	-4.50699000	0.98625400	-0.80741200

Zero-point correction= 0.246288
(Hartree/Particle)
Thermal correction to Energy= 0.264675
Thermal correction to Enthalpy= 0.265619
Thermal correction to Gibbs Free Energy= 0.193201
Sum of electronic and zero-point Energies= -3651.230231
Sum of electronic and thermal Energies= -3651.211843

```
 Sum of electronic and thermal Enthalpies=           -3651.210899
 Sum of electronic and thermal Free Energies=        -3651.283318
```

Sulfoxide product formed from **1** and **5a**.



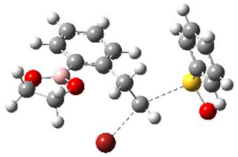


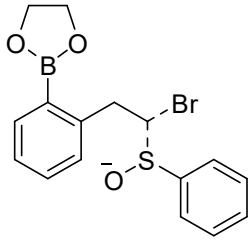
```
0 1
 C                 -0.31785600   -2.29504100    0.35282000
 H                  0.25634900   -3.14044800   -0.03506100
 H                 -1.30244800   -2.66474200    0.65024100
 S                 -0.65751000   -1.26307300   -1.14615400
 O                  0.60484900   -0.44001400   -1.42035000
 C                  0.40985100   -1.61098100    1.51238800
 H                  0.25540000   -2.26504300    2.37726100
 H                 -0.08218200   -0.66648400    1.76178500
 C                  1.92731700   -1.40580700    1.30906900
 H                  2.39010700   -1.33670900    2.30401700
 H                  2.36273200   -2.30089200    0.85194400
 C                  2.63574600    2.05950300   -0.07731600
 C                  3.79494800    1.23288900   -0.67128000
 H                  1.93077800    2.38891200   -0.84430100
 H                  2.97847300    2.92578900    0.49001600
 H                  3.86598400    1.32581300   -1.75572800
 H                  4.76000500    1.48934800   -0.22701200
 B                  2.40622200   -0.12764400    0.53381800
 C                 -1.88747400   -0.12129700   -0.43069300
 C                 -3.21696200   -0.53323000   -0.33650400
 C                 -1.49736800    1.16161600   -0.06056400
 C                 -4.16761500    0.35378200    0.16569800
 H                 -3.51357400   -1.52704800   -0.65473600
 C                 -2.45817700    2.04355700    0.43595300
 H                 -0.45795500    1.45051100   -0.15604000
 C                 -3.78863300    1.64112700    0.55113900
 H                 -5.20314700    0.04358300    0.24466100
 H                 -2.16569400    3.04450900    0.73223000
 H                 -4.53192600    2.33093100    0.93406400
 O                  1.95876500    1.14740400    0.81202200
 O                  3.47932100   -0.13330800   -0.33020100

Zero-point correction=                           0.249620
(Hartree/Particle)
```

```
 Thermal correction to Energy=                    0.265250
 Thermal correction to Enthalpy=                  0.266194
 Thermal correction to Gibbs Free Energy=         0.204535
 Sum of electronic and zero-point Energies=         -1076.944312
 Sum of electronic and thermal Energies=            -1076.928682
 Sum of electronic and thermal Enthalpies=          -1076.927737
 Sum of electronic and thermal Free Energies=       -1076.989397
```

Transition state for reaction of **1** and **3a** w/o precomplexation – **1.3a.TS2**



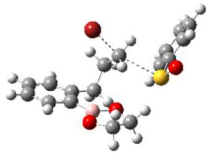


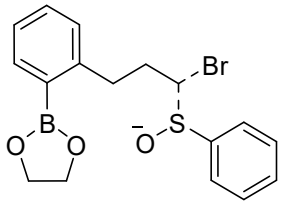

```
-1 1
 C                 -0.96188800    0.21836700   -1.20988200
 C                 -2.26293500    0.74244400   -1.03203900
 C                 -0.52536400   -0.09653100   -2.50373100
 C                 -3.07791600    0.90883200   -2.17032800
 C                 -1.34430700    0.08633800   -3.61411600
 H                  0.47556600   -0.49042900   -2.64455100
 C                 -2.63366000    0.59059700   -3.44863800
 H                 -4.08063400    1.29989400   -2.03933000
 H                 -0.97635500   -0.16388800   -4.60331900
 H                 -3.28259600    0.73375000   -4.30546400
 B                 -2.88939500    1.16610600    0.33248300
 O                 -4.25087400    1.32424100    0.47740700
 O                 -2.20391700    1.46528400    1.48718300
 C                 -3.16734600    1.71854300    2.53550400
 H                 -2.87767400    2.62065700    3.07435300
 H                 -3.15979500    0.86961300    3.22260200
 C                 -4.50893200    1.86313700    1.79254600
 H                 -5.31583300    1.29730600    2.25847400
 H                 -4.81583900    2.90640600    1.68622000
 C                 -0.00336100   -0.00921300   -0.05539200
 H                  0.83539600    0.69567900   -0.15289700
 H                 -0.46780400    0.24373100    0.89471800
 C                  0.57682200   -1.38874700    0.03489500
 H                  0.54652200   -2.06732800   -0.79893200
 H                  1.23940500   -1.63378100    0.84775500
 Br                -1.24732900   -2.67504400    1.09484800
 S                  3.11046300   -1.15846300   -0.91163800
 C                  3.54520000    0.38872200   -0.14308800
```

C	3.20215200	1.59823300	-0.77119500
C	4.22210800	0.41348900	1.08322000
C	3.53154200	2.81162000	-0.17234600
H	2.69483000	1.58898400	-1.73091400
C	4.54852700	1.63400400	1.67167800
H	4.48396900	-0.52793000	1.55173200
C	4.20613600	2.83785600	1.05167500
H	3.26473100	3.74035200	-0.66550600
H	5.07484000	1.64535800	2.62062800
H	4.46369200	3.78433000	1.51316400
O	3.72391500	-2.30420600	-0.01674100

Zero-point correction= 0.299573
(Hartree/Particle)
Thermal correction to Energy= 0.321257
Thermal correction to Enthalpy= 0.322201
Thermal correction to Gibbs Free Energy= 0.241964
Sum of electronic and zero-point Energies= -3842.956054
Sum of electronic and thermal Energies= -3842.934370
Sum of electronic and thermal Enthalpies= -3842.933426
Sum of electronic and thermal Free Energies= -3843.013663

Second transition state for reaction of **1** and **4a** w/o precomplexation – **1.4a.TS2**





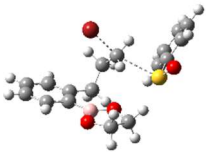
-1 1

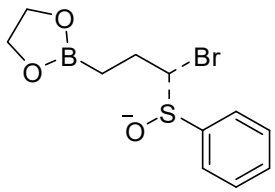
C	-0.57725200	-0.44372500	0.60866300
H	-1.46594400	-0.62360300	1.18889200
H	-0.02160500	0.45276500	0.82118200
Br	0.72085300	-1.69955200	2.24695400
S	-2.24155700	1.55356700	-0.19609100
O	-2.39842200	2.27623700	1.20055200
C	-3.69270900	0.54115500	-0.41588200
C	-4.63474800	0.40628500	0.61261000
C	-3.89563100	-0.13271300	-1.63281800
C	-5.75747800	-0.39907600	0.42696000
H	-4.47105200	0.94138300	1.54067900
C	-5.01780700	-0.93834100	-1.80502600
H	-3.18770500	-0.01205500	-2.44689500
C	-5.95568200	-1.07802900	-0.77703300
H	-6.48269400	-0.49685500	1.22839000
H	-5.16595400	-1.45333100	-2.74843600

H	-6.83078000	-1.70241000	-0.91683600
C	-0.39533000	-1.16825500	-0.69537300
H	-0.16465800	-2.21981600	-0.50325700
H	-1.36880200	-1.18117600	-1.19882900
C	0.64743500	-0.55894400	-1.66036300
H	0.42469800	-0.95004500	-2.65862700
H	0.50258200	0.51901500	-1.70232900
C	2.09612600	-0.89856500	-1.35264800
C	3.02698900	0.01411400	-0.80270600
C	2.52762000	-2.19614500	-1.66565800
C	4.34968700	-0.42678900	-0.58673400
C	3.83531300	-2.61115300	-1.43865700
H	1.81924800	-2.89429100	-2.10133500
C	4.75819400	-1.71923300	-0.89214800
H	5.06622500	0.26913800	-0.16534300
H	4.13384500	-3.62295500	-1.69155700
H	5.78192000	-2.02781300	-0.71163400
B	2.72349400	1.48787600	-0.39276000
O	3.72978800	2.34222600	0.00795300
O	1.48779600	2.08802600	-0.35986400
C	1.65921000	3.47768600	0.00034900
H	1.45224100	4.08987000	-0.88016400
H	0.94843300	3.72957000	0.78717900
C	3.12822500	3.57647300	0.45635300
H	3.22371700	3.63388300	1.54302500
H	3.65760900	4.41622300	0.00529800

Zero-point correction= 0.328066
(Hartree/Particle)
Thermal correction to Energy= 0.351072
Thermal correction to Enthalpy= 0.352016
Thermal correction to Gibbs Free Energy= 0.268506
Sum of electronic and zero-point Energies= -3882.249537
Sum of electronic and thermal Energies= -3882.226531
Sum of electronic and thermal Enthalpies= -3882.225587
Sum of electronic and thermal Free Energies= -3882.309098

Second transition state for reaction of **1** and **5a** w/o precomplexation – **1.5a.TS2**





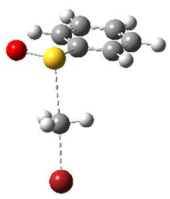
-1 1

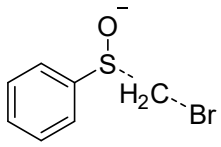
C	0.18315300	1.27697300	0.24287300

H	0.12657000	1.73586400	1.21459000
H	1.10748800	1.39462000	-0.29847200
Br	-0.74847500	3.28817300	-0.76807200
S	1.88076800	-0.16074900	1.79461000
O	2.79519900	1.02519700	2.29657300
C	2.75472900	-0.95431000	0.45668700
C	3.94750600	-0.41076200	-0.03761100
C	2.24511000	-2.13581800	-0.10817500
C	4.61262400	-1.03618900	-1.09134300
H	4.33452900	0.49357800	0.41749200
C	2.91435800	-2.74806800	-1.16410700
H	1.33821700	-2.58245400	0.28720800
C	4.10155200	-2.20291000	-1.66334200
H	5.53642800	-0.60908400	-1.46805100
H	2.51298000	-3.65983100	-1.59388100
H	4.62264100	-2.68592700	-2.48208300
C	-0.79570100	0.21553200	-0.16882400
H	-1.07896700	0.37885900	-1.21171500
H	-0.27084000	-0.74674800	-0.16873200
C	-2.04131700	0.13581300	0.72254200
H	-1.74471600	-0.03254300	1.76540800
H	-2.54696300	1.11069100	0.72258600
C	-4.15391500	-2.60837700	-0.85023800
C	-4.98775500	-2.23329700	0.39262200
H	-4.71815400	-2.52854200	-1.77971100
H	-3.72235900	-3.60899100	-0.77751600
H	-5.92184800	-1.73117800	0.13110000
H	-5.20855600	-3.09021000	1.02967000
B	-3.09295300	-0.95046900	0.31845700
O	-3.07563600	-1.64518700	-0.86776000
O	-4.15449200	-1.30393000	1.12144400

Zero-point correction= 0.246442
(Hartree/Particle)
Thermal correction to Energy= 0.265011
Thermal correction to Enthalpy= 0.265955
Thermal correction to Gibbs Free Energy= 0.192280
Sum of electronic and zero-point Energies= -3651.225521
Sum of electronic and thermal Energies= -3651.206952
Sum of electronic and thermal Enthalpies= -3651.206008
Sum of electronic and thermal Free Energies= -3651.279683

Transition state for direct S-methylation of phenyl sulfenate (**1**)



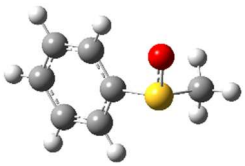


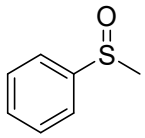
-1 1

C	1.43303400	0.48330100	-0.27048100
H	1.86532900	1.39786200	-0.63541800
H	1.08312100	-0.24659800	-0.97899500
H	1.05893900	0.45432100	0.73762500
Br	3.46388700	-0.58524000	0.17594500
C	-2.57596500	0.26624700	0.96257200
C	-3.38505500	-0.83388400	1.24895500
C	-3.52000200	-1.87536400	0.33029700
C	-2.83588700	-1.80772400	-0.88865000
C	-2.02811300	-0.71449600	-1.18516100
C	-1.89169600	0.33025500	-0.25643600
H	-2.46354500	1.08394100	1.66492100
H	-3.91285500	-0.87615300	2.19625700
H	-2.93514500	-2.61051600	-1.61168200
H	-1.50855700	-0.66908000	-2.13764200
S	-0.85678800	1.73579600	-0.64181500
O	-0.96788400	2.72690900	0.58409100
H	-4.14954900	-2.72837900	0.55659900

Zero-point correction=	0.129526
(Hartree/Particle)	
Thermal correction to Energy=	0.140834
Thermal correction to Enthalpy=	0.141778
Thermal correction to Gibbs Free Energy=	0.088401
Sum of electronic and zero-point Energies=	-3319.204966
Sum of electronic and thermal Energies=	-3319.193658
Sum of electronic and thermal Enthalpies=	-3319.192714
Sum of electronic and thermal Free Energies=	-3319.246091

Methyl phenyl sulfoxide, S-methylation of phenyl sulfenate (**1**)





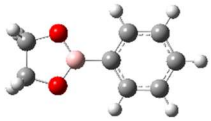
0 1

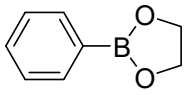
C	-2.19771900	-0.80653400	-0.61548500
C	-0.81587000	-0.94519800	-0.49691100
C	-0.10002200	0.00929400	0.22506200
C	-0.73614100	1.07689000	0.84846700

C	-2.12033800	1.20467700	0.72609700
C	-2.84899700	0.26779300	-0.00626600
H	-2.76470000	-1.54051400	-1.17626200
H	-0.31210300	-1.78901200	-0.95617600
H	-0.15040600	1.78525500	1.42242300
H	-2.62747500	2.03362700	1.20635700
H	-3.92443000	0.36843300	-0.09614600
S	1.70500600	-0.18084300	0.42700000
O	2.15093300	0.88019900	1.43270400
C	2.20269200	0.44031000	-1.22237800
H	3.29197300	0.41623100	-1.24657100
H	1.79460400	-0.22086800	-1.98711000
H	1.83256700	1.45858800	-1.34039700

Zero-point correction= 0.131943
(Hartree/Particle)
Thermal correction to Energy= 0.140651
Thermal correction to Enthalpy= 0.141595
Thermal correction to Gibbs Free Energy= 0.097538
Sum of electronic and zero-point Energies= -744.926577
Sum of electronic and thermal Energies= -744.917870
Sum of electronic and thermal Enthalpies= -744.916925
Sum of electronic and thermal Free Energies= -744.960983

Ethylene glycol ester of phenyl boronic acid (**6a**)





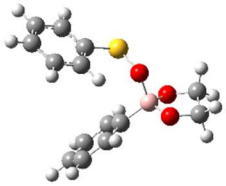
0 1

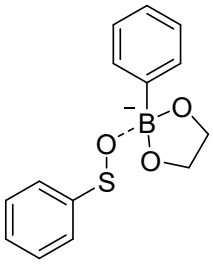
C	1.30367800	1.20555900	0.00547100
C	0.58117300	0.00001200	-0.00005200
C	1.30366200	-1.20554500	-0.00553600
C	2.69718400	-1.20834600	-0.00560700
C	3.39585700	-0.00000900	0.00004000
C	2.69720000	1.20833800	0.00563600
H	0.76706400	2.14815100	0.00913400
H	3.23860100	-2.14793100	-0.00965700
H	4.48037100	-0.00001600	0.00007800
H	3.23863000	2.14791500	0.00972300
B	-0.97161000	0.00002500	-0.00002300
O	-1.73074500	1.14469900	0.05183900
O	-1.73068300	-1.14466700	-0.05184400
C	-3.12149200	-0.76806400	0.07361400
C	-3.12153700	0.76801700	-0.07356800
H	-3.69776700	-1.26915300	-0.70428800
H	-3.48045500	-1.09334400	1.05241600
H	-3.48055200	1.09327400	-1.05235900

```
 H                 -3.69781100    1.26907700    0.70435300
 H                  0.76703600   -2.14813100   -0.00923400

 Zero-point correction=                           0.160516
(Hartree/Particle)
 Thermal correction to Energy=                    0.169671
 Thermal correction to Enthalpy=                  0.170615
 Thermal correction to Gibbs Free Energy=         0.124905
 Sum of electronic and zero-point Energies=           -485.648614
 Sum of electronic and thermal Energies=              -485.639458
 Sum of electronic and thermal Enthalpies=            -485.638514
 Sum of electronic and thermal Free Energies=         -485.684224
```

Complex of phenyl sulfenate (**1**) and **6a**



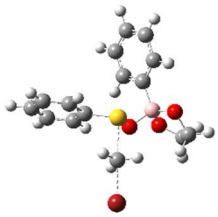


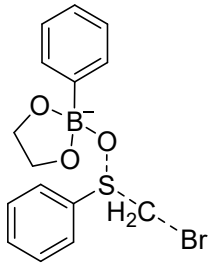

```
-1 1
C -2.20989400 -0.47749500 -1.04890300
C -3.43787400 -0.01990900 -1.52772700
C -4.56861800 -0.02069100 -0.71103200
C -4.46069700 -0.48691000 0.60255900
C -3.24142900 -0.94488600 1.09220800
C -2.10490100 -0.94047700 0.26692400
H -1.32961600 -0.47667400 -1.67788600
H -3.50774100 0.33957400 -2.54914900
H -5.33061300 -0.49297400 1.25067700
H -3.17105900 -1.30449400 2.11412200
S -0.58316000 -1.56758300 0.93978200
O 0.47293100 -1.43281400 -0.32949900
H -5.51987100 0.33591500 -1.08912200
C 0.90185000 1.82481800 -1.06394800
C 1.29103500 1.03664400 0.03332300
C 1.31086300 1.67044700 1.28672400
C 0.95357000 3.01243300 1.44441600
C 0.56835300 3.76865600 0.33688400
C 0.54639400 3.16745900 -0.92344900
H 0.88394200 1.37848800 -2.05392400
H 0.97871700 3.46889400 2.42950600
```

```
H 0.29250900 4.81183900 0.45259100
H 0.25431600 3.74657500 -1.79445400
B 1.72083200 -0.51188200 -0.16529300
O 2.48486400 -0.76548400 -1.40022000
O 2.56832300 -1.00717400 0.93253900
C 3.41647600 -1.99484300 0.36472600
C 3.65730300 -1.49688400 -1.06789800
H 4.33868400 -2.07950600 0.94847300
H 2.92186100 -2.97752100 0.35555200
H 4.53772600 -0.83779400 -1.10988000
H 3.81440400 -2.31912400 -1.77563900
H 1.61961400 1.10113200 2.15766900

Zero-point correction=                           0.253353
(Hartree/Particle)
 Thermal correction to Energy=                    0.270380
 Thermal correction to Enthalpy=                  0.271324
 Thermal correction to Gibbs Free Energy=         0.204934
 Sum of electronic and zero-point Energies=          -1190.837248
 Sum of electronic and thermal Energies=             -1190.820220
 Sum of electronic and thermal Enthalpies=           -1190.819276
 Sum of electronic and thermal Free Energies=        -1190.885667
```

Transition state for S- methylation of phenyl sulfenate (**1**) complexed to **6a**.



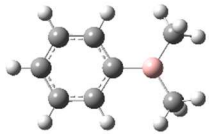


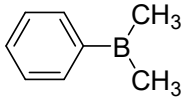

```
-1 1
 C                 -2.64340800   -0.20006700    0.49718300
 H                 -2.46311300   -0.14270300   -0.56154700
 H                 -2.49721300   -1.13172400    1.01352100
 H                 -2.87824600    0.68875100    1.05504100
 Br                -5.01402700   -0.68052800    0.15148300
 C                  0.09713900    2.18185300   -1.23056500
 C                  0.09607200    3.50354600   -1.67621700
 C                 -0.18784000    4.54857800   -0.79716200
 C                 -0.46855100    4.26852200    0.54200200
 C                 -0.46462800    2.95397500    1.00130900
 C                 -0.18146900    1.91165700    0.11016400
```

H	0.31756300	1.36294200	-1.90268000
H	0.31683900	3.71439300	-2.71681200
H	-0.68531700	5.07493900	1.23354200
H	-0.67290500	2.74327900	2.04516800
S	-0.23318400	0.23988700	0.73860800
O	0.26720500	-0.65311400	-0.52673700
H	-0.18773500	5.57339100	-1.15005500
C	3.40363600	0.13162400	-0.82671100
C	2.82056800	-0.76047000	0.09030400
C	3.45035300	-0.88512500	1.33890300
C	4.59833800	-0.15702600	1.66344300
C	5.15568600	0.72043700	0.73330000
C	4.55232700	0.86150100	-0.51842700
H	2.95092100	0.25660900	-1.80596100
H	5.05894700	-0.27616300	2.63946200
H	6.04829900	1.28658800	0.97857100
H	4.97891600	1.53901100	-1.25178900
B	1.51661300	-1.62698900	-0.30286000
O	1.60354400	-2.33027300	-1.58127600
O	1.15708200	-2.62847100	0.69676800
C	0.50642900	-3.68122200	-0.00672400
C	1.17911300	-3.67636900	-1.38784100
H	0.63811300	-4.62558200	0.52957800
H	-0.57042200	-3.48050300	-0.09639300
H	2.04992700	-4.34715100	-1.40489800
H	0.49530300	-3.98285300	-2.18674100
H	3.03368900	-1.57160900	2.06882700

Zero-point correction=	0.290773
(Hartree/Particle)	
Thermal correction to Energy=	0.312277
Thermal correction to Enthalpy=	0.313221
Thermal correction to Gibbs Free Energy=	0.233450
Sum of electronic and zero-point Energies=	-3804.859015
Sum of electronic and thermal Energies=	-3804.837511
Sum of electronic and thermal Enthalpies=	-3804.836567
Sum of electronic and thermal Free Energies=	-3804.916338

Dimethylphenylborane (**6b**)





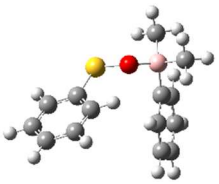
0 1

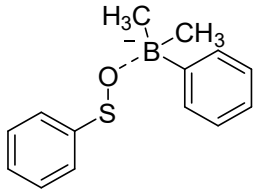
C	-0.60174900	-1.20047300	-0.03450400
C	0.13789500	0.00000000	0.00000000
C	-0.60174900	1.20047300	0.03450400

C	-1.99484700	1.20620200	0.04194500
C	-2.69537400	0.00000000	0.00000000
C	-1.99484700	-1.20620200	-0.04194500
H	-0.07896600	-2.14983500	-0.06035100
H	-2.53475100	2.14623000	0.07596000
H	-3.77998600	0.00000000	0.00000000
H	-2.53475100	-2.14623000	-0.07596000
B	1.70993900	0.00000000	0.00000000
H	-0.07896600	2.14983500	0.06035200
C	2.53150800	-1.34482800	0.07135100
H	2.01634800	-2.20037700	0.51450900
H	2.78367300	-1.62845400	-0.96268400
H	3.49180700	-1.21291600	0.58100600
C	2.53150800	1.34482700	-0.07135100
H	2.01634600	2.20038000	-0.51450000
H	2.78368400	1.62844700	0.96268400
H	3.49180300	1.21291700	-0.58101500

Zero-point correction=	0.167037
(Hartree/Particle)	
Thermal correction to Energy=	0.176563
Thermal correction to Enthalpy=	0.177507
Thermal correction to Gibbs Free Energy=	0.131597
Sum of electronic and zero-point Energies=	-336.275335
Sum of electronic and thermal Energies=	-336.265809
Sum of electronic and thermal Enthalpies=	-336.264865
Sum of electronic and thermal Free Energies=	-336.310776

Complex of phenyl sulfenate (**1**) and **6b**





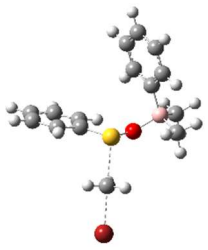
-1 1

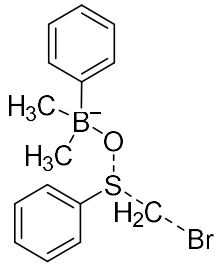
C	2.31163000	-0.11791200	0.98180400
C	3.43091500	0.60593400	1.39459900
C	4.37221700	1.05656500	0.46927000
C	4.18328700	0.77417800	-0.88734500
C	3.07084500	0.05510800	-1.31197400
C	2.12214500	-0.39400200	-0.37739000
H	1.58057400	-0.47362600	1.69583200
H	3.56599400	0.81624800	2.45058400
H	4.90537500	1.11875100	-1.62001900

H	2.93506200	-0.15477500	-2.36845700
S	0.74408200	-1.33805200	-0.97482200
O	-0.11830200	-1.63042400	0.41095300
H	5.23961600	1.61842900	0.79624900
C	-1.32744100	1.18401800	0.78689200
C	-2.02334600	0.16237700	0.11027000
C	-3.05441700	0.59240300	-0.74544500
C	-3.37709800	1.94267100	-0.91677700
C	-2.66390900	2.92596800	-0.23158900
C	-1.63040400	2.53654000	0.62413600
H	-0.51798600	0.90961600	1.45659300
H	-4.18260600	2.22658400	-1.58819100
H	-2.90643000	3.97576400	-0.36173200
H	-1.06307600	3.28934800	1.16426900
B	-1.68071400	-1.41980400	0.37894000
H	-3.62636800	-0.14652200	-1.29891400
C	-2.12663100	-1.84856800	1.89440700
H	-3.21325900	-1.75796900	2.02918600
H	-1.86123600	-2.89220200	2.11525300
H	-1.65680300	-1.22198400	2.66466700
C	-2.33121600	-2.42426800	-0.73791900
H	-2.02704600	-3.46324100	-0.54960300
H	-3.42963200	-2.41266700	-0.71808300
H	-2.03697100	-2.18658600	-1.77045100

Zero-point correction=	0.261392
(Hartree/Particle)	
Thermal correction to Energy=	0.278380
Thermal correction to Enthalpy=	0.279324
Thermal correction to Gibbs Free Energy=	0.214387
Sum of electronic and zero-point Energies=	-1041.476847
Sum of electronic and thermal Energies=	-1041.459859
Sum of electronic and thermal Enthalpies=	-1041.458915
Sum of electronic and thermal Free Energies=	-1041.523852

Transition state for S- methylation of phenyl sulfenate (**1**) complexed to **6b**.





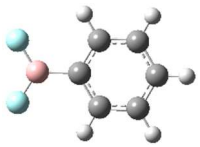
-1 1

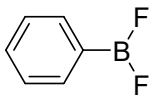
C	2.55300000	-0.51709200	-0.42198300
H	2.41697700	-0.30524600	0.62358000
H	2.36221900	-1.50766300	-0.79384300
H	2.76786200	0.27998000	-1.11108600
Br	4.92131400	-0.99082900	-0.11829600
C	-0.08079200	2.09039500	1.13663900
C	-0.02870900	3.45169000	1.43626700
C	0.25077100	4.38741600	0.44042300
C	0.47633200	3.95613300	-0.86883200
C	0.42096100	2.60068700	-1.18252200
C	0.14131100	1.66830800	-0.17544900
H	-0.29643300	1.35482300	1.90041400
H	-0.20576800	3.77952500	2.45476500
H	0.68962300	4.67654600	-1.65056700
H	0.58596300	2.27326200	-2.20384300
S	0.12561100	-0.06041400	-0.61987600
O	-0.36433500	-0.79032700	0.74865600
H	0.29040900	5.44378400	0.67980500
C	-3.35584400	0.05125600	0.65587100
C	-2.89095000	-1.15430300	0.09335300
C	-3.68685100	-1.69806300	-0.93119800
C	-4.86737400	-1.08892900	-1.36859200
C	-5.29427700	0.10632100	-0.79099800
C	-4.52716200	0.67699100	0.22752700
H	-2.78019300	0.51583900	1.45104600
H	-5.45111700	-1.54586700	-2.16244300
H	-6.20758500	0.58611700	-1.12752300
H	-4.84561000	1.60791000	0.68773100
B	-1.54006900	-1.88590400	0.65694000
H	-3.37994400	-2.62526200	-1.40559400
C	-1.01222000	-3.11444700	-0.27587900
H	-0.83890100	-2.83376900	-1.32466300
H	-0.06721200	-3.52009900	0.10921000
H	-1.72579000	-3.94917600	-0.29356000
C	-1.71135000	-2.33021800	2.21580700
H	-2.48991400	-3.09816800	2.31848700
H	-0.78481000	-2.75698200	2.62370300
H	-2.00160200	-1.49465800	2.86619900

Zero-point correction= 0.298858
(Hartree/Particle)
Thermal correction to Energy= 0.320281
Thermal correction to Enthalpy= 0.321225

```
 Thermal correction to Gibbs Free Energy=         0.243266
 Sum of electronic and zero-point Energies=         -3655.499561
 Sum of electronic and thermal Energies=            -3655.478138
 Sum of electronic and thermal Enthalpies=          -3655.477193
 Sum of electronic and thermal Free Energies=       -3655.555153
```

Difluorophenylborane (**6c**)

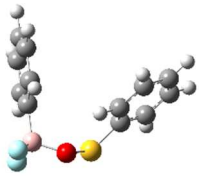


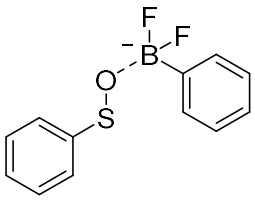



```
0 1
 C                  0.00006400    1.20967500    0.52947600
 C                  0.00000000    0.00000000   -0.18853600
 C                 -0.00006400   -1.20967500    0.52947600
 C                  0.00000000   -1.21057900    1.92122700
 C                  0.00000000    0.00000000    2.61666800
 C                  0.00000000    1.21057900    1.92122700
 H                  0.00013100    2.15165300   -0.00753000
 H                  0.00001200   -2.14854600    2.46440100
 H                  0.00000000    0.00000000    3.70099700
 H                 -0.00001200    2.14854600    2.46440100
 B                  0.00000000    0.00000000   -1.72591300
 H                 -0.00013100   -2.15165300   -0.00753000
 F                 -0.00105200   -1.12920400   -2.44235500
 F                  0.00105200    1.12920400   -2.44235500

Zero-point correction=                           0.100006
(Hartree/Particle)
 Thermal correction to Energy=                    0.107344
 Thermal correction to Enthalpy=                  0.108288
 Thermal correction to Gibbs Free Energy=         0.068038
 Sum of electronic and zero-point Energies=          -456.357775
 Sum of electronic and thermal Energies=             -456.350437
 Sum of electronic and thermal Enthalpies=           -456.349493
 Sum of electronic and thermal Free Energies=        -456.389743
```

Complex of phenyl sulfenate (**1**) and **6c**

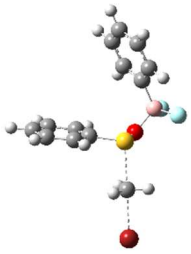


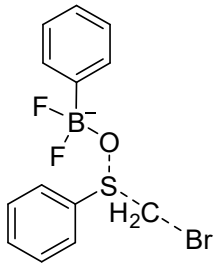


```
-1 1
 C                  1.93679100    0.05199400    1.02521000
 C                  2.94019800    0.95090100    1.38826600
 C                  3.97751100    1.25719300    0.50798000
 C                  4.00538200    0.65208500   -0.75154000
 C                  3.01012800   -0.24529200   -1.12653300
 C                  1.96725200   -0.54792900   -0.23713000
 H                  1.13090800   -0.18718600    1.70597400
 H                  2.90706400    1.41357900    2.36901600
 H                  4.80517100    0.88079900   -1.44762900
 H                  3.04272800   -0.70799600   -2.10797000
 S                  0.74796700   -1.73043900   -0.76714200
 O                 -0.26492600   -1.82025700    0.54614100
 H                  4.75382600    1.95652200    0.79632100
 C                 -1.78022400    1.17178900    1.07244900
 C                 -1.87506000    0.20523400    0.05667900
 C                 -2.13778000    0.67301200   -1.24075200
 C                 -2.29254400    2.03384600   -1.51726200
 C                 -2.19131600    2.97165400   -0.48939000
 C                 -1.93573100    2.53405600    0.81172700
 H                 -1.58705700    0.85089500    2.09185300
 H                 -2.49473600    2.36208000   -2.53220800
 H                 -2.31294500    4.02952300   -0.69803800
 H                 -1.86001600    3.25452200    1.62036500
 B                 -1.69129200   -1.36738000    0.38706900
 H                 -2.22904500   -0.04375900   -2.05042500
 F                 -2.31146800   -2.18067000   -0.62330800
 F                 -2.27688100   -1.70535600    1.64823200

Zero-point correction=                           0.194006
(Hartree/Particle)
 Thermal correction to Energy=                    0.209168
 Thermal correction to Enthalpy=                  0.210112
 Thermal correction to Gibbs Free Energy=         0.148693
 Sum of electronic and zero-point Energies=          -1161.581783
 Sum of electronic and thermal Energies=             -1161.566621
 Sum of electronic and thermal Enthalpies=           -1161.565677
 Sum of electronic and thermal Free Energies=        -1161.627097
```

Transition state for S-methylation of phenyl sulfenate (**1**) complexed to **6c**.





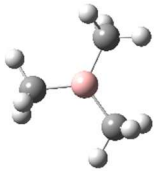
-1 1

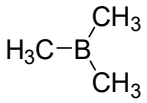
C	2.62370400	-0.41148000	-0.40743800
H	2.42788700	-0.25707800	0.63898100
H	2.57607100	-1.40364900	-0.81962200
H	2.83739000	0.42525900	-1.04836400
Br	5.03761500	-0.68792400	0.05169600
C	-0.31255700	1.84885000	1.07583000
C	-0.43802100	3.19031900	1.43601800
C	-0.22335500	4.19972300	0.49790400
C	0.11427400	3.86500300	-0.81485400
C	0.23591900	2.52962500	-1.19068500
C	0.02255400	1.52575900	-0.23928600
H	-0.47858300	1.05835200	1.79561700
H	-0.70305600	3.44423900	2.45625100
H	0.27714700	4.64338900	-1.55155100
H	0.48678800	2.27518000	-2.21508800
S	0.24162600	-0.16846900	-0.76594900
O	-0.22491400	-1.02378800	0.54410900
H	-0.32160200	5.24011400	0.78519300
C	-3.49813800	-0.52864500	1.09948000
C	-2.80877100	-1.21779700	0.08720400
C	-3.38576300	-1.21644900	-1.19231900
C	-4.58881800	-0.55643100	-1.45562000
C	-5.25143000	0.12198900	-0.43278500
C	-4.70124900	0.13248000	0.85066900
H	-3.08798200	-0.51413500	2.10492500
H	-5.01019900	-0.57431000	-2.45582100
H	-6.18696200	0.63431200	-0.63146000
H	-5.21175000	0.65336800	1.65460700
B	-1.41942000	-1.97263200	0.40312100
H	-2.88737500	-1.74803500	-1.99658800
F	-1.08893100	-2.92271300	-0.61017800
F	-1.43707100	-2.62710400	1.66301700

Zero-point correction= 0.231352
(Hartree/Particle)

```
 Thermal correction to Energy=                  0.250959
 Thermal correction to Enthalpy=                0.251903
 Thermal correction to Gibbs Free Energy=       0.176792
 Sum of electronic and zero-point Energies=         -3775.600892
 Sum of electronic and thermal Energies=            -3775.581286
 Sum of electronic and thermal Enthalpies=          -3775.580341
 Sum of electronic and thermal Free Energies=       -3775.655453
```

Trimethylborane (**7**)

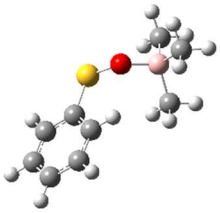


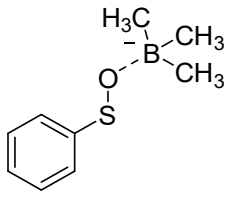



```
0 1
 B                 -0.00312800   -0.00021000   -0.00757800
 C                  0.65270800    1.43153000    0.00936600
 H                  1.71244800    1.45174900    0.28016100
 H                  0.57465500    1.83135400   -1.01422600
 H                  0.10601800    2.14122900    0.64046200
 C                 -1.57104100   -0.15118000   -0.00714300
 H                 -1.91444600   -0.90304000   -0.72720800
 H                 -1.86747700   -0.53962400    0.97965100
 H                 -2.12535800    0.77771800   -0.16939100
 C                  0.91651000   -1.27988600   -0.00584500
 H                  1.39323000   -1.35563400    0.98302500
 H                  0.40035700   -2.22484100   -0.19732300
 H                  1.74714700   -1.18064700   -0.71553100

Zero-point correction=                          0.111804
(Hartree/Particle)
 Thermal correction to Energy=                  0.118907
 Thermal correction to Enthalpy=                0.119851
 Thermal correction to Gibbs Free Energy=       0.080920
 Sum of electronic and zero-point Energies=          -144.545787
 Sum of electronic and thermal Energies=             -144.538685
 Sum of electronic and thermal Enthalpies=           -144.537740
 Sum of electronic and thermal Free Energies=        -144.576671
```

Complex of phenyl sulfenate (**1**) and **7**



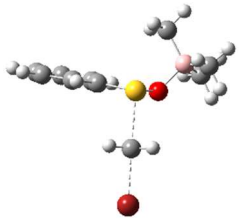


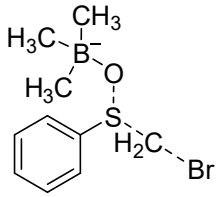
-1 1

C	-1.38469300	0.93155800	-0.35617600
C	-2.61731800	1.56497800	-0.19606400
C	-3.75506500	0.83710700	0.15375400
C	-3.64793200	-0.54410000	0.34391300
C	-2.42388300	-1.18693100	0.18716400
C	-1.27918000	-0.45034400	-0.16179400
H	-0.49831800	1.49068300	-0.62571600
H	-2.68605400	2.63748200	-0.34687800
H	-4.52307400	-1.12470600	0.61625200
H	-2.35529600	-2.26018100	0.33680800
S	0.25228100	-1.32767700	-0.37880400
O	1.32069700	-0.15662400	-0.83092000
H	-4.71012500	1.33482600	0.27703500
B	2.49722800	0.28272100	0.15268400
C	3.28683100	1.40236700	-0.74024900
H	4.15114400	1.80655400	-0.19343400
H	3.67319400	0.98923600	-1.68334300
H	2.64868900	2.25906300	-1.00113800
C	3.44216800	-1.01975200	0.46214600
H	3.83635000	-1.47654600	-0.45791000
H	4.31259000	-0.74342700	1.07512900
H	2.91409100	-1.81186000	1.01284200
C	1.87376100	0.92052600	1.52483300
H	2.67570300	1.22193700	2.21476800
H	1.26405900	1.81597800	1.33893900
H	1.24069800	0.21072300	2.07627600

Zero-point correction=	0.207102
(Hartree/Particle)	
Thermal correction to Energy=	0.221106
Thermal correction to Enthalpy=	0.222050
Thermal correction to Gibbs Free Energy=	0.166113
Sum of electronic and zero-point Energies=	-849.745116
Sum of electronic and thermal Energies=	-849.731111
Sum of electronic and thermal Enthalpies=	-849.730167
Sum of electronic and thermal Free Energies=	-849.786105

Transition state for S-methylation of phenyl sulfenate (**1**) complexed to **7**.





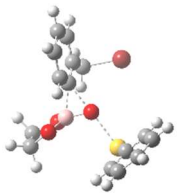
-1 1

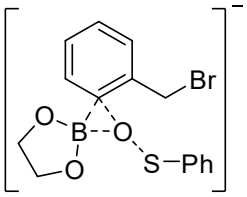
C	1.75539000	-0.33386700	-0.39574900
H	1.43412600	-0.36955400	0.63010100
H	1.82045600	-1.24412500	-0.96416000
H	1.89515100	0.61260900	-0.88659300
Br	4.10293600	-0.44562000	0.22554100
C	-1.51395200	1.61722600	0.96039400
C	-1.75308100	2.92670500	1.37709100
C	-1.49963000	4.00047700	0.52348500
C	-1.00585200	3.75985900	-0.76082400
C	-0.76810100	2.45672900	-1.19051500
C	-1.02273700	1.38510500	-0.32534100
H	-1.70794000	0.77512800	1.61193300
H	-2.13834400	3.10604500	2.37492900
H	-0.80949000	4.58790900	-1.43279000
H	-0.39308900	2.27627300	-2.19283500
S	-0.66786100	-0.26921600	-0.90575000
O	-1.14273000	-1.22767800	0.31047800
H	-1.68671900	5.01591000	0.85324700
B	-2.41223500	-2.22712500	0.11460700
C	-2.05375500	-3.26289400	-1.09522700
H	-1.93375800	-2.76651100	-2.06915300
H	-1.12901200	-3.82603600	-0.90360700
H	-2.85416900	-4.00520700	-1.22500200
C	-2.47240400	-2.96082500	1.56736800
H	-3.29396200	-3.69042100	1.60172000
H	-1.55015900	-3.51157600	1.79919900
H	-2.64349700	-2.25315900	2.39055800
C	-3.74241400	-1.33558400	-0.19666400
H	-4.62099000	-1.98471600	-0.32123000
H	-3.98190900	-0.63202000	0.61261600
H	-3.66144100	-0.74693100	-1.12183700

Zero-point correction= 0.244612
(Hartree/Particle)
Thermal correction to Energy= 0.263060
Thermal correction to Enthalpy= 0.264004

```
 Thermal correction to Gibbs Free Energy=         0.194442
 Sum of electronic and zero-point Energies=          -3463.768130
 Sum of electronic and thermal Energies=             -3463.749682
 Sum of electronic and thermal Enthalpies=           -3463.748738
 Sum of electronic and thermal Free Energies=        -3463.818300
```

Transition state for aryl migration from B to O.



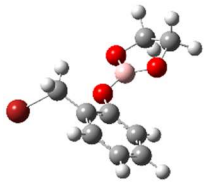


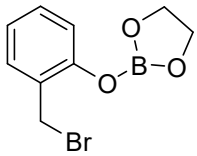

```
-1 1
 C                  0.67281900    1.09101200    2.19594000
 C                  1.13415700    0.78475500    0.91034500
 C                  2.40285400    0.19925400    0.74160500
 C                  3.22026600    0.02907300    1.87044100
 C                  2.77553600    0.37572800    3.14195800
 C                  1.49063400    0.90296200    3.30568200
 H                 -0.32031400    1.50808400    2.31487600
 H                  4.21240500   -0.39372000    1.74413700
 H                  3.42044300    0.22899800    4.00097200
 H                  1.13112100    1.16644700    4.29486400
 B                  0.15219500    1.52001600   -0.46632300
 O                 -0.20749300    0.19301300   -0.29741900
 S                 -1.86069000   -0.46675900   -1.72960700
 C                 -3.13713900   -0.75875300   -0.53908900
 C                 -3.22634500   -1.98735900    0.14420400
 C                 -4.10300000    0.22453000   -0.24832200
 C                 -4.23688000   -2.22128100    1.07445100
 H                 -2.49293500   -2.75813800   -0.06349100
 C                 -5.11460500   -0.01286100    0.67972300
 H                 -4.05100400    1.17905800   -0.75940800
 C                 -5.18892200   -1.23686500    1.34819100
 H                 -4.28192900   -3.17697300    1.58657300
 H                 -5.84702800    0.76174100    0.88276300
 H                 -5.97566300   -1.42028800    2.07143900
 O                 -0.66755000    2.60865200   -0.02795100
 O                  0.91463700    1.96103900   -1.59547500
 C                  0.84084500    3.38548200   -1.64557900
 H                  1.71355400    3.82224500   -1.14285200
 H                  0.83378700    3.71986300   -2.68577400
 C                 -0.46085600    3.72052800   -0.89918500
```

H	-1.30743300	3.80527900	-1.59154200
H	-0.38880100	4.64612300	-0.32134100
C	2.91797100	-0.20703300	-0.59554200
H	3.98823200	-0.05348500	-0.69838000
H	2.37039200	0.23865400	-1.41562900
Br	2.73612800	-2.20692800	-0.90725900

Zero-point correction= 0.270019
(Hartree/Particle)
Thermal correction to Energy= 0.290167
Thermal correction to Enthalpy= 0.291111
Thermal correction to Gibbs Free Energy= 0.215668
Sum of electronic and zero-point Energies= -3803.644516
Sum of electronic and thermal Energies= -3803.624368
Sum of electronic and thermal Enthalpies= -3803.623424
Sum of electronic and thermal Free Energies= -3803.698867

Boronate product after aryl migration.





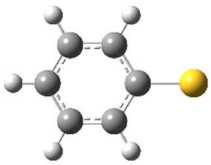
0 1

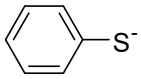
B	2.14664500	-0.45404200	0.12794900
O	2.99217200	0.49629400	-0.38020800
O	2.73903500	-1.66338100	0.38059700
C	4.15344200	-1.50609800	0.12369700
H	4.68101200	-1.51021400	1.07967100
H	4.50083700	-2.34172700	-0.48333900
C	4.26971000	-0.14800000	-0.60464600
H	4.41145800	-0.26414700	-1.68082000
H	5.06148300	0.48296600	-0.20185500
O	0.81131800	-0.28522300	0.36623600
C	0.11122500	0.88902900	0.19794000
C	0.55890800	2.08477100	0.75525200
C	-1.10739900	0.82858500	-0.49716400
C	-0.20375800	3.24134700	0.61263700
H	1.49713000	2.10463700	1.29504800
C	-1.85656700	2.00539400	-0.62603800
C	-1.41383900	3.20583700	-0.08084800
H	0.14943400	4.16931100	1.04725800
H	-2.79792700	1.96948900	-1.16379800
H	-2.00644000	4.10565000	-0.19403200
C	-1.58471100	-0.44241500	-1.10034900

H	-2.27802400	-0.28040400	-1.91892600
H	-0.78337400	-1.11078700	-1.39381100
Br	-2.65917400	-1.55390800	0.21025600

Zero-point correction=	0.183567
(Hartree/Particle)	
Thermal correction to Energy=	0.196418
Thermal correction to Enthalpy=	0.197362
Thermal correction to Gibbs Free Energy=	0.140418
Sum of electronic and zero-point Energies=	-3173.777660
Sum of electronic and thermal Energies=	-3173.764810
Sum of electronic and thermal Enthalpies=	-3173.763866
Sum of electronic and thermal Free Energies=	-3173.820810

Phenyl thiolate by-product after aryl migration.





-1 1

S	2.35083400	0.00000500	-0.00007300
C	0.58015100	0.00006400	0.00008000
C	-0.16428100	-1.20172300	0.00012100
C	-0.16439300	1.20179200	0.00010600
C	-1.55765200	-1.20088600	-0.00002000
H	0.37024900	-2.14573200	0.00020100
C	-1.55776200	1.20082000	-0.00000900
H	0.37002600	2.14585800	0.00020800
C	-2.27233100	-0.00006500	-0.00010400
H	-2.08960200	-2.14775600	-0.00003200
H	-2.08979100	2.14764600	-0.00002500
H	-3.35663000	-0.00011000	-0.00021900

Zero-point correction=	0.089620
(Hartree/Particle)	
Thermal correction to Energy=	0.095184
Thermal correction to Enthalpy=	0.096128
Thermal correction to Gibbs Free Energy=	0.059807
Sum of electronic and zero-point Energies=	-629.968246
Sum of electronic and thermal Energies=	-629.962682
Sum of electronic and thermal Enthalpies=	-629.961738
Sum of electronic and thermal Free Energies=	-629.998060