Electronic Supporting Information

A Computational Investigation of the Thermal Elimination Chemistry of β-Borylated Sulfoxides. Sulfenic Acid vs Boryl Sulfenate Elimination

Eric A. Nicol,[a] and Adrian L. Schwan*[a]

a Department of Chemistry, University of Guelph, Guelph, ON, Canada, N1G 2W1. Email: schwan@uoguelph.ca

Table of Contents

1. Data table and explanations for thermal chemistry of **1B**, **1BH**, **1BF**, **1BC**, **1BO**

Table S1 *Important geometric parameters for starting materials and transition states for the internal MeSOH elimination reaction of compounds **1**.*

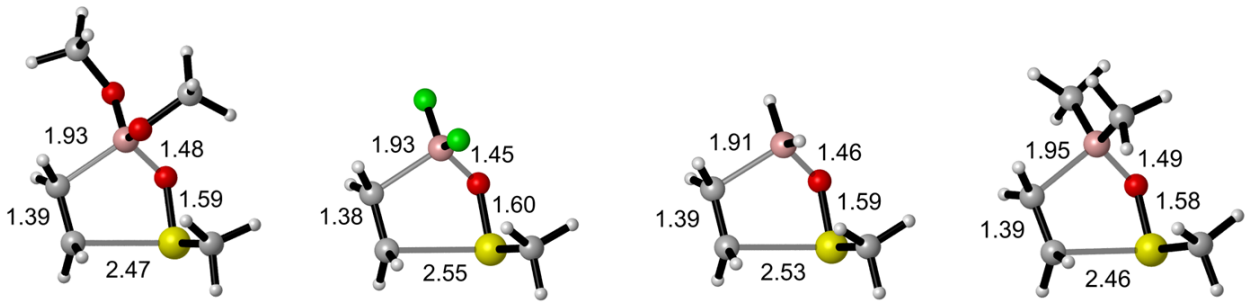
Compound	**1**		**1BH-H**		**1BF-H**		**1BC-H**		**1BO-H**	
Bond	**S.M.**	**T.S.**	**S.M.**	**T.S.**	**S.M.**	**T.S.**	**S.M.**	**T.S.**	**S.M.**	**T.S.**
S-O (Å)	1.491	1.562	1.493	1.558	1.492	1.562	1.493	1.556	1.493	1.561
S-C_α (Å)	1.841	2.436	1.845	2.067	1.844	2.183	1.844	2.186	1.840	2.317
C_α-C_β (Å)	1.521	1.400	1.523	1.449	1.524	1.430	1.521	1.430	1.522	1.414
C_β-H (Å)	1.091	1.378	1.111	1.514	1.101	1.474	1.104	1.462	1.100	1.401
H-O (Å)	2.598	1.242	2.435	1.191	2.449	1.185	2.500	1.208	2.536	1.237
C_β-BR_2	-	-	1.549	1.493	1.561	1.517	1.575	1.525	1.583	1.550
O-S-C_α-C_β dihedral	43.1˚	3.7˚	39.7˚	17.3˚	40.1˚	10.3˚	42.5˚	12.4˚	43.7˚	7.7˚

Table S2. *Bond orders (Angstroms) and NPA charges for the starting sulfoxides (**1**), transition states and products of the MeSOH elimination reaction.*

	Bond Orders						NPA Charges					
Compound	**S-O**	**S-C_α**	**C_α-C_β**	**C_β-H**	**H-O**	**Cβ-BR_2**	**O**	**S**	**C_α**	**C_β**	**H**	**B**
1	1.26	0.81	1.14	0.95	0.00	-	-0.96	1.22	-0.59	-0.62	0.23	-
1‡	1.27	0.43	1.56	0.49	0.46	-	-0.84	0.80	-0.35	-0.70	0.38	-
Products	0.97	0.00	2.11	0.00	0.99	-	-0.82	0.47	-0.39	-0.39	0.47	-
1BH-H	1.26	0.84	1.09	0.88	0.00	1.08	-0.96	1.22	-0.57	-0.82	0.29	0.48
1BH-H‡	1.20	0.69	1.29	0.27	0.66	1.44	-0.85	1.00	-0.43	-0.80	0.43	0.26
Products	0.97	0.00	1.93	0.00	0.99	1.13	-0.82	0.47	-0.24	-0.56	0.47	0.40
1BF-H	1.26	0.82	1.13	0.95	0.00	0.93	-0.95	1.23	-0.58	-0.84	0.28	1.29
1BF-H‡	1.21	0.58	1.41	0.39	0.54	1.19	-0.85	0.93	-0.38	-0.92	0.41	1.23
Products	0.97	0.00	2.04	0.00	0.99	1.00	-0.82	0.47	-0.27	-0.61	0.47	1.24
1BC-H	1.37	0.83	1.09	0.89	0.00	1.00	-0.96	1.22	-0.57	-0.79	0.28	0.88
1BC-H‡	1.26	0.62	1.36	0.30	0.63	1.33	-0.86	0.92	-0.38	-0.82	0.42	0.75
Products	0.97	0.00	1.96	0.00	0.99	1.09	-0.82	0.47	-0.27	-0.53	0.47	0.80
1BO-H	1.25	0.82	1.14	0.95	0.00	0.94	-0.96	1.22	-0.57	-0.76	0.26	1.12
1BO-H‡	1.25	0.50	1.45	0.45	0.50	1.04	-0.85	0.85	-0.34	-0.84	0.40	1.10
Products	0.97	0.00	2.05	0.00	0.99	0.98	-0.82	0.47	-0.31	-0.52	0.47	1.07

Table S3. *Bond lengths starting sulfoxides (**1B**) and transition states of the boryl sulfenate elimination reaction.*

Compound	S-O (Å)	S-C_α (Å)	C_α-C_β (Å)	BR_2-O (Å)	C_β-BR_2 (Å)	O-S-C_α-C_β dihedral
1BH-B	1.539	1.831	1.529	1.639	1.654	32.9
1BH-B‡	1.600	2.485	1.395	1.468	1.873	6.5˚
1BF-B	1.543	1.843	1.527	1.635	1.648	27.9
1BF-B‡	1.606	2.514	1.388	1.455	1.895	2.2˚
1BC-B	1.534	1.833	1.525	1.709	1.648	31.1˚
1BC-B‡	1.591	2.413	1.400	1.493	1.900	6.2˚
1BO	1.501	1.870	1.527	2.591	1.590	12.1˚
1BO-B	1.537	1.838	1.526	1.678	1.653	30.2˚
1BO-B‡	1.595	2.431	1.396	1.487	1.877	2.4˚



syn-1BO-H‡ syn-1BF-B‡ syn-1BH-B‡ syn-1BC-B‡

Figure S1: *Syn transition states related to anti boro sulfoxide elimination structures **1B** (see Figure 4)*

Table S4. *Bond orders (Angstroms) and NPA Charges for starting sulfoxides, transition states and products for the boryl sulfenate elimination of the sulfoxides **1B.***

	Bond Orders					NPA Charges				
Compound	**S-O**	**S-C_α**	**C_α-C_β**	**O-BR_2**	**C_β-BR_2**	**O**	**S**	**Cα**	**Cβ**	**B**
1BH-B	1.19	0.87	1.11	1.00	0.97	-0.78	1.20	-0.55	-0.68	0.14
1BH-B‡	1.18	0.50	1.52	1.38	0.59	-0.78	0.77	-0.26	-0.63	0.25
Products	0.96	-	2.11	2.01	-	-0.79	0.50	-0.39	-0.39	0.59
1BF-B	1.18	0.89	1.08	0.74	0.92	-0.81	1.19	-0.54	-0.75	1.11
1BF-B‡	1.09	0.45	1.48	1.02	0.54	-0.82	0.76	-0.24	-0.68	1.20
Products	1.06	-	2.11	1.40	-	-0.84	0.51	-0.39	-0.39	1.38
1BC-B	1.26	0.86	1.12	0.92	0.94	-0.80	1.20	-0.55	-0.68	0.60
1BC-B‡	1.19	0.51	1.46	1.22	0.59	-0.79	0.81	-0.28	-0.64	0.71
Products	1.00	-	2.11	1.87	-	-0.79	0.48	-0.39	-0.39	0.96
1BO	1.25	0.81	1.13	-	0.92	-0.95	1.19	-0.56	-0.76	1.14
1BO-B	1.26	0.87	1.09	0.75	0.92	-0.81	1.19	-0.54	-0.73	1.03
1BO-B‡	1.19	0.48	1.53	0.95	0.57	-0.81	0.79	-0.26	-0.67	1.10
Products	1.05	-	2.11	1.32	-	-0.81	0.50	-0.39	-0.39	1.25

Discussion of hyperconjugation effects on bond orders in the boryl elimination reaction: In contrast with **1BO-B‡** and **1BF-B‡**, the strongest interactions of the $\sigma^*_{O\text{-}B}$ orbital in **1BH-B‡** and **1BC-B‡** are 2.34 and 3.99 kcal/mol, from the sulfur lone pair and a methyl $\sigma_{C\text{-}H}$, respectively (Figure S2). The interaction of the sulfur lone pair with the $\sigma^*_{O\text{-}B}$ orbital is present in all 4 transition states with stabilization energies of 0.72 kcal/mol, 1.45 kcal/mol, and 1.99 kcal/mol in **1BF-B‡**, **1BO-B‡**, and**1BC-B‡**, respectively. Hence, the delocalization of the lone pairs of O and F retards bond formation to a greater extent for the F and MeO substituted compounds than with Me or H analogs, contributing significantly to the asynchronicity and higher barrier for elimination.

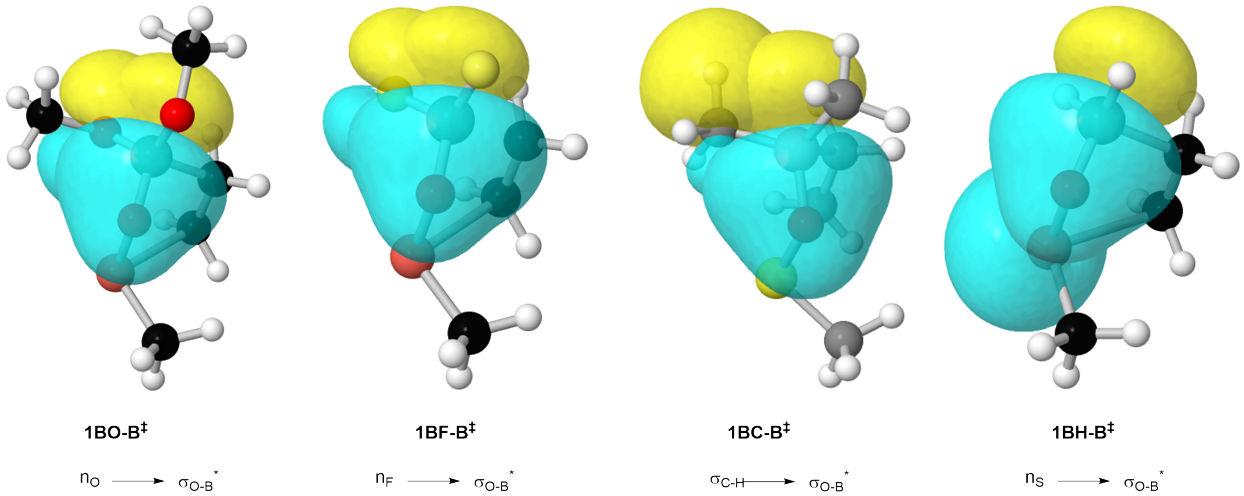


Figure S2: Natural bond orbital diagrams of the transition states for **1BO-B‡**, **1BF-B‡**, **1BC-B‡** and **1BH-B** showing the overlap of the $\sigma_{O\text{-}B^*}$ with the orbital responsible for the strongest second -order perturbation energy interaction identified.

2. Details, discussion and data for boryl sulfenate eliminations of **2B**, **3B** and **4B**

To determine the role of conjugation on the energetics of boron transfer three additional compound families were investigated, all possessing the H, F, Me and OMe boron substituents: **2B** with a vinyl sulfoxide, **3B** with a phenyl sulfoxide, and **4B** still with a methyl sulfoxide, but harbouring an alkene between the sulfur and boron atoms which leads to alkyne formation upon boryl sulfenate loss. Paralleling compounds **1B**, the sulfinyl to boron coordinated structures **2B**/**3B** with H, F and Me groups proved to be the lowest energy identified structures. Whereas for methoxy groups on the boron, the structures lacking significant oxygen to boron interaction (**2BO**/**3BO**) prevailed as global minima, lying 4.5 kcal/mol and 1.7 kcal/mol lower than coordinated local minima **2BO-B** and **3BO-B**, respectively. Bond orders for systems with an S-conjugated group in the starting sulfoxides can be found in Table S5. Considering differences of 10% or greater as significant changes between compound families, the only significant changes are reductions in the S-O bond orders for **3BO-B**, **3BF-B** and **3BH-B** by 27%, 17% and 13%, respectively when compared to **1BO-B**, **1BF-B** and **1BH-B**.

Starting sulfoxide structures and their corresponding transition states for boryl sulfenate elimination for the **2B** and **3B** family of compounds can be found in Figure S3 and Figure S4, respectively. Minimal changes in bond order are observed in the transition states when comparing to compound family **1B**, signifying that the synchronicity of the reaction is relatively unchanged by substitution of the sulfinyl methyl for a vinyl or phenyl group.

These conjugating sulfur substituents bring about a reduction of the barrier for elimination of the boryl sulfenate by 1.9 – 2.6 kcal/mol for pre-coordinated compounds compared to **1B**, and by 2.3 kcal/mol and 4.9 kcal/mol for uncoordinated structures **2BO** and **3BO**, respectively (Table S6). Inspection of the NPA charges, found in Table S5, for both starting sulfoxides shows minor differences in charge (0.01e-0.02e) for most compounds, however, a noticeable change in charge is observed for compounds **3BC-B** and **3BO**, where boron's charge is more negative by 0.44e in **3BC-B** and sulfur is more positive by 0.04e in **3BO**. The more positive charge on sulfur is a consistent feature of each transition state for compound families **2B** and **3B**, with values becoming more positive by 0.03e-0.06e.

	Bond Orders					NPA Charges				
Compound	**S-O**	**S-Cα**	**Cα-Cβ**	**O-BR_2**	**Cβ-BR_2**	**O**	**S**	**C_α**	**C_β**	**B**
2BH-B	1.15	0.88	1.11	0.99	0.98	-0.78	1.19	-0.54	-0.68	0.15
2BH-B‡	1.16	0.51	1.50	1.36	0.61	-0.77	0.82	-0.25	-0.64	0.24
Products	0.96	-	2.11	2.00	-	-0.78	0.55	-0.39	-0.39	0.59
2BF-B	1.20	0.87	1.08	0.75	0.92	-0.81	1.18	-0.53	-0.76	1.13
2BF-B‡	1.08	0.45	1.46	0.97	0.56	-0.81	0.80	-0.24	-0.69	1.19
Products	0.98	-	2.11	1.40	-	-0.84	0.56	-0.39	-0.39	1.14
2BC-B	1.18	0.88	1.12	0.91	0.94	-0.79	1.19	-0.54	-0.69	0.60
2BC-B‡	1.16	0.53	1.49	1.27	0.60	-0.79	0.85	-0.28	-0.65	0.69
Products	1.00	-	2.11	1.87	-	-0.79	0.55	-0.39	-0.39	0.97
2BO	1.22	0.81	1.12	-	0.92	-0.95	1.21	-0.56	-0.77	1.14
2BO-B	1.26	0.85	1.09	0.76	0.92	-0.80	1.18	-0.53	-0.73	1.03
2BO-B‡	1.18	0.50	1.51	0.92	0.59	-0.80	0.84	-0.26	-0.68	1.09
Products	1.08	-	2.11	1.19	-	-0.81	0.56	-0.39	-0.39	1.26
3BH-B	1.04	0.85	1.12	0.98	0.98	-0.79	1.21	-0.53	-0.69	0.16
3BH-B‡	1.16	0.47	1.53	1.36	0.57	-0.78	0.83	-0.25	-0.64	0.25
Products	0.99	-	2.11	1.94	-	0.58	-0.79	-0.39	-0.39	0.60
3BF-B	0.98	0.85	1.13	0.76	0.88	-0.82	1.21	-0.52	-0.76	1.12
3BF-B‡	1.13	0.44	1.57	0.98	0.52	-0.82	0.81	-0.23	-0.68	1.20
Products	0.97	-	2.11	1.44	-	-0.83	0.51	-0.39	-0.39	1.39
3BC-B	1.27	0.85	1.12	0.98	0.98	-0.79	1.21	-0.53	-0.69	0.16
3BC-B‡	1.16	0.49	1.53	1.27	0.57	-0.79	0.86	-0.27	-0.65	0.70
Products	1.03	-	2.11	1.85	-	-0.81	0.58	-0.39	-0.39	1.01
3BO	1.36	0.82	1.12	-	0.91	-0.96	1.23	-0.55	-0.76	1.15
3BO-B	0.92	0.84	1.14	0.75	0.90	-0.82	1.21	-0.52	-0.74	1.05
2BO-B‡	1.18	0.46	1.55	0.91	0.55	-0.81	0.85	-0.25	-0.68	1.10
Products	1.12	-	2.11	1.15	-	-0.81	0.59	-0.39	-0.39	1.26

Table S5**. Bond orders (Angstroms) and NPA Charges for starting sulfoxides, transition states and products for the boryl sulfenate elimination of the sulfoxide families **2B**/**3B.

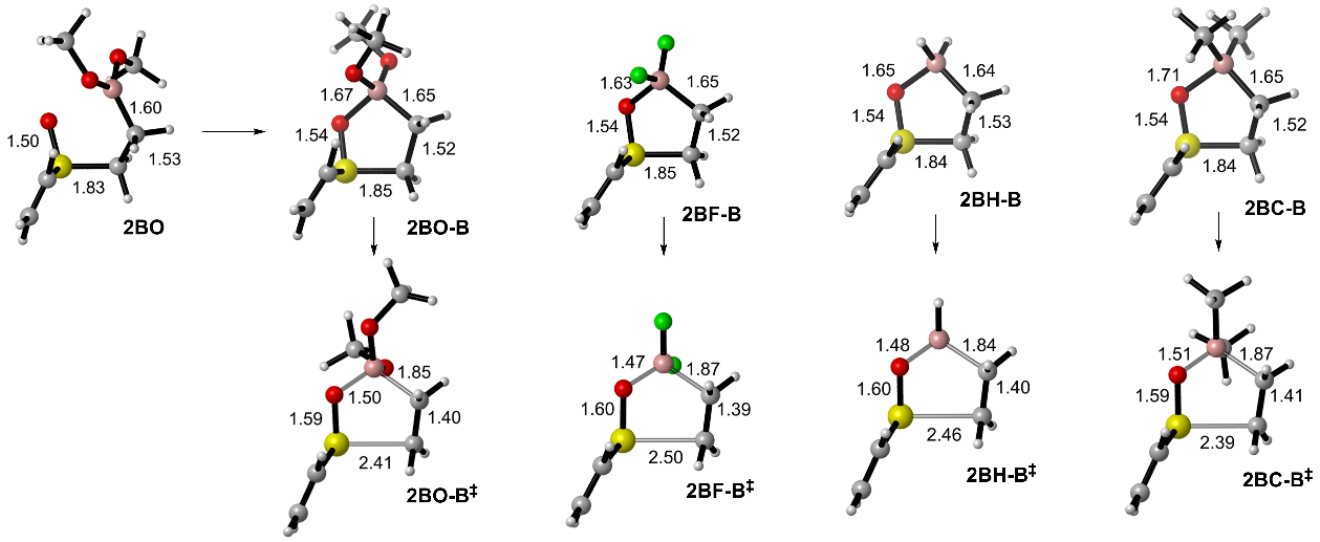


Figure S3. Starting sulfoxides and transition states for the boryl sulfenate elimination of sulfoxides **2B**. Bond lengths are listed in angstroms.

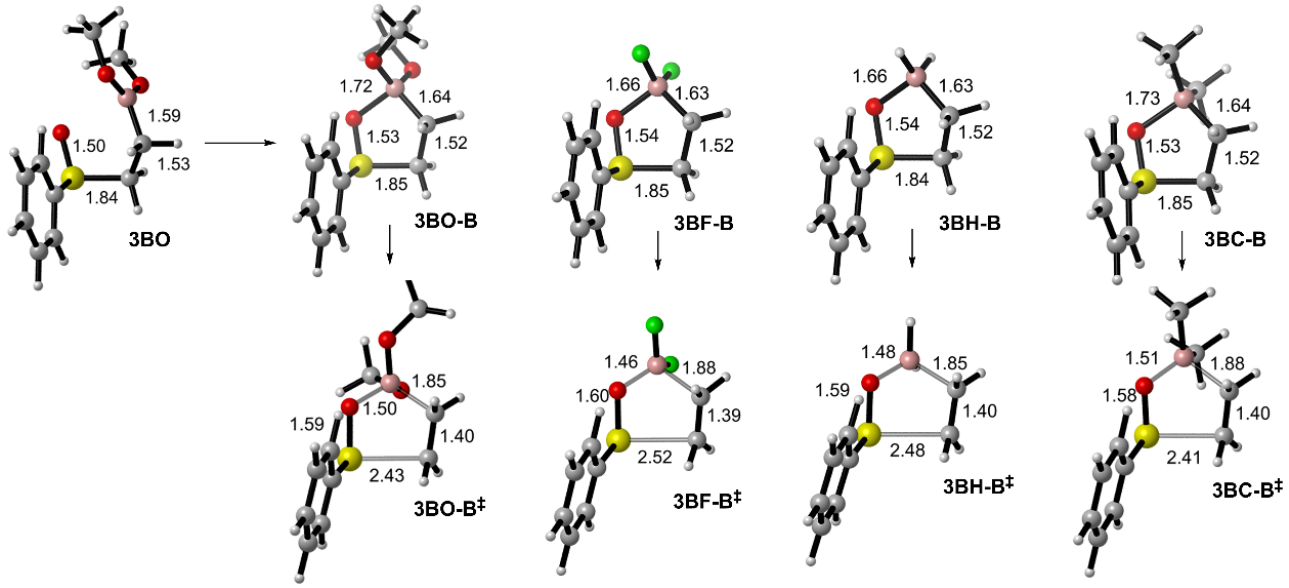


Figure S4. Starting sulfoxides and transition states for the boryl sulfenate elimination of sulfoxides **3B**. Bond lengths are listed in angstroms.

Table S6: *Thermodynamics of boryl sulfenate elimination from sulfoxides **2** and **3**.*[a]

Compound	$\Delta H^{‡}$	$\Delta G^{‡}$	$\Delta S^{‡}$	ΔH	ΔG	ΔS
2BH-B	16.9	16.8	0.3	4.3	-9.4	46.0
2BF-B	19.3	19.0	0.8	4.1	-9.5	45.9
2BC-B	16.4	16.3	0.6	-2.0	-16.6	48.9
2BO[b]	20.9	21.1	-0.8	0.0	-13.6	45.7
3BH-B	17.8	17.0	2.7	7.1	-7.9	50.1
3BF-B	20.1	19.1	3.2	6.4	-8.2	48.8
3BC-B	16.5	16.0	1.7	-0.7	-15.4	49.6
3BO[c]	18.7	18.7	-0.1	-1.1	-15.0	46.6

a Energy units are kcal/mol; entropy units are cal/K•mol. *b* **2BO-B** is a stationary point on the path of **2BO** to the transition state. *c* **3BO-B** is a stationary point on the path of **3BO** to the transition state.

This decrease in negative charge can be attributed to delocalization of the electron density in the S-C_α bond into the π* orbitals of the phenyl and vinyl groups. For example, in compounds **1BO-B** and **1BO**, delocalization of $\sigma_{S\text{-}C\alpha}$ into a Me $\sigma_{C\text{-}H}$* orbital does occur with stabilization energies of 1.38 kcal/mol and 1.62 kcal/mol, respectively. In transition state **1BO‡**, this value increases to 3.43 kcal/mol. But, in the starting sulfoxides **2BO** and **2BO-B**, the strongest delocalization of the $\sigma_{S\text{-}C\alpha}$ density is into the $\pi_{C=C}$* orbital of the vinyl group, with energies of 2.41 kcal/mol and 2.56 kcal/mol, respectively. In transition state **2BO-B‡** , this delocalization increases to 9.72 kcal/mol. For compounds **3BO-B** and **3BO** the $\sigma_{S\text{-}C\alpha} \rightarrow \pi_{C=C}$* stabilization energies are 3.38 kcal/mol and 3.42 kcal/mol, respectively, and increase to 11.85 kcal/mol in the transition state (**3BO-B‡**). These delocalizations into the available π* orbitals of the sulfur substituent aid in stabilizing the increased charge on sulfur in the transition state to a greater extent, leading to a reduced barrier for elimination.

The effect of a π-bond connecting sulfur and boron on the boron elimination was investigated through compound family **4B**, whose starting sulfoxides and transition states can be found in Figure S5. As observed previously, two starting sulfoxide structures were located for the methoxy substituted sulfoxide where pre-coordination of the sulfinyl oxygen to boron (**4BO-B**) proved to be a local minimum, whereas the form (**4BO**), exhibited additional stability, lying 4.3 kcal/mol lower. Unique to this family, the transition states displayed a boron atom that enveloped itself to be syn to the sulfinyl methyl group. This represents a molecular motion that brings one boron substituent *closer* to the methyl group as it approaches the transition state. Thermodynamics for the boron elimination reaction for compound family **4B** can be found in Table S7.

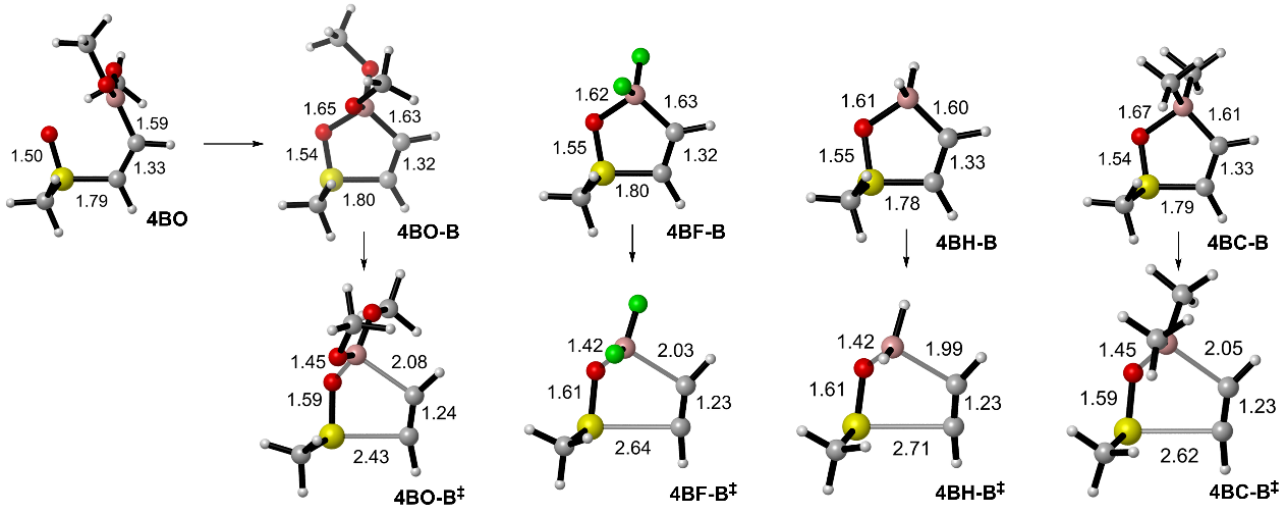


Figure S5. Starting sulfoxides and transition states for the boryl sulfenate elimination of sulfoxides 4**B**. Bond lengths are listed in angstroms.

Table S7: *Thermodynamics of boryl sulfenate elimination from sulfoxides **4**.*[a]

Compound	4BH-B	4BF-B	4BC-B	4BO [b]
$\Delta H^{‡}$	36.2	35.0	36.1	30.8
$\Delta G^{‡}$	34.9	33.7	34.6	31.4
$\Delta S^{‡}$	4.5	4.5	5.0	-2.0
ΔH	24.1	20.3	16.3	15.0
ΔG	10.5	6.3	2.4	3.1
ΔS	45.5	47.0	46.7	39.8

a Energy units are kcal/mol; entropy units are cal/K•mol; *b* **4BO-B** is a stationary point on the path of 4**BO** to the transition state.

As observed previously,[1] barriers for the elimination are increased significantly compared to **1B**, with free energy barriers increasing by 12.6 – 15.9 kcal/mol for the lowest energy starting sulfoxide starting structures. There is also a change in the free energy trend where **4BO-B** has the lowest energy free energy of activation, followed by **4BF-B**, **4BC-B** and surprisingly, the highest

barrier is for **4BH-B**. It should be noted that for hydrogen, methyl and fluoro substituted compounds, barriers only differ by a maximum of 1.2 kcal/mol. Barriers for compound **4BO-B** are overall the lowest at 27.1 kcal/mol; however, this is due to the increase in energy of the compound upon pre-coordination of the sulfinyl oxygen to the boron moiety. Overall, an increase in barrier is to be expected as bond strengths of the C_β-B and C_α-S bonds should be increased due to the sp^2 character of the carbons involved. Natural resonance theory bond orders for starting sulfoxides, transition states and products can be found in Table S8. Some significant changes in bond order are immediately obvious in the starting sulfoxides: S-O bond orders are generally reduced by 0.06-0.09; S-C_α bond orders increase by 0.03-0.09; and C_β-B bond orders are increased particularly in **4BH-B** and **4BC-B**, the two compounds with the highest barriers.

Breakage of the strong bonds during the reaction contributes significantly to the increase in the free energy barrier observed across all four compounds in family **4B**. The bond orders of the hydrogen and methyl compounds for C_β-B are the highest of the four, with bond order of 1.08 and 1.02, approximately 13-18% higher than the F or MeO compounds. A definitive change in the synchronicity of the reactions is also observed compared to the **1B** family of compounds: most noticeably, compounds **4BH-B** and **4BC-B** show significantly more advanced cleavage of the S-C_α than C_β-B (0.37 vs 0.48 and 0.37 vs 0.45, respectively) in the transition states, while **4BF-B‡** and **4BO-B‡** are more symmetric (0.36 vs 0.37 and 0.39 vs 0.44, respectively).

1. J. W. Cubbage, Y. Guo, R. D. McCulla and W. S. Jenks, *J. Org. Chem.*, 2001, **66**, 8722-8736.

Table S8: *Natural bond orders for the boron transfer reaction of compound family **4B.***

Compound	S-O	S-C_α	C_α-C_β	O- BR_2	C_β-BR_2
4BH-B	1.10	0.92	1.97	1.00	1.08
4BH-B‡	1.19	0.37	2.52	1.54	0.48
Products	0.96	-	2.99	2.01	-
4BF-B	1.12	0.92	2.06	0.75	0.91
4BF-B‡	1.18	0.36	2.57	1.10	0.37
Products	1.06	-	2.99	1.40	-
4BC-B	1.17	0.91	2.01	0.92	1.02
4BC-B‡	1.21	0.37	2.53	1.45	0.45
Products	1.00	-	2.99	1.87	-
4BO	1.24	0.85	2.06	-	0.91
4BO-B	1.18	0.90	2.03	0.76	0.90
4BO-B‡	1.18	0.39	2.54	0.90	0.44
Products	1.05	-	2.99	1.32	-

3. Data tables and graphics for thermal chemistry of **1Bpin 1Bcat**, **1Bmida**

Table S9: *Natural resonance theory bond orders for the internal elimination reaction for various sulfoxides substituted with boronic esters*

Compound	S-O	S-C_α	C_α-C_β	C_β-H	H-O	C_β-BR_2
1Bcat-H	1.39	0.81	1.12	0.94	-	0.93
1Bcat-H‡	1.26	0.55	1.41	0.43	0.51	1.10
Products	0.97	-	2.01	-	0.99	1.03
1Bpin-H	1.37	0.82	1.11	0.94	-	0.92
1Bpin-H‡	1.26	0.54	1.44	0.45	0.51	1.03
Products	0.97	-	2.03	-	0.99	0.97
1Bmida-H	1.39	0.79	1.11	0.93	-	0.90
1Bmida-H‡	1.29	0.49	1.45	0.45	0.50	1.03
Products	0.97	-	2.05	-	0.99	0.96

Table S10: *NRT bond orders for various boronic ester substituted sulfoxides in the boryl sulfenate elimination reaction.*

Compound	S-O	S-C_α	C_α-C_β	O-BR_2	C_β-BR_2
1BCat	1.32	0.79	1.15	0.04	0.94
1Bcat-B	1.26	0.85	1.12	0.78	0.89
1Bcat-B‡	1.17	0.47	1.53	0.99	0.56
Products	1.00	-	2.11	1.42	-
1BPin	1.36	0.82	1.09	-	0.94
1Bpin-B‡	1.20	0.49	1.56	0.92	0.55
Products	1.07	-	2.11	1.31	-
1Bmida	1.34	0.84	1.08	-	0.94
1Bmida-B	1.22	0.88	1.10	0.84	0.88
1Bmida-B‡	1.17	0.48	1.56	1.10	0.55
Products	1.04	-	2.11	1.17	-

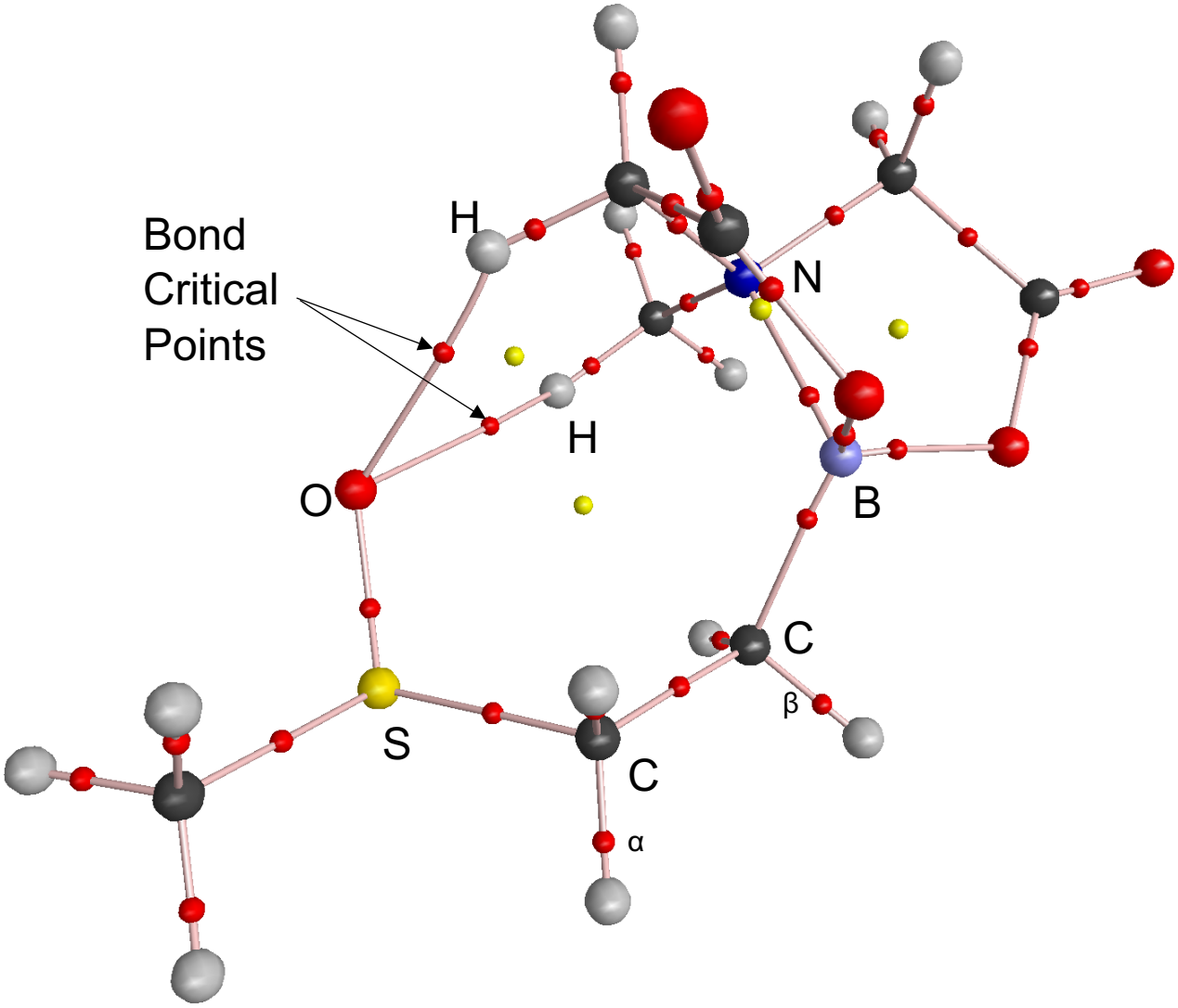


Figure S6*: Bond critical points within compound **1Bmida**, highlighting the interaction between the sulfinyl oxygen and hydrogens within the BMIDA group.*

4. Composite table of all thermodynamic parameters.

Table S11: *Composite table of all thermodynamic parameters.*

$\Delta G^{\ddagger}$ values represent free energy barrier for sulfenic acid elimination compared to the lowest energy conformation
$\Delta\Delta G^{\ddagger}$ values represent transition state free energy difference for the competing thermal eliminations. A positive values indicates boryl sulfenate elimination is preferred.

	Sulfenic acid eliminations								Boryl sulfenate eliminations					
	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta S^{\ddagger}$	ΔH	ΔG	ΔS	$\Delta G^{\ddagger}$	$\Delta\Delta G^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$	$\Delta S^{\ddagger}$	ΔH	ΔG	ΔS
1	34	34.3	-1	19.2	7.5	39								
1BH	17.4	18.5	-3.7	14.8	2.3	42	34.7	15.3	19.4	19.4	0	6.8	-6.9	45.8
1BF	32.3	24.4	-3.7	16	3.8	41	34.0	12.7	21.8	21.3	1.7	7.1	-7.6	49.3
1BC	22.3	23.3	-2.7	16.2	3.6	42.3	31.6	12.0	18.9	18.6	0.9	0.4	-14.2	49
1BO	27.3	28.1	-2.7	17.2	4.1	44.1	33.1	9.5	23.1	23.6	-1.7	2.6	-10.8	45
1Bcat	25.6	26.5	-3.1	16.6	4.4	41.0	28.5	6.7	23.5	24.5	-3.1	-1.3	-13.4	40.7
1Bpin	26.7	27.4	-2.5	7.2	4.9	41.3	28.2	3.7	22.3	21.8	1.6	2.2	11.3	45.4
1Bmida	27.3	27.5	-0.6	15	2.1	43.2	34.3	-4.6	40.5	38.9	5.4	-1.1	-13.6	41.9
2BH-B									16.9	16.8	0.3	4.3	-9.4	46.0
2BF-B									19.3	19.0	0.8	4.1	-9.5	45.9
2BC-B									16.4	16.3	0.6	-2.0	-16.6	48.9
2BO									20.9	21.1	-0.8	0.0	-13.6	45.7
3BH-B									17.8	17.0	2.7	7.1	-7.9	50.1
3BF-B									20.1	19.1	3.2	6.4	-8.2	48.8
3BC-B									16.5	16.0	1.7	-0.7	-15.4	49.6
3BO									18.7	18.7	-0.1	-1.1	-15.0	46.6
4BH-B									36.2	34.9	4.5	24.1	10.5	45.5
4BF-B									35	33.7	4.5	20.3	6.3	47
4BC-B									36.1	34.6	5	16.3	2.4	46.7
4BO									30.8	31.4	-2	15	3.1	39.8

5. Second order perturbation theory stabilization energies of donor and acceptor orbitals involved in proton and boryl transfer

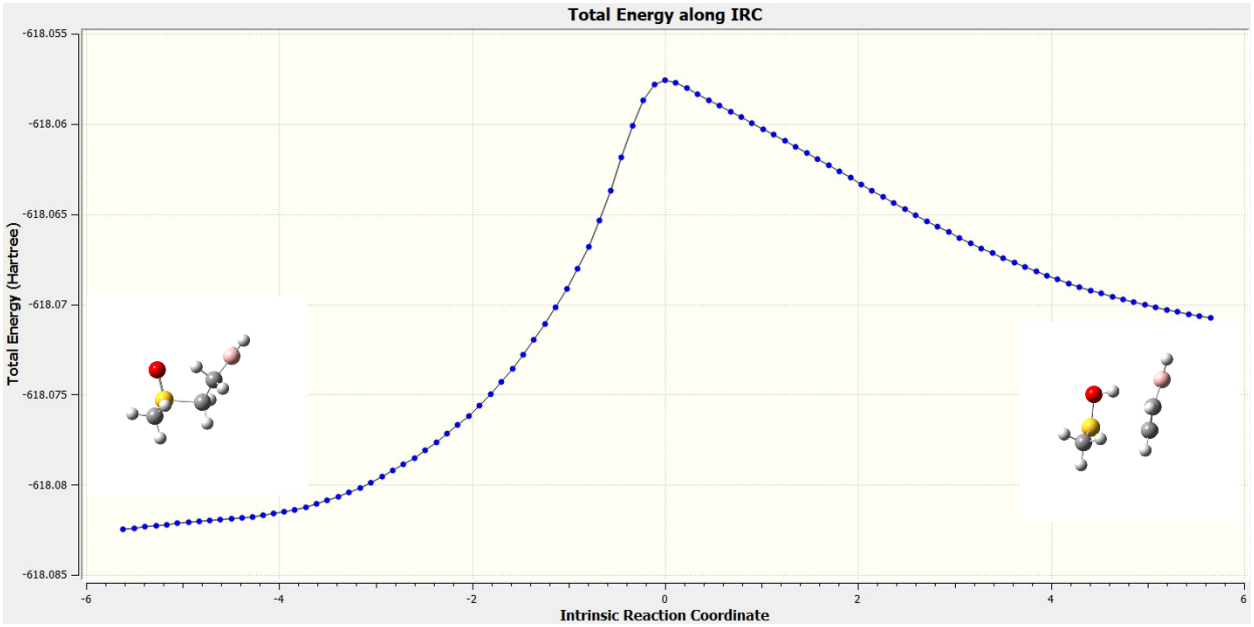
Table S12: *Second Order Perturbation Theory Stabilization Energies of Donor and Acceptor Orbitals Involved in Proton and Boryl Transfer*

Compound	Donor orbital	Acceptor orbital	Stabilization Energy (kcal/mol)	E(acceptor)-E(donor) (a.u.)	F(donor,acceptor) (a.u.)
1‡	LP (1) O 3	BD*(1) C 8- H 13	19.20	0.85	0.114
	LP (3) O 3	BD*(1) C 8- H 13	114.41	0.61	0.236
	LP (3) O 3	BD*(1) S 2- C 4	9.16	0.30	0.047
	BD (1) C 8- H 13	BD*(1) S 2- C 4	35.88	0.26	0.086
1BH-H	BD (1) C 8- H 12	LV (1) B 13	14.19	0.43	0.070
1BH-H	BD (1) C 8- H 12	LV (1) B 13	9.57	0.45	0.059
	LP (3) F 14	LV (1) B 13	47.50	0.41	0.124
	LP (3) F 15	LV (1) B 13	46.91	0.41	0.124
1BC-H	BD (1) C 8- H 12	LV (1) B 13	11.30	0.46	0.064
1BO-H	BD (1) C 8- H 12	LV (1) B 13	9.00	0.46	0.057
	LP (2) O 15	LV (1) B 13	59.24	0.33	0.125
	LP (2) O 14	LV (1) B 13	59.61	0.33	0.124
1BH-H‡	LP (1) O 3	BD*(1) C 8- H 12	17.47	0.77	0.104
	LP (3) O 3	BD*(1) C 8- H 12	140.81	0.59	0.257
	BD (1) C 8- H 12	LV (1) B 13	62.60	0.27	0.115
	BD (1) C 8- H 12	BD*(1) S 2- C 4	22.75	0.27	0.070
	LP (3) O 3	BD*(1) S 2- C 4	7.24	0.44	0.050
1BF-H‡	LP (1) C 8	BD*(1) S 2- C 4	100.52	0.11	0.090
	LP (1) C 8	BD*(1) O 3- H 12	132.67	0.34	0.188
	LP (1) C 8	BD*(2) B 13- F 14	4.39	0.52	0.043
1BC-H‡	LP (1) O 3	BD*(1) S 2- C 4	1.49	0.59	0.026
	LP (1) O 3	BD*(1) C 8- H 12	18.14	0.80	0.107
	LP (3) O 3	BD*(1) S 2- C 4	7.69	0.39	0.049
	LP (3) O 3	BD*(1) C 8- H 12	131.52	0.59	0.249
	BD (1) C 8- H 12	LV (1) B 13	46.57	0.31	0.107
	BD (1) C 8- H 12	BD*(1) S 2- C 4	28.81	0.25	0.076
1BO-H‡	LP (1) O 3	BD*(1) S 2- C 4	1.36	0.57	0.025
	LP (1) C 8	BD*(1) S 2- C 4	168.76	0.07	0.100
	LP (1) C 8	BD*(1) O 3- H 12	176.39	0.31	0.210
	LP (1) C 8	BD*(2) B 13- O 14	48.29	0.20	0.088
	LP (2) O 15	BD*(1) O 3- B 13	13.09	0.62	0.080
	LP (1) O 15	BD*(1) O 3- B 13	1.76	0.76	0.033
	LP (1) O 14	BD*(1) O 3- B 13	4.86	0.74	0.054
	LP (2) O 3	BD*(1) C 8- B 13	8.47	0.57	0.062

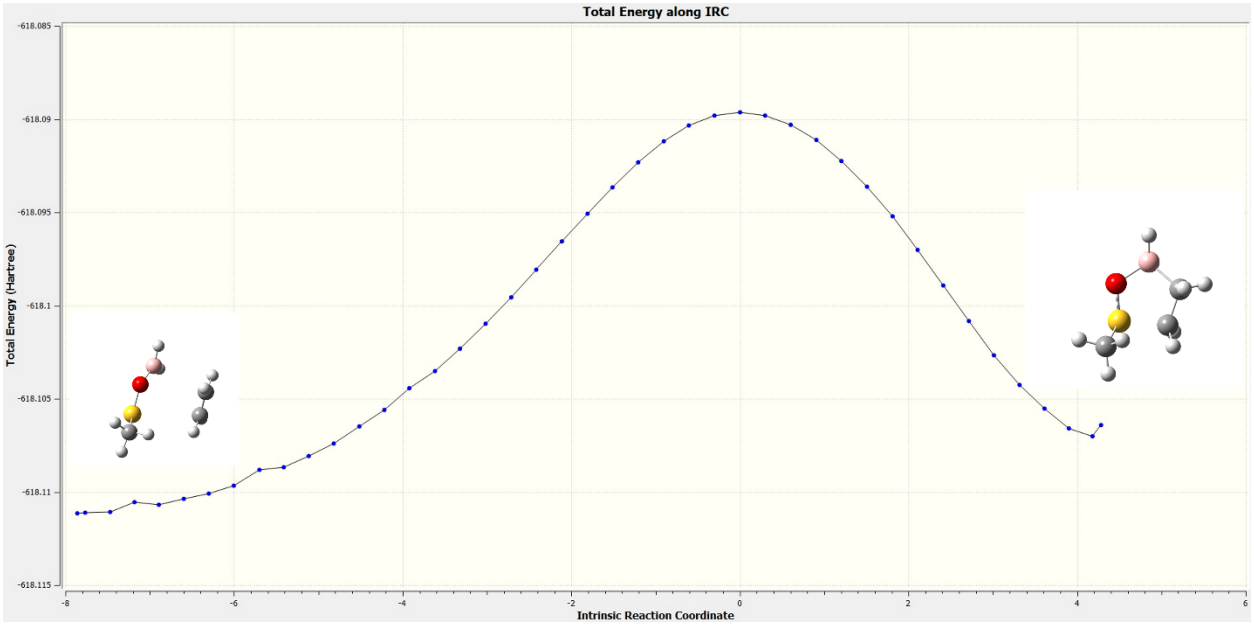
	LP (2) O 3	BD*(1) S 2- C 4	4.46	0.26	0.030
1BO-B‡	LP (2) O 14	BD*(1) C 8- B 13	18.85	0.51	0.088
	LP (1) O 15	BD*(1) C 8- B 13	4.29	0.65	0.047
	LP (2) O 3	BD*(1) S 2- C 4	3.83	0.25	0.028
	LP (1) C 8	LV (1) B 13	326.52	0.18	0.217
	LP (1) C 8	BD*(1) S 2- C 4	414.10	0.04	0.114
	LP (1) C 8	BD*(1) O 3- B 13	9.61	0.50	0.062
1BF-B‡	LP (2) F 14	BD*(1) O 3- B 13	10.09	0.74	0.077
	LP (3) F 14	BD*(1) O 3- B 13	3.14	0.74	0.043
	LP (2) F 15	BD*(1) O 3- B 13	11.66	0.74	0.083
	LP (3) F 15	LV (1) B 13	34.02	0.42	0.107
	LP (3) F 15	BD*(1) O 3- B 13	1.14	0.74	0.026
1Bcat-H	BD (1) C 8- H 12	LV (1) B 13	9.67	0.45	0.059
1Bpin-H	BD (1) C 8- H 12	LV (1) B 13	9.37	0.46	0.059
	BD (1) C 8- H 12	LV (1) B 13	36.64	0.30	0.093
1Bcat-H‡	BD (1) C 8- H 12	BD*(1) S 2- C 4	29.64	0.26	0.078
	LP (1) O 3	BD*(1) C 8- H 12	19.01	0.81	0.111
	LP (1) O 3	BD*(1) S 2- C 4	1.36	0.58	0.025
	LP (1) O 3	BD*(1) S 2- C 4	1.43	0.57	0.025
1Bpin-H‡	LP (1) C 8	BD*(1) S 2- C 4	153.97	0.08	0.099
	LP (1) C 8	BD*(1) O 3- H 12	166.82	0.32	0.206
1Bmida-H‡	BD (1) C 8- H 12	BD*(1) B 13- N 22	14.12	0.50	0.075

6. Sample Intrinsic Reaction Coordinates

1BH-H‡ IRC Pathway



1BH-B‡ IRC Pathway



7. Atomic Coordinates, Energies and Frequencies of Computed Species

Sulfenic Acid Elimination Starting Materials for Sulfoxide Family **1/1B**

1

C 1.8186630000 0.7975030000 0.8758680000
S 1.2099630000 -0.1395170000 -0.5627100000
O 1.0393950000 -1.5496830000 -0.1084750000
C -0.4748740000 0.5969170000 -0.6563330000
H 1.8172750000 1.8647890000 0.6511290000
H 2.8376180000 0.4566440000 1.0520550000
H 1.2033380000 0.5753350000 1.7462250000
C -1.3650570000 0.2434700000 0.5251170000
H -0.8757160000 0.1842320000 -1.5842230000
H -0.3453420000 1.6728630000 -0.7962250000
H -1.0722610000 0.7756240000 1.4303280000
H -1.3141420000 -0.8278390000 0.7227640000
H -2.4013130000 0.5058640000 0.3054500000
Zero-point correction= 0.107860 (Hartree/Particle)
Thermal correction to Energy= 0.114752
Thermal correction to Enthalpy= 0.115696
Thermal correction to Gibbs Free Energy= 0.077441
Sum of electronic and zero-point Energies= -592.538013
Sum of electronic and thermal Energies= -592.531121
Sum of electronic and thermal Enthalpies= -592.530177
Sum of electronic and thermal Free Energies= -592.568432
CBS-DLPNO-CCSD(T) Single Point Energy = -591.883142299323

1BH-H

C 1.8344740000 0.7973290000 0.8655040000
S 1.1920110000 -0.1537950000 -0.5480160000
O 0.9535550000 -1.5415200000 -0.0509550000
C -0.4712960000 0.6369080000 -0.6607920000
H 1.8983180000 1.8533690000 0.6003320000
H 2.8293100000 0.4054760000 1.0710560000
H 1.1943410000 0.6451900000 1.7330290000
C -1.3883320000 0.2721750000 0.4990960000
H -0.8687200000 0.2619310000 -1.6057240000
H -0.3153470000 1.7127990000 -0.7658440000
H -1.0974590000 0.7716820000 1.4259030000
H -1.2396950000 -0.8084070000 0.7124290000
B -2.9162570000 0.3169010000 0.2469560000

H -3.6740690000 0.3642020000 1.1672660000
H -3.3562810000 0.2371320000 -0.8608480000
Zero-point correction= 0.117838 (Hartree/Particle)
Thermal correction to Energy= 0.126221
Thermal correction to Enthalpy= 0.127166
Thermal correction to Gibbs Free Energy= 0.085272
Sum of electronic and zero-point Energies= -617.967915
Sum of electronic and thermal Energies= -617.959532
Sum of electronic and thermal Enthalpies= -617.958588
Sum of electronic and thermal Free Energies= -618.000482
CBS-DLPNO-CCSD(T) Single Point Energy = -617.253672166473

1BF-H
C 1.8111170000 0.8170390000 0.8636630000
S 1.2003290000 -0.1529870000 -0.5507510000
O 1.0097260000 -1.5478970000 -0.0571570000
C -0.4858210000 0.5859210000 -0.6617550000
H 1.8357310000 1.8756420000 0.6022960000
H 2.8203240000 0.4610320000 1.0642140000
H 1.1813490000 0.6378940000 1.7338030000
C -1.3825000000 0.1947330000 0.5071830000
H -0.8760330000 0.1950250000 -1.6024830000
H -0.3653040000 1.6654090000 -0.7735130000
H -1.1184080000 0.7293510000 1.4221010000
H -1.2066110000 -0.8685250000 0.7317390000
B -2.9134370000 0.3511250000 0.2451620000
F -3.7828400000 0.4057300000 1.2448290000
F -3.4203260000 0.4147450000 -0.9801120000
Zero-point correction= 0.107841 (Hartree/Particle)
Thermal correction to Energy= 0.117500
Thermal correction to Enthalpy= 0.118444
Thermal correction to Gibbs Free Energy= 0.071369
Sum of electronic and zero-point Energies= -816.709575
Sum of electronic and thermal Energies= -816.699916
Sum of electronic and thermal Enthalpies= -816.698972
Sum of electronic and thermal Free Energies= -816.746047
CBS-DLPNO-CCSD(T) Single Point Energy = -815.793129728549

1BC-H

C 1.7831100000 0.7466080000 0.9143940000
S 1.1990810000 -0.1512890000 -0.5579150000
O 0.9805180000 -1.5654280000 -0.1317090000
C -0.4730130000 0.6143170000 -0.6875680000
H 1.8193460000 1.8163750000 0.7044730000
H 2.7850840000 0.3748710000 1.1226250000
H 1.1290060000 0.5309910000 1.7576290000
C -1.4088610000 0.2471570000 0.4540790000
H -0.8390150000 0.2328920000 -1.6422760000
H -0.3243650000 1.6915250000 -0.7970780000
H -1.1237860000 0.7581590000 1.3788180000
H -1.2648390000 -0.8239580000 0.6798570000
B -2.9617570000 0.3773850000 0.2243580000
C -3.9077360000 0.3646270000 1.4768540000
H -3.4328240000 0.0622070000 2.4124360000
H -4.2765730000 1.3911020000 1.6173390000
H -4.8035960000 -0.2423210000 1.3164760000
C -3.5645800000 0.4895050000 -1.2231370000
H -3.1402580000 1.3421820000 -1.7653090000
H -3.2775060000 -0.3914090000 -1.8114260000
H -4.6521800000 0.5707050000 -1.2538860000
Zero-point correction= 0.174508 (Hartree/Particle)
Thermal correction to Energy= 0.186358
Thermal correction to Enthalpy= 0.187302
Thermal correction to Gibbs Free Energy= 0.135956
Sum of electronic and zero-point Energies= -696.611634
Sum of electronic and thermal Energies= -696.599784
Sum of electronic and thermal Enthalpies= -696.598840
Sum of electronic and thermal Free Energies= -696.650186
CBS-DLPNO-CCSD(T) Single Point Energy = -695.809247626510

1BO-H

C 1.7247330000 0.7798550000 0.8805910000
S 1.1325410000 -0.1225520000 -0.5861100000
O 0.9594400000 -1.5440600000 -0.1631090000
C -0.5516570000 0.6116190000 -0.6831280000
H 1.7300820000 1.8517600000 0.6785150000
H 2.7392740000 0.4315040000 1.0673990000
H 1.0912430000 0.5422640000 1.7336930000
C -1.4570800000 0.2491070000 0.4848350000
H -0.9467470000 0.2146210000 -1.6191020000
H -0.4193490000 1.6891750000 -0.8109160000
H -1.1774690000 0.7911110000 1.3904490000

H -1.3051500000 -0.8139540000 0.7154840000
B -3.0053010000 0.4513090000 0.2232330000
O -3.7731120000 0.6042110000 1.3421050000
O -3.4195990000 0.4323760000 -1.0779880000
C -5.1874840000 0.6479280000 1.4611870000
H -5.6648290000 -0.1963030000 0.9602660000
H -5.4232190000 0.5965930000 2.5237060000
H -5.5939700000 1.5793280000 1.0613290000
C -4.7257930000 0.5955610000 -1.6106510000
H -5.3628570000 -0.2588150000 -1.3738200000
H -5.2006020000 1.5093570000 -1.2488680000
H -4.6263830000 0.6622680000 -2.6936380000
Zero-point correction= 0.188006 (Hartree/Particle)
Thermal correction to Energy= 0.201774
Thermal correction to Enthalpy= 0.202718
Thermal correction to Gibbs Free Energy= 0.144929
Sum of electronic and zero-point Energies= -847.182082
Sum of electronic and thermal Energies= -847.168314
Sum of electronic and thermal Enthalpies= -847.167369
Sum of electronic and thermal Free Energies= -847.225159
CBS-DLPNO-CCSD(T) Single Point Energy = -846.214257925244

Transition States for Sulfenic Acid Elimination for Sulfoxide Family **1/1B**

1‡
C -1.6366080000 -0.8216500000 0.6055880000
S -0.7679340000 0.2439580000 -0.5780840000
O -0.1534510000 1.3715650000 0.3104170000
C 1.3787550000 -0.8979260000 -0.4254600000
H -2.4915600000 -0.2882970000 1.0189380000
H -0.9576030000 -1.1135000000 1.4062020000
H -1.9789350000 -1.7067810000 0.0654970000
C 2.0039410000 0.0019200000 0.4454070000
H 1.5900870000 -0.8779230000 -1.4861780000
H 0.9640450000 -1.8304590000 -0.0641320000
H 2.7944150000 0.6297930000 0.0457200000
H 2.1397570000 -0.2987080000 1.4797830000
H 0.9778220000 0.9159590000 0.5469720000
Zero-point correction= 0.101485 (Hartree/Particle)
Thermal correction to Energy= 0.108132
Thermal correction to Enthalpy= 0.109076
Thermal correction to Gibbs Free Energy= 0.071295
Sum of electronic and zero-point Energies= -592.492962

Sum of electronic and thermal Energies= -592.486315
Sum of electronic and thermal Enthalpies= -592.485371
Sum of electronic and thermal Free Energies= -592.523152
CBS-DLPNO-CCSD(T) Single Point Energy = -591.822266804104
Imaginary frequency: -1281.25 cm-1

1BH-H‡
C 1.9719770000 0.5418540000 0.7065060000
S 0.9828220000 -0.2937400000 -0.5554380000
O 0.2003680000 -1.3832900000 0.2379540000
C -0.5962400000 1.0389250000 -0.5912700000
H 2.4728400000 1.3879400000 0.2329790000
H 2.7092790000 -0.1611520000 1.0895520000
H 1.3186340000 0.8821260000 1.5085770000
C -1.4817490000 0.5524260000 0.4476040000
H -0.9455240000 0.9142990000 -1.6127480000
H -0.0955630000 1.9937620000 -0.4478490000
H -1.2923420000 0.9566050000 1.4405300000
H -0.7953480000 -0.7953150000 0.5227460000
B -2.7262970000 -0.2202380000 0.1594560000
H -3.4840930000 -0.5189650000 1.0344620000
H -2.9484240000 -0.5911720000 -0.9591800000
Zero-point correction= 0.113533 (Hartree/Particle)
Thermal correction to Energy= 0.121259
Thermal correction to Enthalpy= 0.122204
Thermal correction to Gibbs Free Energy= 0.081982
Sum of electronic and zero-point Energies= -617.944029
Sum of electronic and thermal Energies= -617.936303
Sum of electronic and thermal Enthalpies= -617.935359
Sum of electronic and thermal Free Energies= -617.975580
CBS-DLPNO-CCSD(T) Single Point Energy = -617.220945012162
Imaginary frequency: -935.99 cm-1

1BF-H‡
C -2.8655540000 0.7469770000 0.2675570000
S -1.7557330000 -0.5994860000 -0.2111540000
O -0.9067760000 0.0097320000 -1.3717000000
C -0.1903520000 -0.1851970000 1.2525930000
H -2.2812890000 1.6442510000 0.4681520000
H -3.4007470000 0.4331130000 1.1656800000
H -3.5715150000 0.9290620000 -0.5407250000
C 0.7093740000 0.6427170000 0.5116710000
H 0.1198940000 -1.2017310000 1.4691840000
H -0.7900230000 0.2520520000 2.0443230000

H 0.5977330000 1.7160910000 0.6350720000
H 0.0259340000 0.4360770000 -0.7783480000
B 2.0632080000 0.1164060000 0.0731790000
F 3.0325370000 0.9144770000 -0.3794560000
F 2.3462520000 -1.1926990000 0.0830010000
Zero-point correction= 0.102528 (Hartree/Particle)
Thermal correction to Energy= 0.111799
Thermal correction to Enthalpy= 0.112743
Thermal correction to Gibbs Free Energy= 0.067348
Sum of electronic and zero-point Energies= -816.678664
Sum of electronic and thermal Energies= -816.669394
Sum of electronic and thermal Enthalpies= -816.668450
Sum of electronic and thermal Free Energies= -816.713845
CBS-DLPNO-CCSD(T) Single Point Energy = -815.750257955567
Imaginary frequency: -1006.35 cm-1

1BC-H‡
C 2.0556900000 0.5622320000 0.7348460000
S 1.0755140000 -0.3361170000 -0.4932060000
O 0.2587020000 -1.3589070000 0.3553870000
C -0.6014890000 1.0647490000 -0.5649440000
H 2.5668600000 1.3787870000 0.2216170000
H 2.7855000000 -0.1167270000 1.1723990000
H 1.3941480000 0.9539500000 1.5066170000
C -1.4862730000 0.5221320000 0.4187750000
H -0.8644830000 0.9554940000 -1.6113750000
H -0.0833110000 1.9970520000 -0.3607800000
H -1.3795800000 0.9538580000 1.4136520000
H -0.7507080000 -0.7324270000 0.5733640000
B -2.7518260000 -0.2652140000 0.0961450000
C -3.7907660000 -0.5942620000 1.2405750000
H -3.8469780000 -1.6785120000 1.3958690000
H -3.5685330000 -0.1300760000 2.2040480000
H -4.8020350000 -0.2932690000 0.9440430000
C -3.0530430000 -0.8026040000 -1.3622300000
H -3.7771820000 -0.1301070000 -1.8402900000
H -2.1876680000 -0.8587080000 -2.0267830000
H -3.5274700000 -1.7877980000 -1.3458410000
Zero-point correction= 0.169425 (Hartree/Particle)
Thermal correction to Energy= 0.180963
Thermal correction to Enthalpy= 0.181907
Thermal correction to Gibbs Free Energy= 0.131662
Sum of electronic and zero-point Energies= -696.581634
Sum of electronic and thermal Energies= -696.570097

Sum of electronic and thermal Enthalpies= -696.569152
Sum of electronic and thermal Free Energies= -696.619398
CBS-DLPNO-CCSD(T) Single Point Energy = -695.768361047184
Imaginary frequency: -1097.17 cm-1

1BO-H‡
C 3.6874940000 -0.6696160000 0.0448860000
S 2.4518870000 0.6157820000 -0.2817290000
O 1.5086780000 -0.0340650000 -1.3416830000
C 0.9792640000 -0.0101540000 1.3934200000
H 4.3068380000 -0.3322480000 0.8783720000 246

H 4.3047600000 -0.8137090000 -0.8406210000
H 3.1829730000 -1.5996670000 0.3050160000
C 0.0869440000 -0.8098480000 0.6432310000
H 0.6729710000 0.9887500000 1.6785130000
H 1.7007540000 -0.4649960000 2.0630370000
H 0.2379870000 -1.8851510000 0.7031800000
H 0.6429140000 -0.5348220000 -0.6134480000
B -1.3373450000 -0.3073630000 0.2950070000
O -2.2087220000 -1.2297370000 -0.2254850000
O -1.6025640000 1.0251140000 0.5038140000
C -3.6141130000 -1.0909730000 -0.3477440000
H -3.8867130000 -0.5293880000 -1.2445280000
H -4.0362200000 -2.0929920000 -0.4269530000
H -4.0515060000 -0.5990560000 0.5247700000
C -2.5864880000 1.8070980000 -0.1530240000
H -2.2703380000 2.8488800000 -0.0940540000
H -2.6828430000 1.5353810000 -1.2069790000
H -3.5627780000 1.7137780000 0.3285480000
Zero-point correction= 0.182074 (Hartree/Particle)
Thermal correction to Energy= 0.195491
Thermal correction to Enthalpy= 0.196435
Thermal correction to Gibbs Free Energy= 0.141087
Sum of electronic and zero-point Energies= -847.146147
Sum of electronic and thermal Energies= -847.132730
Sum of electronic and thermal Enthalpies= -847.131786
Sum of electronic and thermal Free Energies= -847.187134
CBS-DLPNO-CCSD(T) Single Point Energy = -846.164554081751
Imaginary frequency: -1251.09 cm-1

Products of the Sulfenic Acid Elimination of Sulfoxide Family **1/1B**

Methane sulfenic acid
S -0.0752400000 -0.6276610000 -0.0679310000
C 1.3850750000 0.4317230000 -0.0213780000
H 1.3525500000 1.0904030000 0.8462760000
H 1.4933650000 1.0143140000 -0.9370250000
H 2.2398430000 -0.2426760000 0.0735250000
O -1.2967820000 0.5185580000 -0.0763390000
H -1.5047140000 0.7248400000 -0.9968370000
Zero-point correction= 0.051654 (Hartree/Particle)
Thermal correction to Energy= 0.056152
Thermal correction to Enthalpy= 0.057096
Thermal correction to Gibbs Free Energy= 0.025131
Sum of electronic and zero-point Energies= -513.937443
Sum of electronic and thermal Energies= -513.932945
Sum of electronic and thermal Enthalpies= -513.932001
Sum of electronic and thermal Free Energies= -513.963966
CBS-DLPNO-CCSD(T) Single Point Energy = -513.373425142364

Ethene
H 0.0000000000 0.9215270000 1.2326950000
C 0.0000000000 0.0000000000 0.6625340000
C 0.0000000000 0.0000000000 -0.6625340000
H 0.0000000000 -0.9215270000 1.2326950000
H 0.0000000000 0.9215270000 -1.2326950000
H 0.0000000000 -0.9215270000 -1.2326950000
Zero-point correction= 0.050944 (Hartree/Particle)
Thermal correction to Energy= 0.053980
Thermal correction to Enthalpy= 0.054925
Thermal correction to Gibbs Free Energy= 0.030082
Sum of electronic and zero-point Energies= -78.573649
Sum of electronic and thermal Energies= -78.570613
Sum of electronic and thermal Enthalpies= -78.569669
Sum of electronic and thermal Free Energies= -78.594512
CBS-DLPNO-CCSD(T) Single Point Energy = -78.475515953077

Vinylborane
C 0.4295240000 -0.2842550000 -0.1873420000
H 0.9419380000 -1.2408940000 -0.1873420000
H -0.6557550000 -0.3218130000 -0.1873420000
C 1.1192150000 0.8666590000 -0.1873420000
H 0.5496490000 1.7936230000 -0.1873420000
B 2.6558060000 0.8755310000 -0.1873420000
H 3.2777570000 1.8936280000 -0.1873420000
H 3.2409410000 -0.1660830000 -0.1873420000

Zero-point correction= 0.062658 (Hartree/Particle)
Thermal correction to Energy= 0.066811
Thermal correction to Enthalpy= 0.067755
Thermal correction to Gibbs Free Energy= 0.037763
Sum of electronic and zero-point Energies= -104.010936
Sum of electronic and thermal Energies= -104.006783
Sum of electronic and thermal Enthalpies= -104.005839
Sum of electronic and thermal Free Energies= -104.035830
CBS-DLPNO-CCSD(T) Single Point Energy = -103.854204758511

Vinyldifluoroborane
C 0.4317620000 -0.2877820000 -0.1873420000
H 0.9313520000 -1.2503820000 -0.1873420000
H -0.6523650000 -0.3074590000 -0.1873420000
C 1.1264120000 0.8519240000 -0.1873420000
H 0.5921040000 1.7972900000 -0.1873420000
B 2.6708670000 0.8681230000 -0.1873420000
F 3.3558800000 2.0055250000 -0.1873420000
F 3.3829800000 -0.2539490000 -0.1873420000
Zero-point correction= 0.052270 (Hartree/Particle)
Thermal correction to Energy= 0.057455
Thermal correction to Enthalpy= 0.058399
Thermal correction to Gibbs Free Energy= 0.023739
Sum of electronic and zero-point Energies= -302.750527
Sum of electronic and thermal Energies= -302.745343
Sum of electronic and thermal Enthalpies= -302.744398
Sum of electronic and thermal Free Energies= -302.779058
CBS-DLPNO-CCSD(T) Single Point Energy = -302.391298549709

Dimethyl vinylborane
C 0.3536100000 -0.2603420000 -0.2989260000
H 0.7864310000 -1.2521920000 -0.3720830000
H -0.7309130000 -0.2172370000 -0.3158370000
C 1.1162940000 0.8328670000 -0.1929460000
H 0.5950350000 1.7877670000 -0.1231820000
B 2.6759410000 0.8318070000 -0.1545420000
C 3.4152150000 2.2170020000 -0.0553560000
H 3.3869280000 2.6757280000 -1.0547330000
H 2.9050620000 2.9263310000 0.6031890000
H 4.4662260000 2.1542810000 0.2336260000
C 3.5272980000 -0.4874600000 -0.2274380000
H 4.0256300000 -0.6274170000 0.7408050000
H 2.9836530000 -1.4054930000 -0.4533590000
H 4.3418110000 -0.3812510000 -0.9520070000

Zero-point correction= 0.119020 (Hartree/Particle)
Thermal correction to Energy= 0.126530
Thermal correction to Enthalpy= 0.127475
Thermal correction to Gibbs Free Energy= 0.087436
Sum of electronic and zero-point Energies= -182.652262
Sum of electronic and thermal Energies= -182.644752
Sum of electronic and thermal Enthalpies= -182.643807
Sum of electronic and thermal Free Energies= -182.683846
CBS-DLPNO-CCSD(T) Single Point Energy = -182.407260208567

Dimethyl vinylboronate
C 0.2495460000 -0.3644410000 -0.5227850000
H 0.8210960000 -1.2151460000 -0.8780030000
H -0.8308430000 -0.4570860000 -0.5592090000
C 0.8604480000 0.7292140000 -0.0668740000
H 0.2486860000 1.5586650000 0.2796820000
B 2.4134010000 0.8950940000 0.0033930000
O 2.8535780000 2.1048980000 0.4679360000
O 3.1727220000 -0.1693090000 -0.3970120000
C 4.1771590000 2.5017780000 0.7879430000
H 4.8001000000 2.5930510000 -0.1043180000
H 4.1152090000 3.4788000000 1.2666610000
H 4.6499820000 1.8052750000 1.4839830000
C 4.5713250000 -0.2347500000 -0.6162140000
H 5.1318640000 -0.1790280000 0.3194260000
H 4.7811250000 -1.1953420000 -1.0864690000
H 4.9132400000 0.5584140000 -1.2851150000
Zero-point correction= 0.132189 (Hartree/Particle)
Thermal correction to Energy= 0.141457
Thermal correction to Enthalpy= 0.142402
Thermal correction to Gibbs Free Energy= 0.096766
Sum of electronic and zero-point Energies= -333.221213
Sum of electronic and thermal Energies= -333.211944
Sum of electronic and thermal Enthalpies= -333.211000
Sum of electronic and thermal Free Energies= -333.256636
CBS-DLPNO-CCSD(T) Single Point Energy = -332.810157319290

Starting Sulfoxides for Boryl Sulfenate Elimination from Sulfoxide Family **1B**

1BO

H	3.4231790000	-1.2254830000	-1.4732370000
C	2.8584820000	-1.2559780000	-0.5426860000
H	1.9188740000	-1.7907550000	-0.6738300000
S	2.4730470000	0.4626080000	-0.0958380000
H	3.4625120000	-1.7039630000	0.2477350000
O	1.5130420000	0.9579900000	-1.1385700000
C	1.4451270000	0.0943000000	1.4218030000
C	0.0517490000	0.6873270000	1.2267900000
H	0.1082750000	1.7762100000	1.1999060000
H	-0.5426990000	0.4293920000	2.1114090000
H	1.9820090000	0.5344460000	2.2632530000
H	1.3960670000	-0.9855340000	1.5545890000
B	-0.6843360000	0.1104260000	-0.0590280000
O	-0.5509070000	-1.2372080000	-0.2750070000
C	-1.1311960000	-1.8389380000	-1.4289760000
H	-0.7246350000	-1.3948410000	-2.3403470000
H	-0.8897180000	-2.9014100000	-1.4011950000
H	-2.2159610000	-1.7150140000	-1.4365040000
O	-1.5391890000	0.8064390000	-0.8602160000
C	-1.5907570000	2.2255790000	-0.8659620000
H	-2.2830970000	2.5261450000	-1.6517850000
H	-1.9547430000	2.6170190000	0.0886700000
H	-0.6033660000	2.6414670000	-1.0772870000

Zero-point correction= 0.188681 (Hartree/Particle)
Thermal correction to Energy= 0.201854
Thermal correction to Enthalpy= 0.202798
Thermal correction to Gibbs Free Energy= 0.148887
Sum of electronic and zero-point Energies= -847.191814
Sum of electronic and thermal Energies= -847.178641
Sum of electronic and thermal Enthalpies= -847.177697
Sum of electronic and thermal Free Energies= -847.231608
CBS-DLPNO-CCSD(T) Single Point Energy = -846.2250225713010

1BO-B

C -1.9879170000 -0.4518890000 1.6536740000
S -1.8321690000 0.9415760000 0.5113480000
O -0.3244150000 1.2227710000 0.4064960000
C -2.0531180000 0.0664340000 -1.0898480000
H -1.7760950000 -0.0714890000 2.6513080000
H -1.2570080000 -1.2107690000 1.3818540000
H -3.0126290000 -0.8212910000 1.6016450000
C -0.7218850000 -0.6270760000 -1.3632310000
H -2.2619310000 0.8701520000 -1.7965220000

H -2.9352550000 -0.5710810000 -1.0146200000
H -0.4888920000 -0.5438350000 -2.4246220000
H -0.8028960000 -1.6883150000 -1.1212100000
B 0.4962030000 0.0596100000 -0.4821390000
O 1.0225500000 -0.7705800000 0.5744100000
O 1.4218640000 0.7455910000 -1.2965930000
C 2.4763400000 1.4549730000 -0.6766540000
H 3.1990050000 1.7341190000 -1.4456840000
H 2.1071530000 2.3677630000 -0.1953820000
H 2.9847720000 0.8550360000 0.0854190000
C 1.8622180000 -1.8301710000 0.1792800000
H 1.3288220000 -2.5737210000 -0.4312860000
H 2.7217080000 -1.4809780000 -0.4050920000
H 2.2332880000 -2.3308890000 1.0759650000
Zero-point correction= 0.187989 (Hartree/Particle)
Thermal correction to Energy= 0.200646
Thermal correction to Enthalpy= 0.201590
Thermal correction to Gibbs Free Energy= 0.149495
Sum of electronic and zero-point Energies= -847.180826
Sum of electronic and thermal Energies= -847.168169
Sum of electronic and thermal Enthalpies= -847.167224
Sum of electronic and thermal Free Energies= -847.219320
CBS-DLPNO-CCSD(T) Single Point Energy = -846.218000263779

1BF-B
C -1.9821640000 -1.3577080000 0.3416250000
S -1.2189330000 -0.4590200000 -1.0291240000
O -0.6227970000 0.8202400000 -0.4056110000
C 0.3441260000 -1.4184360000 -1.2073270000
H -2.8433650000 -0.7749110000 0.6634330000
H -1.2692160000 -1.4544810000 1.1574950000
H -2.3057240000 -2.3282770000 -0.0360940000
C 1.2605490000 -0.8981010000 -0.1027360000
H 0.6936510000 -1.1681680000 -2.2089920000
H 0.0957130000 -2.4797360000 -1.1787370000
H 2.2600590000 -0.7424550000 -0.5082470000
H 1.3359830000 -1.6310290000 0.7008350000
B 0.6960080000 0.5220070000 0.5131600000
F 0.2156230000 0.3915110000 1.8089330000
F 1.4985400000 1.6162170000 0.3485980000
Zero-point correction= 0.108559 (Hartree/Particle)
Thermal correction to Energy= 0.117205
Thermal correction to Enthalpy= 0.118149
Thermal correction to Gibbs Free Energy= 0.074977

Sum of electronic and zero-point Energies= -816.723909
Sum of electronic and thermal Energies= -816.715263
Sum of electronic and thermal Enthalpies= -816.714319
Sum of electronic and thermal Free Energies= -816.757491
CBS-DLPNO-CCSD(T) Single Point Energy = -815.812168821988

1BH-B
C -1.5523300000 -0.9525020000 0.4709310000
S -0.8140440000 0.0627280000 -0.8328230000
O -0.2511550000 1.3079790000 -0.1240990000
C 0.7628020000 -0.8381960000 -1.0675510000
H -2.4352440000 -0.4231540000 0.8246530000
H -0.8376550000 -1.0807880000 1.2805240000
H -1.8400770000 -1.9101190000 0.0359960000
C 1.6060890000 -0.4597710000 0.1506830000
H 1.1572260000 -0.4316560000 -1.9997570000
H 0.5432750000 -1.8979620000 -1.2093240000
H 2.6544960000 -0.4398290000 -0.1527880000
H 1.5104920000 -1.2369510000 0.9116300000
B 1.1321430000 1.0233230000 0.7083910000
H 0.8273520000 1.0192130000 1.8777150000
H 1.8489450000 1.9384300000 0.3919430000
Zero-point correction= 0.120539 (Hartree/Particle)
Thermal correction to Energy= 0.127796
Thermal correction to Enthalpy= 0.128740
Thermal correction to Gibbs Free Energy= 0.089045
Sum of electronic and zero-point Energies= -617.991236
Sum of electronic and thermal Energies= -617.983978
Sum of electronic and thermal Enthalpies= -617.983034
Sum of electronic and thermal Free Energies= -618.022730
CBS-DLPNO-CCSD(T) Single Point Energy = -617.283622778840

1BC-B
C -1.7922600000 -1.4913820000 0.6296800000
S -1.2960410000 -0.4686250000 -0.7801040000
O -0.7545160000 0.8343790000 -0.1772620000
C 0.2952900000 -1.2761240000 -1.1979640000
H -2.6401990000 -0.9939660000 1.0971700000
H -0.9679230000 -1.5755870000 1.3335730000
H -2.0951500000 -2.4689260000 0.2525580000
C 1.2685940000 -0.7721230000 -0.1378970000
H 0.5319630000 -0.8996300000 -2.1939760000
H 0.1332050000 -2.3541880000 -1.2569990000
H 2.2799340000 -0.8193600000 -0.5491930000

H 1.2485500000 -1.4383880000 0.7287800000
B 0.8978500000 0.7847420000 0.2571370000
C 0.9405070000 1.1043050000 1.8283350000
H 1.9739030000 1.0674200000 2.1918130000
H 0.5596050000 2.1033990000 2.0598870000
H 0.3691150000 0.3875850000 2.4296870000
C 1.5689660000 1.8861060000 -0.6992280000
H 1.4885700000 1.6425910000 -1.7655070000
H 1.1221570000 2.8748340000 -0.5592700000
H 2.6370660000 1.9840970000 -0.4749830000
Zero-point correction= 0.176204 (Hartree/Particle)
Thermal correction to Energy= 0.186786
Thermal correction to Enthalpy= 0.187730
Thermal correction to Gibbs Free Energy= 0.141308
Sum of electronic and zero-point Energies= -696.624157
Sum of electronic and thermal Energies= -696.613575
Sum of electronic and thermal Enthalpies= -696.612631
Sum of electronic and thermal Free Energies= -696.659054
CBS-DLPNO-CCSD(T) Single Point Energy = -695.828328396497

Syn Transition States Boryl Sulfenate Elimination for Sulfoxide Family **1B**

Syn-1BO-B‡
O 0.2347990000 2.0489450000 2.2098350000
C -1.4597260000 1.6275030000 -0.0731280000
C -0.2819410000 0.8954220000 -0.1458580000
H -1.5840330000 2.5272060000 -0.6631570000
H -2.3760670000 1.1909030000 0.2983710000
H 0.3614290000 1.0915650000 -0.9976840000
H -0.3131280000 -0.1352670000 0.1883210000
B 1.0349000000 1.6807180000 1.0219850000
O 1.9309540000 0.6739170000 1.3927090000
O 1.5033820000 2.7762060000 0.2385440000
C 2.5329230000 3.5672270000 0.8080140000
H 2.8646930000 4.2854790000 0.0568820000
H 2.1771930000 4.1179380000 1.6869270000
H 3.3904640000 2.9618830000 1.1191280000
C 2.8496320000 0.1744370000 0.4464010000
H 2.3562530000 -0.5109660000 -0.2544740000
H 3.3222440000 0.9709490000 -0.1370280000
H 3.6223110000 -0.3799130000 0.9805350000
S -1.1591730000 2.7999040000 2.0808040000
C -0.7875600000 4.4613190000 1.4686560000

H -0.1946240000 5.0040870000 2.2039860000
H -0.2669290000 4.4134560000 0.5160180000
H -1.7575940000 4.9508180000 1.3563250000
Zero-point correction= 0.185579 (Hartree/Particle)
Thermal correction to Energy= 0.198566
Thermal correction to Enthalpy= 0.199510
Thermal correction to Gibbs Free Energy= 0.146663
Sum of electronic and zero-point Energies= -847.161793
Sum of electronic and thermal Energies= -847.148805
Sum of electronic and thermal Enthalpies= -847.147861
Sum of electronic and thermal Free Energies= -847.200709
CBS-DLPNO-CCSD(T) Single Point Energy = -846.184338820186
Imaginary frequency: -378.57 cm-1

Syn-1BF-B‡
O -0.7209900000 0.9618000000 1.1534100000
C 1.0728500000 -0.4719100000 -0.6098800000
C 1.7282600000 0.1729400000 0.4220200000
H 1.0755100000 -0.0623400000 -1.6122500000
H 0.7569800000 -1.5018800000 -0.5290800000
H 2.4626300000 0.9258600000 0.1532300000
H 1.9450200000 -0.3925600000 1.3207100000
B 0.5846000000 1.5852000000 1.0854200000
F 1.0743800000 1.8971800000 2.3051700000
F 0.7039600000 2.5745800000 0.1419800000
S -1.3414000000 0.1890800000 -0.1052800000
C -1.6428400000 1.4605900000 -1.3545300000
H -2.3535100000 2.1910500000 -0.9705000000
H -0.7217200000 1.9524200000 -1.6546300000
H -2.0879500000 0.9292900000 -2.1987800000
Zero-point correction= 0.105852 (Hartree/Particle)
Thermal correction to Energy= 0.114949
Thermal correction to Enthalpy= 0.115893
Thermal correction to Gibbs Free Energy= 0.071871
Sum of electronic and zero-point Energies= -816.702808
Sum of electronic and thermal Energies= -816.693711
Sum of electronic and thermal Enthalpies= -816.692766
Sum of electronic and thermal Free Energies= -816.736788
CBS-DLPNO-CCSD(T) Single Point Energy = -815.775820896996
Imaginary frequency: -364.35 cm-1

Syn-1BH-B‡
O -0.5514020000 1.0698420000 1.3002350000
C 0.8820370000 -0.5487550000 -0.5812720000

C 1.7087310000 0.1024640000 0.3249380000
H 0.8055680000 -0.2071170000 -1.6063980000
H 0.5170570000 -1.5494300000 -0.3995740000
H 2.4727660000 0.7548960000 -0.0865290000
H 1.9996910000 -0.4476730000 1.2121930000
B 0.7696450000 1.6191870000 1.0171890000
H 1.3554380000 1.9052160000 2.0218490000
H 0.8143530000 2.4090360000 0.1100530000
S -1.3685280000 0.3442680000 0.1408440000
C -1.5908020000 1.5699700000 -1.1701090000
H -2.2132520000 1.0768480000 -1.9196550000
H -2.1205100000 2.4348180000 -0.7713640000
H -0.6465280000 1.8772390000 -1.6111600000
Zero-point correction= 0.118133 (Hartree/Particle)
Thermal correction to Energy= 0.125643
Thermal correction to Enthalpy= 0.126587
Thermal correction to Gibbs Free Energy= 0.086744
Sum of electronic and zero-point Energies= -617.972275
Sum of electronic and thermal Energies= -617.964764
Sum of electronic and thermal Enthalpies= -617.963820
Sum of electronic and thermal Free Energies= -618.003664
CBS-DLPNO-CCSD(T) Single Point Energy = -617.250441926999
Imaginary frequency: -331.54 cm-1

Syn-1BC-B‡
O -0.4559450000 1.3335920000 1.1067180000
C 0.7870520000 -0.6847580000 -0.4811570000
C 1.6991920000 0.0011260000 0.3174750000
H 0.7208460000 -0.4813390000 -1.5434500000
H 0.3732210000 -1.6355510000 -0.1756340000
H 2.5118240000 0.5028300000 -0.1970200000
H 1.9742350000 -0.4687520000 1.2549770000
B 0.9645580000 1.7119600000 0.8827850000
C 1.6560040000 2.0569690000 2.2775610000
H 2.7452050000 2.0964050000 2.1856640000
H 1.3343840000 3.0444950000 2.6270980000
H 1.4082710000 1.3367880000 3.0616800000
C 1.2423030000 2.7390320000 -0.3229540000
H 1.0460130000 2.3511880000 -1.3248730000
H 0.6308930000 3.6393870000 -0.1976010000
H 2.2860380000 3.0653720000 -0.3100940000
S -1.3119160000 0.4292950000 0.1362290000
C -1.6657980000 1.3960950000 -1.3553550000
H -2.4148810000 0.8156830000 -1.8983160000

H -2.0969070000 2.3537700000 -1.0664320000
H -0.7897020000 1.5488320000 -1.9787740000
Zero-point correction= 0.173878 (Hartree/Particle)
Thermal correction to Energy= 0.184842
Thermal correction to Enthalpy= 0.185786
Thermal correction to Gibbs Free Energy= 0.138384
Sum of electronic and zero-point Energies= -696.602198
Sum of electronic and thermal Energies= -696.591234
Sum of electronic and thermal Enthalpies= -696.590290
Sum of electronic and thermal Free Energies= -696.637691
CBS-DLPNO-CCSD(T) Single Point Energy = -695.792277783085
Imaginary frequency: -379.52 cm-1

Anti Transition States of Boryl Sulfenate Elimination for Sulfoxide Family **1B**

1BC-B‡
C -2.0311330000 -0.7122870000 0.5540000000
S -1.0405460000 0.5390260000 -0.2777960000
O -0.3867790000 1.2552560000 0.9831840000
C 1.0258030000 -0.6863950000 -0.5068750000
H -2.8089220000 -0.2281490000 1.1426810000
H -1.3989640000 -1.3241720000 1.1966860000
H -2.4897320000 -1.3271270000 -0.2225210000
C 1.8018930000 -0.0559930000 0.4740680000
H 1.2005540000 -0.4832370000 -1.5557440000
H 0.5138600000 -1.6199850000 -0.3090610000
H 2.7429160000 0.3657550000 0.1346220000
H 1.8574740000 -0.5504710000 1.4378640000
B 1.0506690000 1.6441880000 0.8705500000
C 1.6030440000 2.1006130000 2.2952640000
H 2.6945060000 2.1732910000 2.2953580000
H 1.2209700000 3.0934840000 2.5559420000
H 1.3131740000 1.4176600000 3.0987180000
C 1.3846530000 2.5912140000 -0.3834450000
H 1.0939890000 2.1832800000 -1.3580110000
H 0.8587790000 3.5459310000 -0.2716610000
H 2.4523950000 2.8203940000 -0.4376760000
Zero-point correction= 0.173990 (Hartree/Particle)
Thermal correction to Energy= 0.184801
Thermal correction to Enthalpy= 0.185745
Thermal correction to Gibbs Free Energy= 0.138916
Sum of electronic and zero-point Energies= -696.604369
Sum of electronic and thermal Energies= -696.593558

Sum of electronic and thermal Enthalpies= -696.592614
Sum of electronic and thermal Free Energies= -696.639442
CBS-DLPNO-CCSD(T) Single Point Energy = -695.796276433559
Imaginary frequency: -369.39 cm-1

1BH-B‡

C -2.0936650000 -0.6434070000 0.5195870000
S -1.0563960000 0.6262060000 -0.2208110000
O -0.3761400000 1.2275960000 1.0975660000
C 1.0724180000 -0.6234060000 -0.5107140000
H -2.8345790000 -0.1775610000 1.1678880000
H -1.4851280000 -1.3459780000 1.0883280000
H -2.5986200000 -1.1596010000 -0.2987840000
C 1.8211580000 -0.0544920000 0.5198430000
H 1.2473920000 -0.3354770000 -1.5393710000
H 0.5300200000 -1.5506850000 -0.3780700000
H 2.7586960000 0.4133610000 0.2324410000
H 1.8535800000 -0.5930380000 1.4604840000
B 1.0330580000 1.5973360000 0.9195620000
H 1.5192020000 1.9695420000 1.9494530000
H 1.2580360000 2.2486390000 -0.0723300000
Zero-point correction= 0.118075 (Hartree/Particle)
Thermal correction to Energy= 0.125546
Thermal correction to Enthalpy= 0.126490
Thermal correction to Gibbs Free Energy= 0.086774
Sum of electronic and zero-point Energies= -617.971557
Sum of electronic and thermal Energies= -617.964086
Sum of electronic and thermal Enthalpies= -617.963141
Sum of electronic and thermal Free Energies= -618.002858
CBS-DLPNO-CCSD(T) Single Point Energy = -617.250396066158
Imaginary frequency: -317.70 cm-1

1BF-B‡

C -2.0557000000 -0.6389400000 0.5382350000
S -1.0836160000 0.6364360000 -0.2789740000
O -0.3937510000 1.3092790000 1.0054440000
C 1.0714990000 -0.6347510000 -0.5255000000
H -2.7971780000 -0.1748330000 1.1867620000
H -1.4100150000 -1.2982050000 1.1173250000
H -2.5601940000 -1.2024270000 -0.2489140000
C 1.7907910000 -0.0872620000 0.5279040000
H 1.2689350000 -0.3280900000 -1.5440620000
H 0.5062700000 -1.5508360000 -0.4176460000
H 2.7311140000 0.3959430000 0.2775910000

H 1.7806120000 -0.6094220000 1.4776840000
B 1.0282830000 1.6052280000 0.9105790000
F 1.5451130000 2.0038310000 2.0966660000
F 1.3677500000 2.3803380000 -0.1690740000
Zero-point correction= 0.105811 (Hartree/Particle)
Thermal correction to Energy= 0.114879
Thermal correction to Enthalpy= 0.115823
Thermal correction to Gibbs Free Energy= 0.071834
Sum of electronic and zero-point Energies= -816.701168
Sum of electronic and thermal Energies= -816.692100
Sum of electronic and thermal Enthalpies= -816.691156
Sum of electronic and thermal Free Energies= -816.735145
CBS-DLPNO-CCSD(T) Single Point Energy = -815.775126129689
Imaginary frequency: -351.08 cm-1

1BO-B‡
C -2.2972130000 2.3026880000 2.6951710000
S -1.0300580000 3.0068900000 1.6271470000
O 0.2112540000 2.0918730000 2.0355390000
C -1.3352750000 1.5592170000 -0.3015880000
H -2.0298800000 2.4667450000 3.7379520000
H -2.4027130000 1.2361570000 2.4989090000
H -3.2303920000 2.8224560000 2.4699270000
C -0.2555640000 0.6907190000 -0.1332290000
H -1.2888430000 2.3384610000 -1.0505260000
H -2.3317680000 1.3020770000 0.0350680000
H 0.4331750000 0.6254380000 -0.9716050000
H -0.4408040000 -0.2463870000 0.3794850000
B 1.0314880000 1.5787090000 0.9058660000
O 1.9412280000 0.6459090000 1.4198190000
O 1.4873950000 2.5891620000 0.0078580000
C 2.3919480000 3.5446140000 0.5350620000
H 2.6806430000 4.2191220000 -0.2720890000
H 1.9339490000 4.1346820000 1.3375730000
H 3.2944800000 3.0719660000 0.9387940000
C 2.9293290000 0.1074150000 0.5703280000
H 2.4990170000 -0.6313660000 -0.1185850000
H 3.4259880000 0.8771970000 -0.0286720000
H 3.6733830000 -0.3960680000 1.1890620000
Zero-point correction= 0.185405 (Hartree/Particle)
Thermal correction to Energy= 0.198447
Thermal correction to Enthalpy=0.199391
Thermal correction to Gibbs Free Energy= 0.146270
Sum of electronic and zero-point Energies= -847.160681

Sum of electronic and thermal Energies= -847.147639
Sum of electronic and thermal Enthalpies= -847.146695
Sum of electronic and thermal Free Energies= -847.199815
CBS-DLPNO-CCSD(T) Single Point Energy = -846.184769061878
Imaginary Frequency: -359.83 cm-1

Products of Boryl Sulfenate Elimination for Sulfoxide Family **1B**

$MeSOBH_2$
C -1.4285000000 -0.3577840000 -0.0500820000
H -1.4884050000 -1.4479610000 -0.0195540000
H -0.6175000000 -0.0243310000 0.5964520000
H -2.3783530000 0.0634950000 0.2773700000
S -1.0971240000 0.0555450000 -1.7648230000
O -1.0504890000 1.7397120000 -1.5568700000
B -0.8241790000 2.5752870000 -2.5931570000
H -0.6474050000 2.1616910000 -3.7010110000
H -0.8149170000 3.7363320000 -2.3200790000
Zero-point correction= 0.063459 (Hartree/Particle)
Thermal correction to Energy= 0.069388
Thermal correction to Enthalpy= 0.070333
Thermal correction to Gibbs Free Energy= 0.033735
Sum of electronic and zero-point Energies= -539.419159
Sum of electronic and thermal Energies= -539.413230
Sum of electronic and thermal Enthalpies= -539.412286
Sum of electronic and thermal Free Energies= -539.448883
CBS-DLPNO-CCSD(T) Single Point Energy = -538.793812788908

$MeSOBF_2$
C -1.3968610000 -0.3600160000 -0.0602530000
H -1.4787620000 -1.4489710000 -0.0325470000
H -0.5521550000 -0.0465730000 0.5519270000
H -2.3233910000 0.0804080000 0.3059560000
S -1.1278430000 0.0479960000 -1.7860570000
O -1.0372850000 1.7289660000 -1.5616160000
B -0.8434950000 2.5795570000 -2.5912300000
F -0.7845610000 3.8784010000 -2.3364210000
F -0.7087020000 2.1743830000 -3.8498340000
Zero-point correction= 0.052378 (Hartree/Particle)
Thermal correction to Energy= 0.059567
Thermal correction to Enthalpy= 0.060511
Thermal correction to Gibbs Free Energy= 0.018772
Sum of electronic and zero-point Energies= -738.149764
Sum of electronic and thermal Energies= -738.142576

Sum of electronic and thermal Enthalpies= -738.141632
Sum of electronic and thermal Free Energies= -738.183371
CBS-DLPNO-CCSD(T) Single Point Energy = -737.322684517995

MeSOBMe$_2$
C -1.4791810000 -0.1391670000 0.0618700000
H -0.9915360000 -0.5937480000 0.9267890000
H -2.3526400000 0.4214050000 0.3936620000
H -1.7719260000 -0.9204320000 -0.6389760000
S -0.2564130000 0.9529300000 -0.6695760000
O -1.2316260000 1.5042400000 -1.9340480000
B -0.8006230000 2.4085030000 -2.8704950000
C 0.6562080000 3.0029180000 -2.8284910000
H 0.8386230000 3.5171370000 -1.8780170000
H 1.4038450000 2.2035050000 -2.8836460000
H 0.8538990000 3.7071580000 -3.6371340000
C -1.8598120000 2.7945720000 -3.9667560000
H -2.0329210000 3.8763110000 -3.9591380000
H -1.4700510000 2.5651560000 -4.9645810000
H -2.8181570000 2.2888200000 -3.8437880000
Zero-point correction= 0.119757 (Hartree/Particle)
Thermal correction to Energy= 0.128991
Thermal correction to Enthalpy= 0.129935
Thermal correction to Gibbs Free Energy= 0.085082
Sum of electronic and zero-point Energies= -618.062763
Sum of electronic and thermal Energies= -618.053529
Sum of electronic and thermal Enthalpies= -618.052585
Sum of electronic and thermal Free Energies= -618.097438
CBS-DLPNO-CCSD(T) Single Point Energy = -617.349298515391

MeSOB(OMe)$_2$
C -1.2317170000 -0.3401880000 -0.1913150000
H -0.5870570000 -0.8996970000 0.4901770000
H -2.0077010000 0.1679620000 0.3809680000
H -1.6797270000 -1.0277440000 -0.9085340000
S -0.1592960000 0.8402150000 -1.0167280000
O -1.3579330000 1.5197740000 -1.9865760000
B -1.1397490000 2.6972060000 -2.6620770000
O 0.1293320000 3.2065250000 -2.6841840000
O -2.2534320000 3.2242300000 -3.2518990000
C -2.2456730000 4.0934710000 -4.3730490000
H -1.4273010000 3.8653950000 -5.0608040000
H -3.1893920000 3.9560210000 -4.9005840000
H -2.1687550000 5.1389540000 -4.0649390000

C 0.4783970000 4.5555590000 -2.9526350000
H 1.4298050000 4.7508940000 -2.4587460000
H 0.5990350000 4.7272670000 -4.0245050000
H -0.2673670000 5.2516800000 -2.5616930000
Zero-point correction= 0.132438 (Hartree/Particle)
Thermal correction to Energy= 0.143603
Thermal correction to Enthalpy= 0.144548
Thermal correction to Gibbs Free Energy= 0.094114
Sum of electronic and zero-point Energies= -768.620023
Sum of electronic and thermal Energies= -768.608858
Sum of electronic and thermal Enthalpies= -768.607914
Sum of electronic and thermal Free Energies= -768.658348
CBS-DLPNO-CCSD(T) Single Point Energy = -767.742074644994

Starting Materials of the Boryl Sulfenate Elimination of Sulfoxide Families **2B** and **3B**

2BO-B
C -1.6775820000 -1.5019370000 0.2055970000
S -1.2813950000 -0.6056650000 -1.2810330000
O -0.7201730000 0.7490090000 -0.8153040000
C 0.3216410000 -1.4029810000 -1.7361220000
H -0.9967720000 -1.3125200000 1.0282970000
C 1.3704990000 -0.7738340000 -0.8273590000
H 0.4479470000 -1.1280430000 -2.7841670000
H 0.1879100000 -2.4826410000 -1.6670050000
H 2.2661830000 -0.5602250000 -1.4102920000
H 1.6413100000 -1.4774840000 -0.0382420000
B 0.8121690000 0.6277070000 -0.1535850000
C -2.7544850000 -2.2719840000 0.2471930000
H -3.0070640000 -2.8251220000 1.1432740000
H -3.4192110000 -2.3807880000 -0.6022730000
O 0.4962730000 0.5310630000 1.2539540000
O 1.5371400000 1.7588050000 -0.5815630000
C 1.1201640000 3.0379890000 -0.1460040000
H 0.9304700000 3.0650160000 0.9321450000
H 1.9092570000 3.7538930000 -0.3833830000
H 0.2014710000 3.3472880000 -0.6571890000
C 1.5900620000 0.5040490000 2.1413340000
H 2.2112500000 -0.3931240000 2.0033750000
H 2.2418350000 1.3770700000 2.0199290000
H 1.2063590000 0.4974460000 3.1636840000
Zero-point correction= 0.193004 (Hartree/Particle)

Thermal correction to Energy= 0.206576
Thermal correction to Enthalpy= 0.207520
Thermal correction to Gibbs Free Energy= 0.152623
Sum of electronic and zero-point Energies= -885.266353
Sum of electronic and thermal Energies= -885.252782
Sum of electronic and thermal Enthalpies= -885.251838
Sum of electronic and thermal Free Energies= -885.306734
CBS-DLPNO-CCSD(T) Single Point Energy = -884.237324580703

2BO

C 0.7948060000 -0.3075460000 -0.7123510000
S -0.3385830000 0.6869420000 0.2569950000
O -1.0467490000 1.5906510000 -0.7055710000
C -1.5640020000 -0.6205670000 0.6498510000
C -2.1827750000 -1.2840350000 -0.5850220000
H -2.3093360000 -0.0745500000 1.2320970000
H -1.0681450000 -1.3311620000 1.3152170000
H -1.5069620000 -2.0582960000 -0.9517840000
H -3.0910710000 -1.8004890000 -0.2554930000
C 2.0169320000 -0.5677480000 -0.2728890000
H 0.4106730000 -0.6049240000 -1.6823570000
H 2.7156310000 -1.1458460000 -0.8654900000
H 2.3633850000 -0.2152000000 0.6921470000
B -2.5438820000 -0.3337900000 -1.8182600000
O -3.6225120000 0.4983020000 -1.8835210000
O -1.7878540000 -0.5081170000 -2.9430060000
C -4.3254890000 0.9323160000 -0.7336870000
H -5.2502080000 1.4046970000 -1.0640320000
H -4.5794520000 0.0987040000 -0.0702320000
H -3.7255250000 1.6613360000 -0.1843420000
C -1.9598110000 0.3595360000 -4.0621390000
H -1.7580300000 1.3931370000 -3.7740670000
H -1.2510990000 0.0472500000 -4.8283860000
H -2.9751260000 0.2959480000 -4.4585880000
Zero-point correction= 0.193995 (Hartree/Particle)
Thermal correction to Energy= 0.207946
Thermal correction to Enthalpy= 0.208890
Thermal correction to Gibbs Free Energy= 0.153034
Sum of electronic and zero-point Energies= -885.277587
Sum of electronic and thermal Energies= -885.263636
Sum of electronic and thermal Enthalpies= -885.262692
Sum of electronic and thermal Free Energies= -885.318548
CBS-DLPNO-CCSD(T) Single Point Energy = -884.244958642563

2BF-B

C -1.7145520000 -1.1954860000 0.0121480000
S -0.7386210000 -0.3118570000 -1.1842490000
O -0.2680890000 0.9800550000 -0.4807440000
C 0.8528930000 -1.2506870000 -1.0733280000
H -1.3209870000 -1.1910010000 1.0218730000
C 1.5678550000 -0.6942140000 0.1530320000
H 1.3547860000 -1.0117170000 -2.0114530000
H 0.6100520000 -2.3128330000 -1.0635230000
H 2.6115190000 -0.5008710000 -0.0940810000
H 1.5421410000 -1.4211400000 0.9651890000
B 0.8613850000 0.7025880000 0.6638870000
C -2.8517800000 -1.7615980000 -0.3636830000
H -3.4590350000 -2.3101530000 0.3454360000
H -3.2166500000 -1.7004650000 -1.3824500000
F 1.6487530000 1.8191950000 0.6692860000
F 0.1485250000 0.5353480000 1.8453630000
Zero-point correction= 0.113635 (Hartree/Particle)
Thermal correction to Energy= 0.123179
Thermal correction to Enthalpy= 0.124123
Thermal correction to Gibbs Free Energy= 0.078079
Sum of electronic and zero-point Energies= -854.809145
Sum of electronic and thermal Energies= -854.799601
Sum of electronic and thermal Enthalpies= -854.798657
Sum of electronic and thermal Free Energies= -854.844701
CBS-DLPNO-CCSD(T) Single Point Energy = -853.831209269752

2BH-B

C -1.2675940000 -0.8444210000 0.1690090000
S -0.3459770000 0.2391970000 -0.9016440000
O 0.0319630000 1.4615640000 -0.0449730000
C 1.2808940000 -0.6136860000 -0.8789950000
H -0.8524170000 -0.9862210000 1.1594720000
C 1.8702110000 -0.2547710000 0.4814640000
H 1.8264060000 -0.1577930000 -1.7072540000
H 1.1147840000 -1.6704630000 -1.0941630000
H 2.9588940000 -0.3112220000 0.4131260000
H 1.5574550000 -0.9969590000 1.2200310000
B 1.3965630000 1.2705620000 0.8634950000
H 1.0539740000 1.4118830000 2.0108680000
H 2.1338140000 2.1336800000 0.4538800000
C -2.4037120000 -1.3806740000 -0.2516930000
H -2.9810640000 -2.0379970000 0.3865670000
H -2.7960250000 -1.1856290000 -1.2430340000

Zero-point correction= 0.125625 (Hartree/Particle)
Thermal correction to Energy= 0.133691
Thermal correction to Enthalpy= 0.134635
Thermal correction to Gibbs Free Energy= 0.092611
Sum of electronic and zero-point Energies= -656.076525
Sum of electronic and thermal Energies= -656.068459
Sum of electronic and thermal Enthalpies= -656.067515
Sum of electronic and thermal Free Energies= -656.109539
CBS-DLPNO-CCSD(T) Single Point Energy = -655.302761264093

2BC-B

C -1.5722150000 -1.2756560000 0.2181260000
S -0.8236440000 -0.2517810000 -1.0329510000
O -0.3945060000 1.0409380000 -0.3243160000
C 0.8209040000 -1.0638050000 -1.1471270000
H -1.0375020000 -1.3324860000 1.1583800000
C 1.5683970000 -0.5802100000 0.0887830000
H 1.2446670000 -0.6702820000 -2.0726150000
H 0.6636100000 -2.1382950000 -1.2538300000
H 2.6412710000 -0.6438690000 -0.1094450000
H 1.3593950000 -1.2476890000 0.9294850000
B 1.1480560000 0.9802390000 0.4072670000
C -2.7308660000 -1.8718470000 -0.0211510000
H -3.2045690000 -2.4939570000 0.7281120000
H -3.2451690000 -1.7622320000 -0.9688890000
C 0.9004530000 1.3025660000 1.9586290000
H 1.8474600000 1.2558500000 2.5085110000
H 0.4926500000 2.3055480000 2.1151240000
H 0.2192430000 0.5928040000 2.4424280000
C 1.9947910000 2.0738680000 -0.4086180000
H 2.1152300000 1.8273770000 -1.4704610000
H 1.5363750000 3.0658600000 -0.3576140000
H 3.0020860000 2.1661300000 0.0127100000
Zero-point correction= 0.181339 (Hartree/Particle)
Thermal correction to Energy= 0.192777
Thermal correction to Enthalpy= 0.193721
Thermal correction to Gibbs Free Energy= 0.144756
Sum of electronic and zero-point Energies= -734.709486
Sum of electronic and thermal Energies= -734.698049
Sum of electronic and thermal Enthalpies= -734.697104
Sum of electronic and thermal Free Energies= -734.746070
CBS-DLPNO-CCSD(T) Single Point Energy = -733.847764081969

3BO-B

S -0.7104790000 0.0418990000 -1.5499660000
O -0.2131290000 1.2914430000 -0.8131190000
C 0.9118280000 -0.8005410000 -1.8146490000
C 1.7609710000 -0.3754330000 -0.6302830000
H 1.2756930000 -0.3865050000 -2.7561410000
H 0.7154480000 -1.8667280000 -1.9338450000
H 2.8141570000 -0.4518270000 -0.9052350000
H 1.5810670000 -1.0398970000 0.2168760000
B 1.4066130000 1.1768650000 -0.2476760000
C -1.4215720000 -1.0288070000 -0.2969600000
C -1.2398660000 -0.7475940000 1.0522080000
C -2.1766510000 -2.1177290000 -0.7229250000
C -1.8174720000 -1.5972430000 1.9894760000
H -0.6534260000 0.1120740000 1.3529540000
C -2.7392360000 -2.9620830000 0.2257410000
H -2.3298280000 -2.3045380000 -1.7796260000
C -2.5590710000 -2.7010430000 1.5809240000
H -1.6837920000 -1.3938060000 3.0441920000
H -3.3260180000 -3.8140400000 -0.0924570000
H -3.0050760000 -3.3555100000 2.3189160000
O 1.2174120000 1.4873690000 1.1367430000
O 2.1548270000 2.0817770000 -1.0321990000
C 2.3777450000 1.4954920000 1.9365800000
H 2.1019020000 1.8159790000 2.9431000000
H 2.8324260000 0.4969600000 2.0067500000
H 3.1399560000 2.1826910000 1.5494550000
C 1.8982050000 3.4667620000 -0.9038430000
H 2.6638710000 4.0084960000 -1.4619850000
H 0.9151320000 3.7253110000 -1.3132480000
H 1.9239840000 3.7931440000 0.1408980000
Zero-point correction= 0.241207 (Hartree/Particle)
Thermal correction to Energy= 0.257006
Thermal correction to Enthalpy= 0.257950
Thermal correction to Gibbs Free Energy= 0.197652
Sum of electronic and zero-point Energies= -1038.938902
Sum of electronic and thermal Energies= -1038.923103
Sum of electronic and thermal Enthalpies= -1038.922159
Sum of electronic and thermal Free Energies= -1038.982457
CBS-DLPNO-CCSD(T) Single Point Energy = -1037.674800600020

3BO

C -1.7310220000 -0.3871140000 -0.3485640000
S -0.3380630000 -1.4799710000 -0.7091980000
O 0.7167450000 -0.6422540000 -1.3673830000

C 0.2413340000 -1.7215930000 1.0223430000
C 0.7796700000 -0.4325470000 1.6376280000
H 1.0286950000 -2.4715340000 0.9254320000
H -0.5975060000 -2.1595950000 1.5682970000
H -0.0321280000 0.2713770000 1.8229410000
H 1.2045420000 -0.6929760000 2.6135870000
C -3.8741430000 1.2833630000 0.1681590000
C -2.9543970000 -0.9376910000 0.0187580000
C -1.5685370000 0.9858660000 -0.4774600000
C -2.6490920000 1.8204670000 -0.2143060000
C -4.0271140000 -0.0954020000 0.2846830000
H -3.0722960000 -2.0128550000 0.0911610000
H -0.6027680000 1.3791550000 -0.7657690000
H -2.5318890000 2.8929720000 -0.3049920000
H -4.9828900000 -0.5143590000 0.5728280000
H -4.7127410000 1.9378220000 0.3695520000
B 1.9261820000 0.2372330000 0.7614000000
O 3.0157640000 -0.5513640000 0.5015750000
O 1.7821670000 1.5689210000 0.4871450000
C 3.8547780000 -0.4822160000 -0.6424640000
H 4.3899480000 -1.4297140000 -0.7102920000
H 3.2578270000 -0.3514420000 -1.5464600000
H 4.5887030000 0.3229990000 -0.5627430000
C 2.7305050000 2.3812030000 -0.1859950000
H 2.8081880000 2.1062970000 -1.2400600000
H 2.3848890000 3.4127100000 -0.1174380000
H 3.7182340000 2.3140690000 0.2767390000
Zero-point correction= 0.241966 (Hartree/Particle)
Thermal correction to Energy= 0.258109
Thermal correction to Enthalpy= 0.259054
Thermal correction to Gibbs Free Energy= 0.197413
Sum of electronic and zero-point Energies= -1038.945381
Sum of electronic and thermal Energies= -1038.929237
Sum of electronic and thermal Enthalpies= -1038.928293
Sum of electronic and thermal Free Energies= -1038.989934
CBS-DLPNO-CCSD(T) Single Point Energy = -1037.677320526108

3BF-B
S -0.2660890000 0.5205610000 -1.2137110000
O 0.2576220000 1.5938790000 -0.2417560000
C 1.3158220000 -0.4017760000 -1.4769750000
C 2.0774340000 -0.2119090000 -0.1775740000
H 1.7834060000 0.1079550000 -2.3207690000
H 1.0604690000 -1.4222150000 -1.7625310000

H 3.1482850000 -0.2971790000 -0.3687740000
H 1.7989520000 -0.9860360000 0.5387390000
B 1.7468040000 1.2699830000 0.4234890000
F 1.5466390000 1.3185870000 1.7854790000
F 2.5487340000 2.2820860000 -0.0400260000
C -1.1688840000 -0.6628400000 -0.2137470000
C -1.1058900000 -0.6131500000 1.1737090000
C -1.9494270000 -1.6049550000 -0.8780380000
C -1.8300970000 -1.5481640000 1.9049340000
H -0.5049670000 0.1392150000 1.6662720000
C -2.6593190000 -2.5381040000 -0.1338170000
H -2.0087770000 -1.6104710000 -1.9603160000
C -2.5986770000 -2.5090310000 1.2563950000
H -1.7896630000 -1.5233380000 2.9860990000
H -3.2672260000 -3.2779310000 -0.6380280000
H -3.1593090000 -3.2321360000 1.8346440000
Zero-point correction= 0.161922 (Hartree/Particle)
Thermal correction to Energy= 0.173569
Thermal correction to Enthalpy= 0.174513
Thermal correction to Gibbs Free Energy= 0.123568
Sum of electronic and zero-point Energies= -1008.481218
Sum of electronic and thermal Energies= -1008.469570
Sum of electronic and thermal Enthalpies= -1008.468626
Sum of electronic and thermal Free Energies= -1008.519571
CBS-DLPNO-CCSD(T) Single Point Energy = -1007.268298310385

3BH-B

S 0.2501780000 1.0788200000 -1.1260060000
O 0.7684800000 2.0926000000 -0.0892340000
C 1.8126630000 0.1411220000 -1.3980820000
C 2.5288770000 0.2336670000 -0.0571130000
H 2.3218120000 0.6947690000 -2.1890020000
H 1.5458630000 -0.8530790000 -1.7595220000
H 3.5980760000 0.0808460000 -0.2224620000
H 2.1795910000 -0.5703600000 0.5946290000
B 2.2489990000 1.7234380000 0.5549490000
H 2.0975710000 1.7618260000 1.7517310000
H 2.9787720000 2.5800890000 0.1181730000
C -0.6910750000 -0.1398150000 -0.2041830000
C -0.6579450000 -0.1436740000 1.1848110000
C -1.4690280000 -1.0469860000 -0.9175150000
C -1.4074480000 -1.0946620000 1.8678330000
H -0.0563160000 0.5844110000 1.7117570000
C -2.2058320000 -1.9976200000 -0.2226530000

H -1.5049200000 -1.0126230000 -2.0001940000
C -2.1742100000 -2.0209950000 1.1685730000
H -1.3889620000 -1.1110070000 2.9498410000
H -2.8116510000 -2.7110090000 -0.7661300000
H -2.7553080000 -2.7578700000 1.7079820000
Zero-point correction= 0.174030 (Hartree/Particle)
Thermal correction to Energy= 0.184090
Thermal correction to Enthalpy= 0.185034
Thermal correction to Gibbs Free Energy= 0.138095
Sum of electronic and zero-point Energies= -809.748261
Sum of electronic and thermal Energies= -809.738201
Sum of electronic and thermal Enthalpies= -809.737257
Sum of electronic and thermal Free Energies= -809.784196
CBS-DLPNO-CCSD(T) Single Point Energy = -808.739872875206

3BC-B
S -0.2920810000 0.6008450000 -1.2929470000
O 0.2313260000 1.7226360000 -0.3855190000
C 1.2877170000 -0.3070810000 -1.5938360000
C 2.1240820000 -0.0066260000 -0.3602510000
H 1.6942670000 0.1436530000 -2.4999460000
H 1.0358350000 -1.3503490000 -1.7883320000
H 3.1758050000 -0.1796750000 -0.6040440000
H 1.8547730000 -0.6991420000 0.4417550000
B 1.8945560000 1.5573960000 0.0659970000
C -1.1138740000 -0.5757270000 -0.2099350000
C -1.1237690000 -0.3671370000 1.1617510000
C -1.7672360000 -1.6619320000 -0.7850830000
C -1.7840890000 -1.2819650000 1.9749090000
H -0.6227550000 0.4966320000 1.5748660000
C -2.4166960000 -2.5726680000 0.0378340000
H -1.7725080000 -1.7983920000 -1.8603620000
C -2.4241150000 -2.3831070000 1.4171380000
H -1.7949060000 -1.1320130000 3.0467670000
H -2.9231810000 -3.4243070000 -0.3975980000
H -2.9362340000 -3.0915040000 2.0554710000
C 1.9498180000 1.8701540000 1.6362820000
H 1.4194390000 1.1382450000 2.2544270000
H 2.9919260000 1.8657490000 1.9753420000
H 1.5492740000 2.8604570000 1.8730140000
C 2.6465680000 2.6253140000 -0.8697560000
H 2.5492550000 2.4213690000 -1.9428460000
H 2.2770740000 3.6413550000 -0.7028690000
H 3.7191280000 2.6359300000 -0.6458710000

Zero-point correction= 0.229584 (Hartree/Particle)
Thermal correction to Energy= 0.243207
Thermal correction to Enthalpy= 0.244152
Thermal correction to Gibbs Free Energy= 0.189608
Sum of electronic and zero-point Energies= -888.380663
Sum of electronic and thermal Energies= -888.367040
Sum of electronic and thermal Enthalpies= -888.366095
Sum of electronic and thermal Free Energies= -888.420639
CBS-DLPNO-CCSD(T) Single Point Energy = -887.283909244478

Transition States of Boryl Sulfenate Elimination for Sulfoxide Families **2B** and **3B**

2BO-B‡
C -1.9467570000 -0.7955370000 0.2851530000
S -1.0171310000 0.5771460000 -0.2845590000
O -0.3570050000 1.0725190000 1.0750520000
C 1.0496130000 -0.5531730000 -0.7829010000
H -1.5519440000 -1.2464590000 1.1893100000
C 1.8217660000 -0.1540560000 0.3157140000
H 1.2094970000 -0.0899800000 -1.7480480000
H 0.5420780000 -1.5089290000 -0.8100640000
H 2.7651070000 0.3282420000 0.0693870000
H 1.8696180000 -0.8359380000 1.1579060000
B 1.1010970000 1.4113650000 0.9807460000
C -3.0090240000 -1.2632530000 -0.3626710000
H -3.5165660000 -2.1544760000 -0.0184130000
H -3.4009880000 -0.7824890000 -1.2509090000
O 1.5627250000 1.6414260000 2.2843100000
O 1.4011700000 2.3529080000 -0.0497880000
C 0.8693640000 3.6575900000 0.1049530000
H 1.1892810000 4.1192090000 1.0456870000
H 1.2251210000 4.2692780000 -0.7251310000
H -0.2269330000 3.6508210000 0.0904110000
C 2.8807200000 2.1049600000 2.4732290000
H 3.6106820000 1.3018180000 2.3061300000
H 3.1301300000 2.9319890000 1.8007500000
H 2.9783210000 2.4451670000 3.5050090000
Zero-point correction= 0.190525 (Hartree/Particle)
Thermal correction to Energy= 0.204346
Thermal correction to Enthalpy= 0.205290
Thermal correction to Gibbs Free Energy= 0.149824
Sum of electronic and zero-point Energies= -885.250191
Sum of electronic and thermal Energies= -885.236370

Sum of electronic and thermal Enthalpies= -885.235426
Sum of electronic and thermal Free Energies= -885.290892
CBS-DLPNO-CCSD(T) Single Point Energy = -884.208084656128
Imaginary frequency: -336.62 cm-1

2BF-B‡

C -1.9810560000 -0.7063430000 0.2191890000
S -0.9819250000 0.5462760000 -0.4906630000
O -0.4408420000 1.2689250000 0.8320720000
C 1.1965370000 -0.6811620000 -0.4884090000
H -1.6729960000 -1.0050050000 1.2153850000
C 1.8072200000 -0.0753370000 0.6052400000
H 1.4777410000 -0.4048320000 -1.4964480000
H 0.6411590000 -1.6049500000 -0.3982800000
H 2.7639620000 0.4057380000 0.4183360000
H 1.7251870000 -0.5718020000 1.5657390000
B 0.9891510000 1.5871470000 0.8622080000
C -2.9938430000 -1.2685550000 -0.4323800000
H -3.5436260000 -2.0894050000 0.0083150000
H -3.3017830000 -0.9386430000 -1.4171880000
F 1.4016290000 2.3504940000 -0.2019010000
F 1.3725460000 2.0364670000 2.0808240000
Zero-point correction= 0.110914 (Hartree/Particle)
Thermal correction to Energy= 0.120771
Thermal correction to Enthalpy= 0.121715
Thermal correction to Gibbs Free Energy= 0.075299
Sum of electronic and zero-point Energies= -854.790515
Sum of electronic and thermal Energies= -854.780658
Sum of electronic and thermal Enthalpies= -854.779714
Sum of electronic and thermal Free Energies= -854.826130
CBS-DLPNO-CCSD(T) Single Point Energy = -853.798078956668
Imaginary frequency: -326.76 cm-1

2BH-B‡

C -2.0165210000 -0.7217320000 0.2363800000
S -0.9689730000 0.5253610000 -0.4075910000
O -0.4338200000 1.1906930000 0.9401080000
C 1.1820680000 -0.6631680000 -0.4774330000
H -1.7600730000 -1.0305280000 1.2441690000
C 1.8297180000 -0.0362810000 0.5940280000
H 1.4331890000 -0.3984600000 -1.4971600000
H 0.6612720000 -1.6049390000 -0.3632470000
H 2.7857130000 0.4273730000 0.3626040000
H 1.8028010000 -0.5554290000 1.5463390000

B 0.9913220000 1.5823480000 0.8705040000
H 1.3680060000 2.0051580000 1.9263310000
H 1.2728230000 2.2238210000 -0.1141780000
C -2.9991010000 -1.2733800000 -0.4690550000
H -3.5763800000 -2.0929150000 -0.0621780000
H -3.2538670000 -0.9361630000 -1.4665280000
Zero-point correction= 0.123224 (Hartree/Particle)
Thermal correction to Energy= 0.131458
Thermal correction to Enthalpy= 0.132403
Thermal correction to Gibbs Free Energy= 0.090257
Sum of electronic and zero-point Energies= -656.060952
Sum of electronic and thermal Energies= -656.052718
Sum of electronic and thermal Enthalpies= -656.051774
Sum of electronic and thermal Free Energies= -656.093920
CBS-DLPNO-CCSD(T) Single Point Energy = -655.273605626012
Imaginary frequency: -296.69 cm-1

2BC-B‡
C -1.9760770000 -0.7275350000 0.2256580000
S -0.9236760000 0.4830260000 -0.4814150000
O -0.4233560000 1.2405120000 0.8191740000
C 1.1417940000 -0.7205060000 -0.4597030000
H -1.7289740000 -0.9759850000 1.2523060000
C 1.8117160000 -0.0504220000 0.5783420000
H 1.4182060000 -0.5406880000 -1.4914640000
H 0.6239490000 -1.6562740000 -0.2915930000
H 2.7876740000 0.3506090000 0.3188790000
H 1.7774280000 -0.5297790000 1.5514240000
B 1.0321050000 1.6265010000 0.8494350000
C -2.9520050000 -1.3170890000 -0.4572070000
H -3.5358560000 -2.1111710000 -0.0109940000
H -3.1951920000 -1.0358660000 -1.4747640000
C 1.4163610000 2.1278400000 2.3142890000
H 2.5002130000 2.2188780000 2.4316200000
H 0.9935970000 3.1196480000 2.5065690000
H 1.0510400000 1.4591370000 3.0989250000
C 1.4792460000 2.5607310000 -0.3800410000
H 1.2970440000 2.1338490000 -1.3730120000
H 0.9341530000 3.5101120000 -0.3397910000
H 2.5443790000 2.8028020000 -0.3282590000
Zero-point correction= 0.179079 (Hartree/Particle)
Thermal correction to Energy= 0.190687
Thermal correction to Enthalpy= 0.191631
Thermal correction to Gibbs Free Energy= 0.142360

Sum of electronic and zero-point Energies= -734.693677
Sum of electronic and thermal Energies= -734.682069
Sum of electronic and thermal Enthalpies= -734.681125
Sum of electronic and thermal Free Energies= -734.730396
CBS-DLPNO-CCSD(T) Single Point Energy = -733.819466189678
Imaginary frequency: -347.07 cm-1

3BO-B‡
S -1.0310150000 0.5764640000 -0.3070750000
O -0.4231480000 1.4118430000 0.8959630000
C 1.0422190000 -0.6833240000 -0.3747840000
C 1.7380750000 -0.0623520000 0.6668080000
H 1.2987050000 -0.4573560000 -1.4016360000
H 0.4838750000 -1.5977280000 -0.2222860000
H 2.7210820000 0.3247140000 0.4078040000
H 1.6773070000 -0.5247520000 1.6457760000
B 1.0572740000 1.6494010000 0.8646070000
C -2.0023200000 -0.6386420000 0.5365990000
C -1.8876520000 -0.8468610000 1.9092310000
C -2.8699570000 -1.4159310000 -0.2320580000
C -2.6487220000 -1.8431820000 2.5083320000
H -1.2211600000 -0.2248470000 2.4901740000
C -3.6150810000 -2.4156530000 0.3787100000
H -2.9674110000 -1.2385670000 -1.2969090000
C -3.5080670000 -2.6312510000 1.7494070000
H -2.5673870000 -2.0034930000 3.5760090000
H -4.2880540000 -3.0197570000 -0.2163280000
H -4.0965540000 -3.4056890000 2.2239630000
O 1.4178470000 2.1603270000 2.1199030000
O 1.5081270000 2.3024130000 -0.3192230000
C 2.7350070000 2.6218570000 2.3211180000
H 2.7602860000 3.1849620000 3.2549900000
H 3.4391900000 1.7836620000 2.4061820000
H 3.0768210000 3.2676850000 1.5062590000
C 1.0304110000 3.6177170000 -0.5436970000
H 1.4998630000 3.9984320000 -1.4516330000
H -0.0574820000 3.6336090000 -0.6781010000
H 1.2756920000 4.2883530000 0.2875130000
Zero-point correction= 0.238764 (Hartree/Particle)
Thermal correction to Energy= 0.254807
Thermal correction to Enthalpy= 0.255751
Thermal correction to Gibbs Free Energy= 0.194150
Sum of electronic and zero-point Energies= -1038.921023
Sum of electronic and thermal Energies= -1038.904979

Sum of electronic and thermal Enthalpies= -1038.904035
Sum of electronic and thermal Free Energies= -1038.965636
CBS-DLPNO-CCSD(T) Single Point Energy = -1037.644243388673
Imaginary frequency: -340.39 cm-1

3BF-B‡
S -1.0871450000 0.5849440000 -0.3384820000
O -0.4359610000 1.4105870000 0.8644670000
C 1.0791190000 -0.7030090000 -0.3717980000
C 1.7556420000 -0.0462790000 0.6478150000
H 1.3213460000 -0.5051010000 -1.4078330000
H 0.4869540000 -1.5887270000 -0.1864920000
H 2.7162050000 0.3931910000 0.3916620000
H 1.6948900000 -0.4663690000 1.6452940000
B 1.0033550000 1.6690820000 0.8031640000
F 1.4608060000 2.1921270000 1.9660320000
F 1.3966890000 2.3278390000 -0.3328380000
C -2.0362070000 -0.6317260000 0.5260480000
C -1.8831440000 -0.8614370000 1.8913480000
C -2.9327800000 -1.3907660000 -0.2280690000
C -2.6341630000 -1.8608860000 2.4980820000
H -1.1975250000 -0.2540110000 2.4648680000
C -3.6664810000 -2.3943010000 0.3898250000
H -3.0621090000 -1.1962470000 -1.2864470000
C -3.5208520000 -2.6314820000 1.7533080000
H -2.5233190000 -2.0365860000 3.5605650000
H -4.3615810000 -2.9838730000 -0.1940590000
H -4.1010750000 -3.4085150000 2.2335230000
Zero-point correction= 0.159169 (Hartree/Particle)
Thermal correction to Energy= 0.171233
Thermal correction to Enthalpy= 0.172177
Thermal correction to Gibbs Free Energy= 0.119693
Sum of electronic and zero-point Energies= -1008.461003
Sum of electronic and thermal Energies= -1008.448939
Sum of electronic and thermal Enthalpies= -1008.447995
Sum of electronic and thermal Free Energies= -1008.500479
CBS-DLPNO-CCSD(T) Single Point Energy = -1007.234008572466
Imaginary frequency: -332.83 cm-1

3BH-B‡
S -1.0513880000 0.5653000000 -0.2801180000
O -0.4195360000 1.3347460000 0.9631630000
C 1.0832750000 -0.6942820000 -0.3509290000
C 1.7908850000 -0.0088690000 0.6400530000

H 1.3022920000 -0.5219400000 -1.3972470000
H 0.5221890000 -1.5938670000 -0.1346300000
H 2.7499630000 0.4074200000 0.3418150000
H 1.7788210000 -0.4423300000 1.6342870000
B 1.0125360000 1.6636690000 0.8004070000
H 1.4490090000 2.1602700000 1.7999740000
H 1.2767170000 2.2017750000 -0.2475810000
C -2.0752570000 -0.6410030000 0.5068490000
C -1.9656330000 -0.9307500000 1.8655910000
C -2.9825010000 -1.3341140000 -0.2966180000
C -2.7717610000 -1.9198800000 2.4150690000
H -1.2678580000 -0.3752820000 2.4759490000
C -3.7700760000 -2.3309460000 0.2632390000
H -3.0781140000 -1.0923430000 -1.3487250000
C -3.6691690000 -2.6251540000 1.6195690000
H -2.6949140000 -2.1411080000 3.4721180000
H -4.4727900000 -2.8694710000 -0.3596420000
H -4.2917170000 -3.3958320000 2.0551080000
Zero-point correction= 0.171504 (Hartree/Particle)
Thermal correction to Energy= 0.181914
Thermal correction to Enthalpy= 0.182858
Thermal correction to Gibbs Free Energy= 0.134619
Sum of electronic and zero-point Energies= -809.731095
Sum of electronic and thermal Energies= -809.720685
Sum of electronic and thermal Enthalpies= -809.719741
Sum of electronic and thermal Free Energies= -809.767980
CBS-DLPNO-CCSD(T) Single Point Energy = -808.709258240299
Imaginary frequency: -299.85 cm-1

3BC-B‡
S -1.0138160000 0.5037480000 -0.3280350000
O -0.4110460000 1.3574430000 0.8604930000
C 1.0577050000 -0.7282150000 -0.3569890000
C 1.7870730000 -0.0086800000 0.6012090000
H 1.2826850000 -0.6159660000 -1.4103480000
H 0.5228740000 -1.6331820000 -0.0991440000
H 2.7545920000 0.3615170000 0.2737340000
H 1.7888070000 -0.4200240000 1.6052290000
B 1.0514600000 1.7060670000 0.7869290000
C -2.0077910000 -0.6832250000 0.5282300000
C -1.8907370000 -0.8868840000 1.9013830000
C -2.8946330000 -1.4468600000 -0.2318660000
C -2.6697090000 -1.8627460000 2.5103020000
H -1.2080740000 -0.2760880000 2.4750230000

C -3.6557840000 -2.4291140000 0.3876980000
H -2.9950020000 -1.2712340000 -1.2965930000
C -3.5474330000 -2.6382220000 1.7591200000
H -2.5874450000 -2.0185080000 3.5785590000
H -4.3433650000 -3.0230740000 -0.2007320000
H -4.1493060000 -3.3978170000 2.2408180000
C 1.5239480000 2.2982200000 2.1909460000
H 1.1919990000 1.6930360000 3.0396600000
H 2.6138000000 2.3752740000 2.2440240000
H 1.1281590000 3.3090000000 2.3358610000
C 1.4508220000 2.5366460000 -0.5284710000
H 1.1945560000 2.0458660000 -1.4742680000
H 0.9352420000 3.5031970000 -0.5246550000
H 2.5232550000 2.7482660000 -0.5580270000
Zero-point correction= 0.227329 (Hartree/Particle)
Thermal correction to Energy= 0.241143
Thermal correction to Enthalpy= 0.242087
Thermal correction to Gibbs Free Energy= 0.186719
Sum of electronic and zero-point Energies= -888.364246
Sum of electronic and thermal Energies= -888.350431
Sum of electronic and thermal Enthalpies= -888.349487
Sum of electronic and thermal Free Energies= -888.404855
CBS-DLPNO-CCSD(T) Single Point Energy = -887.255502215326
Imaginary frequency: -350.21 cm-1

Products of the Boryl Sulfenate Elimination for Sulfoxide Families **2B** and **3B**

$CH_2CHSOB(OMe)_2$
S -1.7420270000 1.3301950000 0.0022180000
O -2.4693460000 2.1557250000 -1.2519940000
B -1.7473010000 2.8936080000 -2.1809500000
O -0.3990120000 2.7242630000 -2.2511260000
O -2.5288030000 3.7085360000 -2.9436900000
C -2.1842820000 4.2242920000 -4.2201230000
H -1.5974400000 3.5103780000 -4.8031870000
H -3.1137800000 4.4253300000 -4.7519390000
H -1.6243330000 5.1580720000 -4.1326120000
C 0.5338020000 3.6206080000 -2.8344920000
H 1.4933900000 3.4529860000 -2.3465360000
H 0.6474690000 3.4317100000 -3.9040090000
H 0.2429860000 4.6627020000 -2.6844610000
C -1.2639220000 -0.1491150000 -0.7931490000
H -1.9392260000 -0.4683960000 -1.5813980000

C -0.2265400000 -0.8888560000 -0.4074200000
H 0.4580990000 -0.5608270000 0.3649410000
H -0.0529120000 -1.8640980000 -0.8433020000
Zero-point correction= 0.137548 (Hartree/Particle)
Thermal correction to Energy= 0.149444
Thermal correction to Enthalpy= 0.150388
Thermal correction to Gibbs Free Energy= 0.097663
Sum of electronic and zero-point Energies= -806.710907
Sum of electronic and thermal Energies= -806.699012
Sum of electronic and thermal Enthalpies= -806.698068
Sum of electronic and thermal Free Energies= -806.750793
CBS-DLPNO-CCSD(T) Single Point Energy = -805.765838800680

$CH_2CHSOBF_2$
S 0.2761230000 0.5463700000 -0.7292140000
O -0.3409950000 2.0376200000 -1.2384590000
B -0.8747420000 2.2102140000 -2.4767400000
F -1.2991870000 3.4214650000 -2.7993770000
F -0.9957980000 1.2404250000 -3.3698430000
C -1.1640780000 -0.1705450000 -0.0465420000
H -1.7595170000 0.4876460000 0.5785140000
C -1.4358540000 -1.4668160000 -0.1777080000
H -0.8475020000 -2.1137250000 -0.8162490000
H -2.2467880000 -1.9191410000 0.3790430000
Zero-point correction= 0.057669 (Hartree/Particle)
Thermal correction to Energy= 0.065474
Thermal correction to Enthalpy= 0.066418
Thermal correction to Gibbs Free Energy= 0.023429
Sum of electronic and zero-point Energies= -776.239741
Sum of electronic and thermal Energies= -776.231936
Sum of electronic and thermal Enthalpies= -776.230992
Sum of electronic and thermal Free Energies= -776.273981
CBS-DLPNO-CCSD(T) Single Point Energy = -775.346301176893

$CH_2CHSOBH_2$
S -1.0723600000 0.0214630000 -1.9129520000
O -1.0821760000 1.6888410000 -1.5994450000
B -1.0031230000 2.5914220000 -2.6028160000
H -1.0224590000 3.7334380000 -2.2616690000
H -0.9191960000 2.2478750000 -3.7445280000
C -0.7700950000 -1.6568790000 0.1847840000
H -0.0692980000 -2.2424060000 -0.3971220000
H -1.0491160000 -2.0386790000 1.1581050000
C -1.3029530000 -0.5272610000 -0.2751600000

H -1.9905160000 0.0726800000 0.3118190000
Zero-point correction= 0.068629 (Hartree/Particle)
Thermal correction to Energy= 0.075292
Thermal correction to Enthalpy= 0.076237
Thermal correction to Gibbs Free Energy= 0.037222
Sum of electronic and zero-point Energies= -577.508954
Sum of electronic and thermal Energies= -577.502290
Sum of electronic and thermal Enthalpies= -577.501346
Sum of electronic and thermal Free Energies= -577.540361
CBS-DLPNO-CCSD(T) Single Point Energy = -576.816860188415

$CH_2CHSOBMe_2$
S -0.2521250000 0.7988030000 -0.8173990000
O -1.2294980000 1.3974220000 -2.0543530000
B -0.8144200000 2.3781900000 -2.9219190000
C 0.6251710000 3.0058880000 -2.8254540000
H 0.7913220000 3.4519810000 -1.8383330000
H 1.3953650000 2.2344920000 -2.9385540000
H 0.8053650000 3.7742070000 -3.5777500000
C -1.8765310000 2.8087260000 -3.9968030000
H -2.0810730000 3.8818080000 -3.9138770000
H -1.4725780000 2.6622340000 -5.0044490000
H -2.8201550000 2.2678770000 -3.9189510000
C -1.4177240000 -0.2933510000 -0.1197500000
H -2.4418880000 0.0623710000 -0.1620040000
C -1.0791730000 -1.4203110000 0.5022180000
H -0.0592270000 -1.7834980000 0.5248450000
H -1.8242760000 -1.9995270000 1.0313520000
Zero-point correction= 0.124837 (Hartree/Particle)
Thermal correction to Energy= 0.134856
Thermal correction to Enthalpy= 0.135800
Thermal correction to Gibbs Free Energy= 0.088435
Sum of electronic and zero-point Energies= -656.152931
Sum of electronic and thermal Energies= -656.142912
Sum of electronic and thermal Enthalpies= -656.141967
Sum of electronic and thermal Free Energies= -656.189333
CBS-DLPNO-CCSD(T) Single Point Energy = -655.372479982757

$PhSOB(OMe)_2$
S 0.1782440000 -0.3069890000 -1.9265110000
O -0.8060380000 0.4747990000 -3.0102580000
B -0.9628650000 1.8583590000 -3.0108920000
O -0.1650010000 2.6154860000 -2.2132880000
O -1.9474450000 2.2778010000 -3.8527240000

C -2.0793680000 3.5928350000 -4.3721420000
H -1.1075740000 4.0474070000 -4.5783500000
H -2.6339980000 3.5190860000 -5.3069020000
H -2.6354640000 4.2352010000 -3.6858980000
C -0.4478130000 3.9240960000 -1.7412280000
H 0.1031620000 4.0586840000 -0.8112390000
H -0.1207740000 4.6816540000 -2.4563250000
H -1.5125890000 4.0576510000 -1.5379530000
C -0.8171450000 -0.3343530000 -0.4698560000
C -0.1943130000 -0.7035980000 0.7271250000
C -2.1785140000 -0.0281960000 -0.4750300000
C -0.9331660000 -0.7758380000 1.8989320000
H 0.8668620000 -0.9233440000 0.7434580000
C -2.9027320000 -0.0874490000 0.7103720000
H -2.6694250000 0.2398480000 -1.4002960000
C -2.2900280000 -0.4634670000 1.8998700000
H -0.4416140000 -1.0643600000 2.8197500000
H -3.9583930000 0.1546050000 0.6972850000
H -2.8606550000 -0.5111110000 2.8181180000
Zero-point correction= 0.185836 (Hartree/Particle)
Thermal correction to Energy= 0.199867
Thermal correction to Enthalpy= 0.200811
Thermal correction to Gibbs Free Energy= 0.141894
Sum of electronic and zero-point Energies= -960.379648
Sum of electronic and thermal Energies= -960.365618
Sum of electronic and thermal Enthalpies= -960.364673
Sum of electronic and thermal Free Energies= -960.423590
CBS-DLPNO-CCSD(T) Single Point Energy = -959.200212214344

PhSOBF$_2$

S -0.8835550000 -0.4330400000 -2.0664300000
O -1.5292960000 1.1177050000 -2.3657350000
B -0.9149630000 2.2461790000 -1.9364710000
F 0.1843650000 2.2568090000 -1.1912640000
F -1.4482000000 3.4120820000 -2.2707300000
C -1.4303740000 -0.7214500000 -0.4070990000
C -0.6215600000 -0.3540950000 0.6728560000
C -2.6598820000 -1.3455590000 -0.1776190000
C -1.0466110000 -0.6037640000 1.9710250000
H 0.3279740000 0.1280960000 0.4847380000
C -3.0780320000 -1.5945520000 1.1229250000
H -3.2772320000 -1.6279600000 -1.0199720000
C -2.2725200000 -1.2232360000 2.1952430000
H -0.4209890000 -0.3181480000 2.8069300000

H -4.0302010000 -2.0779900000 1.3000400000
H -2.6000600000 -1.4191700000 3.2085180000
Zero-point correction= 0.105931 (Hartree/Particle)
Thermal correction to Energy= 0.115921
Thermal correction to Enthalpy= 0.116865
Thermal correction to Gibbs Free Energy= 0.067572
Sum of electronic and zero-point Energies= -929.907807
Sum of electronic and thermal Energies= -929.897818
Sum of electronic and thermal Enthalpies= -929.896874
Sum of electronic and thermal Free Energies= -929.946167
CBS-DLPNO-CCSD(T) Single Point Energy = -928.779907645039

PhSOBH$_2$
S -0.1573440000 0.7898540000 -0.8887550000
O -1.4065330000 1.6742490000 -1.5986160000
B -1.2852000000 2.1950800000 -2.8425820000
H -0.2997470000 2.0260830000 -3.4953530000
H -2.2245610000 2.8252320000 -3.2185060000
C -1.0911670000 -0.1689290000 0.2577550000
C -2.4581660000 -0.4076300000 0.1178350000
C -0.3862280000 -0.7382290000 1.3221570000
C -3.1096930000 -1.2128640000 1.0440890000
H -3.0051490000 0.0412910000 -0.6983470000
C -1.0457330000 -1.5619630000 2.2236710000
H 0.6697490000 -0.5321080000 1.4508460000
C -2.4102120000 -1.7998430000 2.0926010000
H -4.1731800000 -1.3866180000 0.9374910000
H -0.4924980000 -2.0031760000 3.0430710000
H -2.9243250000 -2.4306070000 2.8059120000
Zero-point correction= 0.116822 (Hartree/Particle)
Thermal correction to Energy= 0.125640
Thermal correction to Enthalpy= 0.126584
Thermal correction to Gibbs Free Energy= 0.080671
Sum of electronic and zero-point Energies= -731.176088
Sum of electronic and thermal Energies= -731.167271
Sum of electronic and thermal Enthalpies= -731.166327
Sum of electronic and thermal Free Energies= -731.212239
CBS-DLPNO-CCSD(T) Single Point Energy = -730.249586863283

PhSOBMe$_2$
S -2.0116450000 -0.3242540000 -2.4687600000
O -2.1717800000 1.3353540000 -2.6044950000
B -1.0907810000 2.2031940000 -2.6144970000
C 0.3883430000 1.7048860000 -2.4538530000

H 0.5174940000 1.1938550000 -1.4940400000
H 0.6428660000 0.9641760000 -3.2178430000
H 1.1116920000 2.5191690000 -2.5063670000
C -1.4785090000 3.7152630000 -2.7764730000
H -1.1055770000 4.2886100000 -1.9205260000
H -0.9769430000 4.1389360000 -3.6532920000
H -2.5512410000 3.8856890000 -2.8709650000
C -1.9093560000 -0.5444700000 -0.7192100000
C -2.2311420000 0.4590800000 0.1940640000
C -1.5095240000 -1.8026130000 -0.2574670000
C -2.1468600000 0.2015340000 1.5577150000
H -2.5522520000 1.4289040000 -0.1586200000
C -1.4465080000 -2.0506950000 1.1060870000
H -1.2391030000 -2.5813080000 -0.9610170000
C -1.7599850000 -1.0500620000 2.0216250000
H -2.3940640000 0.9877170000 2.2602910000
H -1.1364370000 -3.0280480000 1.4540840000
H -1.6991190000 -1.2443190000 3.0843760000
Zero-point correction= 0.173066 (Hartree/Particle)
Thermal correction to Energy= 0.185183
Thermal correction to Enthalpy= 0.186127
Thermal correction to Gibbs Free Energy= 0.132851
Sum of electronic and zero-point Energies= -809.821070
Sum of electronic and thermal Energies= -809.808953
Sum of electronic and thermal Enthalpies= -809.808009
Sum of electronic and thermal Free Energies= -809.861285
CBS-DLPNO-CCSD(T) Single Point Energy = -808.806338907030

Starting Materials of Boryl Sulfenate Elimination for Sulfoxide Family **4B**

4BO-B
S -0.1529810000 0.2345650000 -0.5590680000
C -1.1424580000 -0.2062930000 0.8947090000
H -2.0033030000 0.4598830000 0.9263860000
H -0.5025660000 -0.0702370000 1.7656560000
H -1.4685490000 -1.2413730000 0.7863580000
O 0.5818390000 1.5267740000 -0.1451660000
C 1.2066470000 -0.9217160000 -0.3664920000
C 2.2376250000 -0.3137650000 0.2003190000
H 1.0730020000 -1.9316680000 -0.7306750000
H 3.1559020000 -0.8645890000 0.3757890000
B 1.9889880000 1.2294080000 0.6716830000
O 2.9779750000 2.1108590000 0.1994200000

O 1.5766610000 1.3448350000 2.0477740000
C 2.8149680000 3.4972380000 0.4306980000
H 3.7541980000 3.9959330000 0.1858210000
H 2.0229470000 3.9108790000 -0.2034160000
H 2.5611090000 3.7131930000 1.4739530000
C 2.5832750000 1.2238010000 3.0294250000
H 3.4192880000 1.9087670000 2.8482520000
H 2.1459830000 1.4584390000 4.0017700000
H 2.9900400000 0.2039170000 3.0745720000
Zero-point correction= 0.164351 (Hartree/Particle)
Thermal correction to Energy= 0.176607
Thermal correction to Enthalpy= 0.177551
Thermal correction to Gibbs Free Energy= 0.126302
Sum of electronic and zero-point Energies= -845.970798
Sum of electronic and thermal Energies= -845.958542
Sum of electronic and thermal Enthalpies= -845.957598
Sum of electronic and thermal Free Energies= -846.008847
CBS-DLPNO-CCSD(T) Single Point Energy = -844.986487732678

4BO
S -1.4983450000 -0.2530230000 -1.0185760000
C -2.1536190000 -1.8692100000 -0.4914900000
H -3.1468160000 -1.6924280000 -0.0808000000
H -1.4830350000 -2.2672520000 0.2689700000
H -2.2157270000 -2.5361250000 -1.3520700000
O -1.2103220000 0.5128290000 0.2346470000
C 0.0866360000 -0.8547490000 -1.6030550000
C 1.1802880000 -0.6139630000 -0.8920440000
H 0.0588600000 -1.3598180000 -2.5635240000
H 2.1173520000 -0.9752910000 -1.3134470000
B 1.2586160000 0.0838660000 0.5340350000
O 1.5475110000 1.4022280000 0.7230960000
O 1.2794080000 -0.7625670000 1.6014200000
C 1.3578320000 2.3803230000 -0.2881080000
H 1.8570590000 3.2930890000 0.0357860000
H 1.7832520000 2.0628280000 -1.2448140000
H 0.2918360000 2.5739920000 -0.4204610000
C 1.3433660000 -0.2407320000 2.9271530000
H 0.4741690000 0.3875880000 3.1328850000
H 1.3500830000 -1.0891370000 3.6104180000
H 2.2477160000 0.3533190000 3.0751960000
Zero-point correction= 0.164749 (Hartree/Particle)
Thermal correction to Energy= 0.177750
Thermal correction to Enthalpy= 0.178694

Thermal correction to Gibbs Free Energy= 0.124422
Sum of electronic and zero-point Energies= -845.980038
Sum of electronic and thermal Energies= -845.967038
Sum of electronic and thermal Enthalpies= -845.966094
Sum of electronic and thermal Free Energies= -846.020366
CBS-DLPNO-CCSD(T) Single Point Energy = -844.991482048707

4BF-B
S -0.9367760000 -0.5091110000 -1.0424180000
C -1.9534640000 -1.4065940000 0.1578180000
H -2.9296180000 -0.9252420000 0.1904630000
H -1.4524420000 -1.3538420000 1.1229320000
H -2.0525690000 -2.4374830000 -0.1845290000
O -0.5807240000 0.8148990000 -0.3269200000
C 0.6294180000 -1.3598290000 -0.8213660000
C 1.4224020000 -0.6406950000 -0.0435600000
H 0.7740880000 -2.3029180000 -1.3308710000
H 2.4201640000 -0.9935390000 0.1942690000
B 0.7737540000 0.7265260000 0.5597590000
F 0.3819650000 0.5770060000 1.8767210000
F 1.4616310000 1.8807120000 0.3227370000
Zero-point correction= 0.084980 (Hartree/Particle)
Thermal correction to Energy= 0.093183
Thermal correction to Enthalpy= 0.094127
Thermal correction to Gibbs Free Energy= 0.051967
Sum of electronic and zero-point Energies= -815.512938
Sum of electronic and thermal Energies= -815.504736
Sum of electronic and thermal Enthalpies= -815.503791
Sum of electronic and thermal Free Energies= -815.545951
CBS-DLPNO-CCSD(T) Single Point Energy = -814.579940121508

4BF-B
S -0.6480290000 -0.1263130000 -0.6359240000
C -1.6701030000 -0.8874340000 0.6586880000
H -2.6181700000 -0.3527510000 0.6970550000
H -1.1328520000 -0.8138840000 1.6022520000
H -1.8365110000 -1.9294390000 0.3822440000
O -0.2171010000 1.2404800000 -0.0456830000
C 0.8854330000 -1.0048650000 -0.3862170000
C 1.7019260000 -0.2565130000 0.3539190000
H 1.0039390000 -1.9821750000 -0.8332960000
H 2.6827840000 -0.6431710000 0.6139170000
B 1.1394380000 1.1629920000 0.8167490000
H 1.8065590000 2.1093650000 0.4846210000

H 0.8573780000 1.1757980000 1.9967570000
Zero-point correction= 0.096821 (Hartree/Particle)
Thermal correction to Energy= 0.103476
Thermal correction to Enthalpy= 0.104420
Thermal correction to Gibbs Free Energy= 0.066683
Sum of electronic and zero-point Energies= -616.788093
Sum of electronic and thermal Energies= -616.781438
Sum of electronic and thermal Enthalpies= -616.780494
Sum of electronic and thermal Free Energies= -616.818231
CBS-DLPNO-CCSD(T) Single Point Energy = -616.057602018551

4BC-B
S -0.9461810000 -0.3213690000 -1.0192880000
C -2.0714440000 -1.3354790000 -0.0174510000
H -3.0142440000 -0.7973850000 0.0717150000
H -1.6150710000 -1.5003400000 0.9558730000
H -2.2270100000 -2.2788990000 -0.5430460000
O -0.5665870000 0.8746310000 -0.1211920000
C 0.5623560000 -1.2631490000 -0.8611480000
C 1.3688110000 -0.6729950000 0.0156800000
H 0.6838180000 -2.1495860000 -1.4693470000
H 2.3355360000 -1.1240990000 0.2221740000
B 0.8539470000 0.6755330000 0.7253090000
C 0.4831580000 0.4860340000 2.2841350000
H -0.1478750000 -0.3845860000 2.4909390000
H 1.3932510000 0.3668850000 2.8812810000
H -0.0361040000 1.3687850000 2.6690830000
C 1.7306250000 1.9811470000 0.3940780000
H 1.2374280000 2.8861730000 0.7613190000
H 2.7064890000 1.9265930000 0.8880790000
H 1.9131950000 2.1142420000 -0.6763390000
Zero-point correction= 0.152753 (Hartree/Particle)
Thermal correction to Energy= 0.162923
Thermal correction to Enthalpy= 0.163868
Thermal correction to Gibbs Free Energy= 0.118450
Sum of electronic and zero-point Energies= -695.418456
Sum of electronic and thermal Energies= -695.408286
Sum of electronic and thermal Enthalpies= -695.407342
Sum of electronic and thermal Free Energies= -695.452760
CBS-DLPNO-CCSD(T) Single Point Energy = -694.600558151208

Transition States of Boryl Sulfenate Elimination for Sulfoxide Family **4B**

4BO-B‡

S -0.9315230000 0.5722310000 -0.3404700000
C -1.4611940000 -0.7833290000 0.7308800000
H -2.2756880000 -0.4547390000 1.3747760000
H -0.6220990000 -1.1340940000 1.3260300000
H -1.8161930000 -1.5699180000 0.0611210000
O -0.2950190000 1.6471880000 0.6492780000
C 1.3245310000 -0.2179730000 -0.8039590000
C 2.0011540000 0.3859710000 0.0382670000
H 1.0735340000 -0.8633530000 -1.6151020000
H 3.0137260000 0.5023400000 0.3765330000
B 0.9105190000 1.4602390000 1.4392110000
O 1.6553480000 2.6036020000 1.6751940000
O 0.8055030000 0.5342260000 2.4715740000
C 1.7529340000 3.6151230000 0.6887560000
H 2.4152910000 4.3912000000 1.0722290000
H 2.1702970000 3.2202230000 -0.2440440000
H 0.7757290000 4.0531210000 0.4697870000
C 1.8245940000 0.4574510000 3.4520760000
H 1.9846660000 1.4218720000 3.9394590000
H 1.5156310000 -0.2773610000 4.1957700000
H 2.7745940000 0.1314350000 3.0125950000
Zero-point correction= 0.160600 (Hartree/Particle)
Thermal correction to Energy= 0.173761
Thermal correction to Enthalpy= 0.174705
Thermal correction to Gibbs Free Energy= 0.121375
Sum of electronic and zero-point Energies= -845.936373
Sum of electronic and thermal Energies= -845.923212
Sum of electronic and thermal Enthalpies= -845.922267
Sum of electronic and thermal Free Energies= -845.975597
CBS-DLPNO-CCSD(T) Single Point Energy = -844.938384873680
Imaginary frequency: - 443.79cm-1

4BF-B‡

S -0.6775630000 0.0889310000 -0.7636710000
C -1.5448820000 -0.6221930000 0.6534290000
H -2.2781560000 0.0860290000 1.0366910000
H -0.8494240000 -0.9119490000 1.4371300000
H -2.0605860000 -1.5016000000 0.2609570000
O 0.0561420000 1.3979920000 -0.1749290000
C 1.6988260000 -1.0151160000 -0.4377020000
C 2.2631830000 -0.1329940000 0.2033820000
H 1.3867730000 -1.8688870000 -0.9892150000
H 3.1815080000 0.1801090000 0.6620320000

B 1.0575980000 1.3728610000 0.8297340000
F 0.7222300000 0.8901580000 2.0544760000
F 1.8683840000 2.4474950000 0.8278560000
Zero-point correction= 0.080432 (Hartree/Particle)
Thermal correction to Energy= 0.089698
Thermal correction to Enthalpy= 0.090642
Thermal correction to Gibbs Free Energy= 0.046340
Sum of electronic and zero-point Energies= -815.467589
Sum of electronic and thermal Energies= -815.458323
Sum of electronic and thermal Enthalpies= -815.457378
Sum of electronic and thermal Free Energies= -815.501681
CBS-DLPNO-CCSD(T) Single Point Energy = -814.520610402502
Imaginary frequency: -410.41 cm-1

4BH-B‡
S -0.7834780000 0.1390030000 -0.8327590000
C -1.5155390000 -0.6273810000 0.6307150000
H -2.1473830000 0.0915550000 1.1521040000
H -0.7587970000 -1.0273250000 1.3017150000
H -2.1357230000 -1.4391300000 0.2444400000
O 0.0272690000 1.4197180000 -0.2892110000
C 1.6305090000 -1.0252230000 -0.4603160000
C 2.1375200000 -0.1662440000 0.2573190000
H 1.3242520000 -1.8301270000 -1.0828200000
H 3.0235420000 0.1118610000 0.7945510000
B 0.9568000000 1.3500050000 0.7822420000
H 1.6965160000 2.2904520000 0.8147840000
H 0.6071630000 0.8548460000 1.8193180000
Zero-point correction= 0.092597 (Hartree/Particle)
Thermal correction to Energy= 0.100252
Thermal correction to Enthalpy= 0.101196
Thermal correction to Gibbs Free Energy= 0.061315
Sum of electronic and zero-point Energies= -616.739330
Sum of electronic and thermal Energies= -616.731674
Sum of electronic and thermal Enthalpies= -616.730730
Sum of electronic and thermal Free Energies= -616.770612
CBS-DLPNO-CCSD(T) Single Point Energy = -615.996695221179
Imaginary frequency: -366.26 cm-1

4BC-B‡
S -0.7150840000 0.2602030000 -0.7574950000
C -1.6422280000 -0.6357080000 0.5154850000
H -2.2135790000 0.0687920000 1.1190420000
H -0.9992550000 -1.2461290000 1.1446710000

H -2.3349600000 -1.2755520000 -0.0360140000
O 0.0596840000 1.4447730000 -0.0270110000
C 1.5560620000 -1.0137370000 -0.4940980000
C 2.1547270000 -0.2452670000 0.2560330000
H 1.2285860000 -1.7893370000 -1.1434600000
H 3.0764350000 -0.0785450000 0.7773650000
B 1.1207490000 1.3777940000 0.9517180000
C 0.7830340000 0.8788960000 2.4316590000
H 0.2155780000 -0.0483580000 2.4984730000
H 1.6930100000 0.7516690000 3.0233870000
H 0.1951290000 1.6596760000 2.9296980000
C 2.1316470000 2.5958720000 0.7893860000
H 1.6448400000 3.5163100000 1.1315190000
H 3.0322510000 2.4739600000 1.3972620000
H 2.4336000000 2.7582230000 -0.2476960000
Zero-point correction= 0.148383 (Hartree/Particle)
Thermal correction to Energy= 0.159596
Thermal correction to Enthalpy= 0.160540
Thermal correction to Gibbs Free Energy= 0.112733
Sum of electronic and zero-point Energies= -695.370870
Sum of electronic and thermal Energies= -695.359657
Sum of electronic and thermal Enthalpies= -695.358713
Sum of electronic and thermal Free Energies= -695.406520
CBS-DLPNO-CCSD(T) Single Point Energy = -694.539776084582
Imaginary frequency: -391.50 cm-1

Products of Boryl Sulfenate Elimination for Sulfoxide Family **4B**

290
Acetylene
H 0.0000000000 0.0000000000 1.6615070000
C 0.0000000000 0.0000000000 0.5985150000
C 0.0000000000 0.0000000000 -0.5985150000
H 0.0000000000 0.0000000000 -1.6615070000
Zero-point correction= 0.026813 (Hartree/Particle)
Thermal correction to Energy= 0.029650
Thermal correction to Enthalpy= 0.030594
Thermal correction to Gibbs Free Energy= 0.007848
Sum of electronic and zero-point Energies= -77.337992
Sum of electronic and thermal Energies= -77.335156
Sum of electronic and thermal Enthalpies= -77.334211
Sum of electronic and thermal Free Energies= -77.356957
CBS-DLPNO-CCSD(T) Single Point Energy = -77.221939463899

Starting Materials of Sulfenic Acid Elimination for Boronic Esters

1Bcat-H

C 0.0021930000 -0.0067280000 -0.0251740000
S -0.0166270000 -0.0232090000 1.7953960000
O 1.4097760000 -0.0313560000 2.2329680000
C -0.6338930000 1.6916430000 2.0631520000
H -1.0093220000 0.1446460000 -0.4040500000
H 0.3728060000 -0.9822790000 -0.3356740000
H 0.6779340000 0.7705370000 -0.3786710000
C 0.3718780000 2.7652450000 1.6598540000
H -0.8342140000 1.7274790000 3.1350250000
H -1.5906600000 1.7778890000 1.5433600000
H 0.4517470000 2.8539340000 0.5743260000
H 1.3648490000 2.4494530000 2.0075640000
B 0.0696110000 4.1676790000 2.2673800000
O 0.5234010000 5.3704490000 1.7393250000
O -0.6737500000 4.3858850000 3.4223370000
C 0.0623220000 6.3482790000 2.5941610000
C -0.6652420000 5.7507760000 3.6165300000
C 0.2408350000 7.7128680000 2.5257250000
C -1.2521580000 6.4858150000 4.6232210000
C -0.3489330000 8.4712370000 3.5410200000
C -1.0786610000 7.8716330000 4.5662850000
H 0.8098660000 8.1663770000 1.7260990000
H -0.2345350000 9.5471360000 3.5294730000
H -1.5204000000 8.4903490000 5.3362150000
H -1.8146130000 6.0089540000 5.4138880000
Zero-point correction= 0.191686 (Hartree/Particle)
Thermal correction to Energy= 0.204821
Thermal correction to Enthalpy= 0.205765
Thermal correction to Gibbs Free Energy= 0.149821
Sum of electronic and zero-point Energies= -998.470028
Sum of electronic and thermal Energies= -998.456893
Sum of electronic and thermal Enthalpies= -998.455949
Sum of electronic and thermal Free Energies= -998.511894
CBS-DLPNO-CCSD(T) Single Point Energy = -997.232470423489

1Bmida

O -0.6197750000 1.0329460000 -1.2105300000
C -0.3765410000 1.9687500000 -0.2947430000
O -0.1041830000 3.1132470000 -0.5258680000
O -2.0707620000 -0.9393120000 -1.0943510000

C -3.1028930000 -0.6448010000 -0.3123830000
O -4.2385210000 -0.9841300000 -0.4847620000
C -0.4515930000 1.3644510000 1.1036600000
H 0.5682090000 1.1748640000 1.4407220000
H -0.9662020000 2.0179120000 1.8049280000
C -2.6305990000 0.2147380000 0.8574510000
H -2.8886580000 1.2505570000 0.6386300000
H -3.1092790000 -0.0768140000 1.7890450000
B -0.8003690000 -0.3344620000 -0.6785910000
N -1.1452270000 0.0623040000 0.9248580000
C -0.7712820000 -0.9605070000 1.9338620000
H -1.1073640000 -0.6401360000 2.9206560000
H -1.2570860000 -1.8999400000 1.6738060000
H 0.3076490000 -1.0779690000 1.9336710000
C 1.8048750000 -0.6947470000 -1.2390720000
C 0.4203240000 -1.3230140000 -1.0194190000
O 2.2295940000 -0.1425620000 1.3653640000
H 2.3563890000 -1.2012670000 -2.0356210000
H 0.4782850000 -2.1613710000 -0.3181220000
H 0.1195380000 -1.7813940000 -1.9660220000
C 4.2090260000 0.2408490000 -0.3599780000
H 3.7929760000 1.2340980000 -0.5291590000
H 4.9598580000 0.2770210000 0.4274900000
H 4.6457340000 -0.1625840000 -1.2738620000
H 1.7344050000 0.3641630000 -1.4949760000
S 2.8878280000 -0.8572990000 0.2182920000
Zero-point correction= 0.235314 (Hartree/Particle)
Thermal correction to Energy= 0.251145
Thermal correction to Enthalpy= 0.252089
Thermal correction to Gibbs Free Energy= 0.192326
Sum of electronic and zero-point Energies= -1167.444728
Sum of electronic and thermal Energies= -1167.428896
Sum of electronic and thermal Enthalpies= -1167.427952
Sum of electronic and thermal Free Energies= -1167.487716
CBS-DLPNO-CCSD(T) Single Point Energy = -1166.064125176

1Bmida-H

C 1.6717870000 0.5061010000 1.0406130000
S 1.1318700000 -0.0529530000 -0.6080810000
O 0.8735590000 -1.5153490000 -0.4905380000
C -0.5133340000 0.7844450000 -0.6304860000
H 1.7480800000 1.5943160000 1.0578070000
H 2.6529940000 0.0646840000 1.2072240000
H 0.9759300000 0.1430620000 1.7956450000
C -1.5182750000 0.1972620000 0.3513080000

H -0.8575310000 0.6465950000 -1.6565920000
H -0.3090520000 1.8484450000 -0.4889650000
H -1.2512400000 0.4428900000 1.3849100000
H -1.4437760000 -0.8940350000 0.2893050000
B -3.0509110000 0.5412800000 0.0782410000
O -3.9768570000 -0.3307280000 0.8354790000
O -3.4097250000 0.6496070000 -1.3318060000
C -4.5368920000 0.2159100000 1.9042030000
C -4.3187150000 1.5802660000 -1.6038540000
O -4.7922700000 1.8134770000 -2.6773580000
O -5.2462670000 -0.3342820000 2.6971420000
C -4.1329250000 1.6913450000 2.0050780000
C -4.6903540000 2.3336240000 -0.3238700000
N -3.6093700000 2.0439160000 0.6648420000
C -2.6073010000 3.1312050000 0.6884570000
H -2.2535940000 3.3101630000 -0.3248800000
H -1.7683260000 2.8320080000 1.3110810000
H -3.0524500000 4.0448550000 1.0841910000
H -3.3327630000 1.7829900000 2.7398680000
H -4.9663470000 2.3204890000 2.3112120000
H -5.6392990000 1.9377450000 0.0365120000
H -4.8009440000 3.4000900000 -0.5054180000
Zero-point correction= 0.234747 (Hartree/Particle)
Thermal correction to Energy= 0.250869
Thermal correction to Enthalpy= 0.251813
Thermal correction to Gibbs Free Energy= 0.190305
Sum of electronic and zero-point Energies= -1167.431816
Sum of electronic and thermal Energies= -1167.415694
Sum of electronic and thermal Enthalpies= -1167.414750
Sum of electronic and thermal Free Energies= -1167.476258
CBS-DLPNO-CCSD(T) Single Point Energy = -1166.051253403277

1Bpin-H
C 1.7182960000 0.6899220000 0.9475360000
S 1.1281700000 0.0977130000 -0.6700800000
O 0.9721930000 -1.3816670000 -0.5453480000
C -0.5663430000 0.8132120000 -0.6052560000
H 1.7145460000 1.7805160000 0.9660850000
H 2.7363630000 0.3198050000 1.0572910000
H 1.0913060000 0.2790830000 1.7372860000
C -1.4594910000 0.1837170000 0.4568190000
H -0.9610110000 0.6271860000 -1.6052640000
H -0.4532000000 1.8939690000 -0.4910540000
H -1.1880360000 0.5179730000 1.4603360000

H -1.2909750000 -0.9013230000 0.4460180000
B -2.9890520000 0.4269240000 0.2190130000
O -3.9404120000 0.2826270000 1.1947600000
O -3.5216990000 0.7819000000 -0.9942980000
C -5.2050040000 0.7610460000 0.6551590000
C -4.9685060000 0.6481490000 -0.8957100000
C -5.3674990000 2.2022160000 1.1367350000
C -6.3283970000 -0.1063840000 1.1990750000
C -5.3184240000 -0.7278570000 -1.4603500000
C -5.6179720000 1.7413300000 -1.7282130000
H -4.5657260000 2.8358300000 0.7564520000
H -5.3224780000 2.2154690000 2.2257040000
H -6.3233740000 2.6236450000 0.8238230000
H -5.2535250000 2.7276130000 -1.4492820000
H -6.7028030000 1.7210440000 -1.6077530000
H -5.3894140000 1.5820720000 -2.7823500000
H -6.1463590000 -1.1618750000 1.0096400000
H -7.2818540000 0.1727340000 0.7463750000
H -6.4087830000 0.0340560000 2.2773130000
H -4.8532020000 -1.5223470000 -0.8764700000
H -4.9430920000 -0.7946960000 -2.4814440000
H -6.3965250000 -0.8909970000 -1.4754360000
Zero-point correction= 0.279802 (Hartree/Particle)
Thermal correction to Energy= 0.296302
Thermal correction to Enthalpy= 0.297246
Thermal correction to Gibbs Free Energy= 0.235326
Sum of electronic and zero-point Energies= -1003.234452
Sum of electronic and thermal Energies= -1003.217952
Sum of electronic and thermal Enthalpies= -1003.217008
Sum of electronic and thermal Free Energies= -1003.278928
CBS-DLPNO-CCSD(T) Single Point Energy = -1002.081293356374

Transition States of Sulfenic Acid Elimination for Boronic Esters

1Bcat-H‡
C -0.0326450000 0.0341910000 -0.0382920000
S -0.0632790000 0.0204160000 1.7721130000
O 1.4421550000 -0.0682040000 2.1719180000
C -0.0538700000 2.2351210000 2.0473630000
H -1.0472400000 0.2368100000 -0.3866050000
H 0.2955840000 -0.9393980000 -0.3982450000
H 0.6475620000 0.8120250000 -0.3834970000
C 1.3334120000 2.4877580000 2.2484790000

H -0.7176890000 2.2949840000 2.9023560000
H -0.5262070000 2.5231840000 1.1144000000
H 1.8960460000 2.8264140000 1.3828950000
H 1.7203730000 1.0972650000 2.2944490000
B 1.8527750000 2.8794430000 3.6223990000
O 3.1210530000 3.4036760000 3.8889130000
O 1.1329900000 2.7186310000 4.8138710000
C 3.1780530000 3.5605010000 5.2530890000
C 1.9740450000 3.1443320000 5.8139010000
C 4.2127000000 4.0426230000 6.0249090000
C 1.7486370000 3.1899790000 7.1723990000
C 2.7917230000 3.6768700000 7.9670870000
C 3.9966020000 4.0937440000 7.4059090000
H 4.7833950000 4.4646560000 8.0496970000
H 5.1437070000 4.3625810000 5.5776110000
H 0.8092670000 2.8628230000 7.5964930000
H 2.6577800000 3.7291270000 9.0396590000
Zero-point correction= 0.185888 (Hartree/Particle)
Thermal correction to Energy= 0.198753
Thermal correction to Enthalpy= 0.199697
Thermal correction to Gibbs Free Energy= 0.145247
Sum of electronic and zero-point Energies= -998.436082
Sum of electronic and thermal Energies= -998.423218
Sum of electronic and thermal Enthalpies= -998.422274
Sum of electronic and thermal Free Energies= -998.476723
CBS-DLPNO-CCSD(T) Single Point Energy = -997.185669946754
Imaginary frequency: -1152.73 cm-1

1Bmida-H‡

C 3.5308970000 -0.1976280000 -0.4416350000
S 1.9524350000 0.6757280000 -0.6305940000
O 1.0163990000 -0.3788750000 -1.2871970000
C 1.0839510000 0.0857280000 1.4666940000
H 4.1973880000 0.4401230000 0.1425190000
H 3.9626370000 -0.3814210000 -1.4243500000
H 3.3658240000 -1.1425280000 0.0752560000
C 0.2808750000 -1.0096060000 1.0759040000
H 0.6262300000 1.0468510000 1.6711640000
H 2.0326740000 -0.0639820000 1.9696010000
H 0.7246320000 -1.9928480000 1.2303790000
H 0.4701820000 -0.8798420000 -0.2931330000
B -1.2871640000 -0.9229210000 1.0796870000
O -1.9553830000 -1.9767560000 0.3210540000
O -1.8199200000 0.4283170000 0.7981600000
C -3.0821250000 -2.4309130000 0.8549570000

C -2.2368950000 1.1141720000 1.8518590000
O -3.8132040000 -3.2485660000 0.3742180000
O -2.5984890000 2.2573250000 1.8551680000
C -2.1745530000 0.2406500000 3.1098250000
C -3.3360880000 -1.7520570000 2.2036040000
N -2.0415590000 -1.1470290000 2.6208700000
C -1.2994960000 -2.0382520000 3.5359120000
H -1.1996210000 -3.0177420000 3.0709660000
H -1.8310680000 -2.1364630000 4.4836030000
H -0.3071120000 -1.6276240000 3.7012420000
H -3.7148870000 -2.4586300000 2.9388830000
H -4.0808430000 -0.9712010000 2.0515590000
H -3.0463870000 0.3871570000 3.7448850000
H -1.2800260000 0.5111060000 3.6708650000
Zero-point correction= 0.228165 (Hartree/Particle)
Thermal correction to Energy= 0.244322
Thermal correction to Enthalpy= 0.245266
Thermal correction to Gibbs Free Energy= 0.184023
Sum of electronic and zero-point Energies= -1167.396110
Sum of electronic and thermal Energies= -1167.379953
Sum of electronic and thermal Enthalpies= -1167.379008
Sum of electronic and thermal Free Energies= -1167.440252
CBS-DLPNO-CCSD(T) Single Point Energy = -1166.001223596375
Imaginary frequency: -1302.07 cm-1

1Bpin-H‡
C 3.8392900000 -0.6483660000 0.0886220000
S 2.5697920000 0.6077970000 -0.2183380000
O 1.6582850000 -0.0410890000 -1.3059040000
C 1.1198080000 -0.0846560000 1.4183280000
H 4.4365510000 -0.3170520000 0.9403840000
H 4.4721830000 -0.7462020000 -0.7920330000
H 3.3599700000 -1.6006200000 0.3134740000
C 0.2465290000 -0.8960360000 0.6522950000
H 0.7818650000 0.8971240000 1.7277430000
H 1.8451540000 -0.5338460000 2.0877250000
H 0.4207890000 -1.9683080000 0.6904540000
H 0.8052250000 -0.5799310000 -0.6074180000
B -1.1690460000 -0.4031300000 0.3226650000
O -2.1503120000 -1.1814940000 -0.2477170000
O -1.5764260000 0.9015500000 0.5109970000
C -3.3720490000 -0.3978820000 -0.2755040000
C -2.8229310000 1.0740000000 -0.2127160000
C -4.1788200000 -0.7903500000 0.9622780000

C -4.1444830000 -0.7417470000 -1.5391430000
C -2.4600280000 1.6379020000 -1.5866410000
C -3.7000660000 2.0562390000 0.5467720000
H -3.6360590000 -0.5460840000 1.8757770000
H -4.3453320000 -1.8675280000 0.9446440000
H -5.1475390000 -0.2896230000 0.9859630000
H -3.5270320000 -0.6261610000 -2.4272290000
H -5.0251240000 -0.1036490000 -1.6370010000
H -4.4781630000 -1.7789040000 -1.4925940000
H -3.8338600000 1.7536220000 1.5831640000
H -4.6814040000 2.1392890000 0.0753220000
H -3.2346030000 3.0424320000 0.5400090000
H -1.8251960000 0.9450280000 -2.1392920000
H -1.9041640000 2.5653940000 -1.4485570000
H -3.3491700000 1.8510430000 -2.1813160000
Zero-point correction= 0.273787 (Hartree/Particle)
Thermal correction to Energy= 0.290086
Thermal correction to Enthalpy= 0.291031
Thermal correction to Gibbs Free Energy= 0.230316
Sum of electronic and zero-point Energies= -1003.199091
Sum of electronic and thermal Energies= -1003.182791
Sum of electronic and thermal Enthalpies= -1003.181847
Sum of electronic and thermal Free Energies= -1003.242562
CBS-DLPNO-CCSD(T) Single Point Energy = -1002.032570388569
Imaginary frequency: -1250.91 cm-1

Products of Sulfenic Acid Elimination for Boronic Esters

Catechol vinylboronate

C -0.0212640000 2.3005790000 2.0283570000
C 1.2236980000 2.7342030000 2.2370580000
H -0.7023410000 2.1260920000 2.8541230000
H -0.4078690000 2.1038920000 1.0346620000
H 1.8729990000 2.8959080000 1.3812670000
B 1.7834270000 3.0165670000 3.6403930000
O 3.0752950000 3.4686140000 3.8952530000
O 1.0747520000 2.8574500000 4.8296420000
C 3.1617880000 3.5891570000 5.2629520000
C 1.9467210000 3.2179080000 5.8296030000
C 4.2305760000 4.0003370000 6.0299280000
C 1.7401110000 3.2394460000 7.1922570000
C 2.8162860000 3.6545940000 7.9814660000
C 4.0339110000 4.0266060000 7.4133650000
H 4.8453280000 4.3427800000 8.0556090000

H 5.1698700000 4.2863720000 5.5773090000
H 0.7913100000 2.9486610000 7.6214250000
H 2.6998170000 3.6872800000 9.0567610000
Zero-point correction= 0.136023 (Hartree/Particle)
Thermal correction to Energy= 0.144600
Thermal correction to Enthalpy= 0.145545
Thermal correction to Gibbs Free Energy= 0.102093
Sum of electronic and zero-point Energies= -484.510495
Sum of electronic and thermal Energies= -484.501917
Sum of electronic and thermal Enthalpies= -484.500973
Sum of electronic and thermal Free Energies= -484.544424
CBS-DLPNO-CCSD(T) Single Point Energy = -483.829395433420

N-methyliminodiacetyl vinylboronate (N→B coordination)
C 1.0819750000 0.2106100000 1.7919400000
C 0.3174190000 -0.8696830000 1.6435680000
H 0.6664630000 1.2096090000 1.7093160000
H 2.1496050000 0.1497310000 1.9728010000
H 0.7978600000 -1.8451800000 1.7043110000
B -1.2341820000 -0.8176820000 1.3651980000
O -1.7193150000 -1.8284180000 0.4306940000
O -1.7718450000 0.5291800000 1.0888750000
C -2.8979070000 -2.3549770000 0.7466690000
C -2.3715120000 1.1226310000 2.1120020000
O -3.5140730000 -3.1493720000 0.0975480000
O -2.7882750000 2.2456910000 2.1337860000
C -2.4492900000 0.1613130000 3.3032720000
C -3.3786470000 -1.7935360000 2.0886460000
N -2.1862350000 -1.1817840000 2.7405520000
C -1.5556890000 -2.1187750000 3.6966460000
H -1.3424220000 -3.0555670000 3.1843690000
H -2.2252640000 -2.3065740000 4.5368730000
H -0.6215690000 -1.6898240000 4.0495080000
H -3.8281160000 -2.5685810000 2.7051730000
H -4.1265890000 -1.0276950000 1.8855090000
H -3.4079840000 0.2263000000 3.8139980000
H -1.6542750000 0.4178860000 4.0032720000
Zero-point correction= 0.178799 (Hartree/Particle)
Thermal correction to Energy= 0.190471
Thermal correction to Enthalpy= 0.191415
Thermal correction to Gibbs Free Energy= 0.141343
Sum of electronic and zero-point Energies= -653.473651
Sum of electronic and thermal Energies= -653.461979
Sum of electronic and thermal Enthalpies= -653.461035

Sum of electronic and thermal Free Energies= -653.511106
CBS-DLPNO-CCSD(T) Single Point Energy = -652.650630186282

Pinacol vinylboronate
C 1.1080020000 -0.1383610000 1.4169400000
C 0.1720960000 -0.9246000000 0.8834310000
H 0.9357940000 0.9243520000 1.5499750000
H 2.0723470000 -0.5158110000 1.7400780000
H 0.3840630000 -1.9841120000 0.7662620000
B -1.2076100000 -0.3910350000 0.4252470000
O -2.1597190000 -1.1767130000 -0.1751620000
O -1.6116080000 0.9140000000 0.5717530000
C -3.3829830000 -0.3952350000 -0.2636020000
C -2.8404100000 1.0791440000 -0.1864580000
C -4.2388820000 -0.7852740000 0.9411010000
C -4.0989170000 -0.7510060000 -1.5565670000
C -2.4427660000 1.6457720000 -1.5492800000
C -3.7413010000 2.0583560000 0.5488030000
H -3.7354040000 -0.5376520000 1.8758490000
H -4.4038440000 -1.8625340000 0.9201810000
H -5.2078990000 -0.2852220000 0.9222950000
H -3.4462790000 -0.6373980000 -2.4193760000
H -4.9778340000 -0.1182550000 -1.6948750000
H -4.4291230000 -1.7894480000 -1.5173750000
H -3.9025300000 1.7554710000 1.5810480000
H -4.7093760000 2.1380200000 0.0502980000
H -3.2788590000 3.0458260000 0.5549800000
H -1.7934800000 0.9543770000 -2.0869000000
H -1.8941580000 2.5751060000 -1.3958740000
H -3.3169830000 1.8564580000 -2.1663460000
Zero-point correction= 0.224072 (Hartree/Particle)
Thermal correction to Energy= 0.236035
Thermal correction to Enthalpy= 0.236979
Thermal correction to Gibbs Free Energy= 0.187386
Sum of electronic and zero-point Energies= -489.273395
Sum of electronic and thermal Energies= -489.261432
Sum of electronic and thermal Enthalpies= -489.260488
Sum of electronic and thermal Free Energies= -489.310081
CBS-DLPNO-CCSD(T) Single Point Energy = -488.677234073487

Starting Materials for Boryl Sulfenate Elimination for Boronic Esters

1Bpin

C -3.5331180000 -0.4477170000 1.9208920000
S -2.5689240000 0.9401250000 1.2466700000
O -1.1564120000 0.7144160000 1.6839900000
C -2.6480880000 0.4710380000 -0.5289660000
H -3.5306790000 -0.3226230000 3.0024890000
H -3.0557100000 -1.3907370000 1.6597270000
H -4.5551370000 -0.4026530000 1.5432410000
C -1.7634120000 -0.7273600000 -0.8680950000
H -2.3069930000 1.3623680000 -1.0580370000
H -3.7046070000 0.3176090000 -0.7626630000
H -1.9280140000 -0.9648610000 -1.9259470000
H -2.0620310000 -1.6171680000 -0.3119610000
B -0.2221360000 -0.4594710000 -0.6864980000
O 0.6574090000 -1.3743830000 -0.1781500000
O 0.3868890000 0.6725730000 -1.1624710000
C 1.7713960000 0.6464180000 -0.7127820000
C 2.0033970000 -0.8900330000 -0.4388830000
C 2.5090130000 -1.6546650000 -1.6617150000
C 2.8689110000 -1.1988910000 0.7723750000
C 1.8456640000 1.5070570000 0.5467580000
C 2.6447490000 1.2389270000 -1.8080960000
H 1.8846870000 -1.4557880000 -2.5332210000
H 2.4644260000 -2.7232710000 -1.4504290000
H 3.5395600000 -1.3913490000 -1.9028310000
H 2.4309990000 -0.7963420000 1.6827800000
H 3.8701740000 -0.7819010000 0.6471320000
H 2.9609080000 -2.2794260000 0.8882350000
H 2.4903930000 0.7397940000 -2.7625270000
H 3.7003400000 1.1642330000 -1.5394130000
H 2.4004770000 2.2940410000 -1.9347950000
H 1.1893320000 1.1232940000 1.3247780000
H 1.5088120000 2.5143580000 0.2998760000
H 2.8676240000 1.5676970000 0.9237470000
Zero-point correction= 0.280071 (Hartree/Particle)
Thermal correction to Energy= 0.296317
Thermal correction to Enthalpy= 0.297261
Thermal correction to Gibbs Free Energy= 0.236976
Sum of electronic and zero-point Energies= -1003.237619
Sum of electronic and thermal Energies= -1003.221372
Sum of electronic and thermal Enthalpies= -1003.220428
Sum of electronic and thermal Free Energies= -1003.280713
CBS-DLPNO-CCSD(T) Single Point Energy = -1002.084220574448

1Bcat

H 0.0770160000 -0.0724600000 -0.0267720000
C 0.0165220000 -0.0401690000 1.0599370000
H 1.0082170000 0.0695170000 1.4970960000
S -0.6734390000 -1.6313860000 1.6011260000
H -0.6505200000 0.7639690000 1.3741630000
O 0.3851600000 -2.6623540000 1.3258440000
C -0.5773600000 -1.3319720000 3.4443650000
C 0.2793910000 -2.4390890000 4.0569610000
H -0.2399720000 -3.3977600000 4.0225600000
H 0.4338540000 -2.1999130000 5.1148720000
H -1.6020810000 -1.3315260000 3.8159860000
H -0.1381490000 -0.3494010000 3.6151490000
B 1.6719240000 -2.5742970000 3.3477900000
O 2.4503780000 -1.4615730000 2.9971480000
C 3.6420000000 -1.9839410000 2.5513330000
O 2.4071410000 -3.7480320000 3.2269140000
C 3.6144530000 -3.3684580000 2.6923210000
C 4.6840540000 -4.1570850000 2.3291170000
C 4.7384680000 -1.3243220000 2.0413970000
C 5.8034300000 -3.4998240000 1.8081480000
C 5.8306240000 -2.1143890000 1.6672800000
H 4.6501030000 -5.2320370000 2.4404850000
H 6.6645640000 -4.0821350000 1.5073320000
H 6.7125010000 -1.6375210000 1.2598440000
H 4.7487860000 -0.2478330000 1.9377560000
Zero-point correction= 0.191744 (Hartree/Particle)
Thermal correction to Energy= 0.204597
Thermal correction to Enthalpy= 0.205542
Thermal correction to Gibbs Free Energy= 0.151818
Sum of electronic and zero-point Energies= -998.471875
Sum of electronic and thermal Energies= -998.459022
Sum of electronic and thermal Enthalpies= -998.458078
Sum of electronic and thermal Free Energies= -998.511801
CBS-DLPNO-CCSD(T) Single Point Energy = -997.234772562179

1Bcat-B
C -0.7552270000 -0.6690740000 -3.1765750000
S -2.1385890000 -0.5518300000 -2.0168020000
O -1.5186710000 -0.7144050000 -0.6161090000
C -2.3721640000 1.2749060000 -1.9876500000
H -0.4065230000 -1.6999020000 -3.1499790000
H 0.0436060000 0.0012620000 -2.8661800000
H -1.1306230000 -0.4251860000 -4.1710900000
C -1.2823770000 1.8046750000 -1.0589490000

H -3.3770690000 1.4065910000 -1.5866850000
H -2.3542710000 1.6399220000 -3.0147070000
H -1.7068810000 2.5549660000 -0.3922250000
H -0.4933760000 2.2857850000 -1.6373450000
B -0.6154190000 0.6214710000 -0.1571610000
O 0.7686410000 0.2983970000 -0.4748990000
O -0.7253680000 0.6822300000 1.2752320000
C 0.4561510000 0.2068520000 1.7633460000
C 1.3522870000 -0.0243020000 0.7152340000
C 2.6279350000 -0.4917850000 0.9476660000
C 2.9949850000 -0.7303860000 2.2791350000
C 2.1041530000 -0.5005090000 3.3211390000
C 0.8095800000 -0.0232170000 3.0756120000
H 3.3141730000 -0.6644040000 0.1290160000
H 3.9892240000 -1.0995850000 2.4960040000
H 2.4120980000 -0.6934240000 4.3408400000
H 0.1079620000 0.1598200000 3.8784750000
Zero-point correction= 0.191582 (Hartree/Particle)
Thermal correction to Energy= 0.203993
Thermal correction to Enthalpy= 0.204937
Thermal correction to Gibbs Free Energy= 0.152638
Sum of electronic and zero-point Energies= -998.472503
Sum of electronic and thermal Energies= -998.460092
Sum of electronic and thermal Enthalpies= -998.459148
Sum of electronic and thermal Free Energies= -998.511448
CBS-DLPNO-CCSD(T) Single Point Energy = -997.238479481029

1BmidaSO

O	1.4355970000	-1.3388070000	-0.9531120000
C	2.7372120000	-1.1184850000	-0.8107240000
O	3.6205970000	-1.7177790000	-1.3510530000
O	0.2726590000	0.8124470000	-0.9862410000
C	0.5422490000	1.9519290000	-0.3685770000
O	0.2415730000	3.0494980000	-0.7460680000
C	2.9665230000	0.0442890000	0.1572870000
H	3.7920760000	-0.1582940000	0.8355950000
H	3.2056480000	0.9284940000	-0.4325830000
C	1.2809250000	1.6791170000	0.9465190000
H	2.1276340000	2.3503520000	1.0768120000
H	0.5882020000	1.8309920000	1.7733480000
B	0.5717570000	-0.4205170000	-0.2207250000
N	1.6821940000	0.2534380000	0.8903750000
C	1.7084170000	-0.4104770000	2.2132860000
H	0.7259910000	-0.3352180000	2.6717190000

H	1.9541390000	-1.4617970000	2.0761990000
H	2.4543110000	0.0589890000	2.8555000000
C	-1.7430860000	-0.2311440000	1.0834910000
C	-0.7035390000	-1.1334440000	0.4036670000
O	-3.6668840000	-1.6482080000	-0.1496230000
H	-1.9720670000	-0.5622580000	2.0974510000
H	-1.1903420000	-1.6806340000	-0.4120400000
H	-0.3986880000	-1.9277880000	1.0890130000
C	-2.9208190000	0.6480050000	-1.2590290000
H	-2.6041580000	1.6624520000	-1.0155050000
H	-2.1222240000	0.1139710000	-1.7693310000
H	-3.8137200000	0.6716300000	-1.8818660000
H	-1.4677640000	0.8249920000	1.1400310000
S	-3.3968000000	-0.2389570000	0.2537450000

Zero-point correction= 0.234911 (Hartree/Particle)
Thermal correction to Energy= 0.250923
Thermal correction to Enthalpy= 0.251867
Thermal correction to Gibbs Free Energy= 0.190993
Sum of electronic and zero-point Energies= -1167.432104
Sum of electronic and thermal Energies= -1167.416092
Sum of electronic and thermal Enthalpies= -1167.415148
Sum of electronic and thermal Free Energies= -1167.476022
CBS-DLPNO-CCSD(T) Single Point Energy = -1166.051234878

1Bmida-B

O	0.7384220000	-1.6737760000	-0.0897210000
C	1.9985510000	-1.5848650000	-0.5107670000
O	2.6577620000	-2.5668130000	-0.7370110000
O	-0.2310290000	0.4686500000	-0.8715850000
C	0.1550910000	1.7223800000	-0.6725360000
O	-0.5310980000	2.6577090000	-1.0141450000
C	2.5719060000	-0.1778360000	-0.6952080000
H	3.6567910000	-0.2829680000	-0.7761520000
H	2.2121840000	0.1848250000	-1.6606230000
C	1.5331150000	1.9482060000	-0.0538620000
H	2.1068600000	2.5405850000	-0.7867430000
H	1.3824900000	2.6022390000	0.8071940000
B	-0.2636450000	-0.6617480000	0.0789770000
N	2.1840010000	0.7349170000	0.3690540000
C	3.1940350000	0.9005550000	1.3965870000
H	2.7738190000	1.4363490000	2.2499300000
H	3.5203630000	-0.0795990000	1.7467610000
H	4.0833570000	1.4509460000	1.0483620000
C	-2.1095560000	0.2174580000	1.6038210000

C -0.6480170000 -0.2223820000 1.5974470000
O -1.5974150000 -1.4314740000 -0.3477580000
H -2.6682840000 -0.0116950000 2.5097340000
H -0.5008590000 -1.0748520000 2.2613910000
H -0.0210410000 0.5928520000 1.9565790000
C -3.3629350000 0.5352520000 -0.9142180000
H -4.2217310000 1.0358040000 -0.4626410000
H -2.5376700000 1.2245790000 -1.0827740000
H -3.6654350000 0.0510690000 -1.8413780000
H -2.2404820000 1.2685570000 1.3508390000
S -2.8835270000 -0.7775850000 0.2297150000
Zero-point correction= 0.233307 (Hartree/Particle)
Thermal correction to Energy= 0.249454
Thermal correction to Enthalpy= 0.250398
Thermal correction to Gibbs Free Energy= 0.189890
Sum of electronic and zero-point Energies= -1167.425544
Sum of electronic and thermal Energies= -1167.409397
Sum of electronic and thermal Enthalpies= -1167.408453
Sum of electronic and thermal Free Energies= -1167.468961
CBS-DLPNO-CCSD(T) Single Point Energy = -1166.039987284

Transition States of Boryl Sulfenate Elimination for Boronic Esters

1Bpin-B‡
C -2.2924540000 2.0482560000 2.7985680000
S -1.0350640000 2.9333640000 1.8598260000
O 0.2126500000 1.9668900000 2.0818740000
C -1.3632280000 1.8046770000 -0.2799160000
H -2.0174910000 2.0289260000 3.8520220000
H -2.3985970000 1.0318120000 2.4209200000
H -3.2285210000 2.5961470000 2.6743740000
C -0.2794970000 0.9271130000 -0.2588930000
H -1.3362010000 2.6813140000 -0.9142600000
H -2.3511870000 1.5033560000 0.0435730000
H 0.3945570000 0.9858950000 -1.1048230000
H -0.4473210000 -0.0741900000 0.1215080000
B 1.0437310000 1.6536800000 0.8914840000
O 2.0432100000 0.7134890000 1.1839270000
O 1.6027170000 2.7635960000 0.1997080000
C 3.0284530000 2.6954280000 0.3964670000
C 3.2640260000 1.1482120000 0.5542860000
C 3.3898920000 0.4259120000 -0.7898260000
C 4.4330890000 0.7687080000 1.4526750000

C 3.3633180000 3.4749380000 1.6720230000
C 3.7220970000 3.3303800000 -0.7993480000
H 2.5933220000 0.7173120000 -1.4734610000
H 3.3150150000 -0.6480120000 -0.6166800000
H 4.3470810000 0.6342240000 -1.2703040000
H 4.2858290000 1.1336760000 2.4668540000
H 5.3691300000 1.1748890000 1.0629890000
H 4.5240820000 -0.3175410000 1.4956100000
H 3.3795280000 2.8934750000 -1.7352640000
H 4.8050650000 3.2074700000 -0.7292560000
H 3.5018410000 4.3985010000 -0.8253390000
H 2.8838380000 3.0236400000 2.5404570000
H 2.9844190000 4.4919840000 1.5660440000
H 4.4391500000 3.5224800000 1.8481990000
Zero-point correction= 0.277082 (Hartree/Particle)
Thermal correction to Energy= 0.293134
Thermal correction to Enthalpy= 0.294078
Thermal correction to Gibbs Free Energy= 0.235282
Sum of electronic and zero-point Energies= -1003.205907
Sum of electronic and thermal Energies= -1003.189855
Sum of electronic and thermal Enthalpies= -1003.188911
Sum of electronic and thermal Free Energies= -1003.247707
CBS-DLPNO-CCSD(T) Single Point Energy = -1002.043515119510
Imaginary frequency: -377.26 cm-1

1Bcat-B‡
C -0.0388070000 0.1011200000 -0.0821290000
S -0.0997620000 0.0051170000 1.7147160000
O 1.4636940000 -0.1199710000 2.0402150000
C 0.1414590000 2.4076540000 2.2021000000
H 0.3702680000 -0.8249430000 -0.4829950000
H 0.5694390000 0.9483070000 -0.3969360000
H -1.0671270000 0.2263450000 -0.4265920000
C 1.4933990000 2.4488880000 2.5457110000
H -0.6180050000 2.4648430000 2.9710310000
H -0.2006400000 2.6295310000 1.1999200000
H 1.7295240000 2.8772090000 3.5159950000
H 2.1978590000 2.7051940000 1.7617600000
B 2.0100270000 0.7334130000 3.0851520000
O 3.4365120000 0.7073880000 3.1733070000
O 1.4657440000 0.5316990000 4.4114280000
C 2.5411970000 0.5506220000 5.2484060000
C 3.7227380000 0.6516490000 4.5065620000
C 4.9585970000 0.6826190000 5.1171630000

C 4.9850530000 0.6101510000 6.5151510000
C 3.8101460000 0.5108640000 7.2536710000
C 2.5590290000 0.4806040000 6.6257790000
H 5.8649590000 0.7578860000 4.5316730000
H 5.9381300000 0.6318440000 7.0276260000
H 3.8608770000 0.4564620000 8.3334900000
H 1.6393660000 0.3998710000 7.1895660000
Zero-point correction= 0.189054 (Hartree/Particle)
Thermal correction to Energy= 0.201754
Thermal correction to Enthalpy= 0.202698
Thermal correction to Gibbs Free Energy= 0.149651
Sum of electronic and zero-point Energies= -998.449139
Sum of electronic and thermal Energies= -998.436440
Sum of electronic and thermal Enthalpies= -998.435496
Sum of electronic and thermal Free Energies= -998.488542
CBS-DLPNO-CCSD(T) Single Point Energy = -997.200716819352
Imaginary frequency: -333.72 cm-1

1Bmida-B‡
H 2.8293890000 -1.0399100000 -2.1287790000
C 2.6562690000 -1.2931400000 -1.0836190000
H 1.8697700000 -2.0374010000 -0.9997060000
S 2.3112590000 0.2175100000 -0.1519330000
H 3.5867260000 -1.6648870000 -0.6473970000
O 1.0783320000 0.9432920000 -0.8874000000
C 0.4944470000 -0.4939890000 1.5818950000
C -0.5785630000 0.1942440000 1.0612170000
H -0.7505750000 1.2110790000 1.3935050000
H -1.4755590000 -0.3486980000 0.7811320000
H 1.1528010000 -0.0561670000 2.3170370000
H 0.5993680000 -1.5619920000 1.4335250000
B -0.2593680000 0.4149250000 -0.8722510000
O -0.3172610000 -0.8995380000 -1.4546800000
C -0.9265140000 -2.0617020000 -1.2029640000
O -1.1473130000 1.4329230000 -1.2823020000
C -2.3317600000 1.4105530000 -1.9161950000
O -2.8656040000 2.4331600000 -2.2484760000
C -2.9505240000 0.0418050000 -2.1761640000
C -2.4425080000 -2.0621890000 -1.0352810000
O -0.3070670000 -3.0938910000 -1.1735840000
N -3.0300140000 -0.7483160000 -0.9525090000
H -2.3341090000 -0.4650150000 -2.9209060000
H -3.9333780000 0.2099560000 -2.6227250000
C -4.3406010000 -0.7078150000 -0.3243830000

H -2.6478060000 -2.6132080000 -0.1159680000
H -2.8399910000 -2.6825280000 -1.8564400000
H -4.6513640000 0.3300110000 -0.2011090000
H -4.2918020000 -1.1631060000 0.6660820000
H -5.1144460000 -1.2300540000 -0.9089010000
Zero-point correction= 0.230201 (Hartree/Particle)
Thermal correction to Energy= 0.247052
Thermal correction to Enthalpy= 0.247996
Thermal correction to Gibbs Free Energy= 0.185662
Sum of electronic and zero-point Energies= -1167.397652
Sum of electronic and thermal Energies= -1167.380801
Sum of electronic and thermal Enthalpies= -1167.379857
Sum of electronic and thermal Free Energies= -1167.442191
CBS-DLPNO-CCSD(T) Single Point Energy = -1165.995412290850
Imaginary frequency: -397.67 cm-1

Products of Boryl Sulfenate Elimination for Boronic Esters

MeSOBpin
C -1.7264700000 2.3945120000 1.6420380000
S -0.8330840000 2.4372960000 3.2058140000
O 0.3671260000 1.2979370000 2.9156830000
H -2.1028990000 1.3919000000 1.4372780000
H -1.0979930000 2.7494780000 0.8263860000
H -2.5724550000 3.0737460000 1.7717020000
B 1.4223380000 1.5675850000 2.0873920000
O 2.5125650000 0.7380230000 2.0528010000
O 1.5001260000 2.6201540000 1.2091000000
C 2.8604390000 2.6317460000 0.6913350000
C 3.3042640000 1.1350620000 0.9000620000
C 2.8937730000 0.2224720000 -0.2547860000
C 4.7752930000 0.9431900000 1.2295360000
C 3.6502340000 3.6174440000 1.5504470000
C 2.8266620000 3.0970010000 -0.7547400000
H 1.8399290000 0.3529260000 -0.5029690000
H 3.0444190000 -0.8137950000 0.0472450000
H 3.4888040000 0.4145790000 -1.1482510000
H 5.0482810000 1.4553310000 2.1495070000
H 5.4017950000 1.3184100000 0.4179910000
H 4.9847480000 -0.1188560000 1.3595160000
H 2.1355940000 2.5037700000 -1.3497020000
H 3.8205240000 3.0304150000 -1.2012930000
H 2.5033820000 4.1375350000 -0.7967400000

H 3.6833640000 3.2925380000 2.5906600000
H 3.1563250000 4.5883540000 1.5145490000
H 4.6722700000 3.7330830000 1.1882690000
Zero-point correction= 0.224301 (Hartree/Particle)
Thermal correction to Energy= 0.238138
Thermal correction to Enthalpy= 0.239082
Thermal correction to Gibbs Free Energy= 0.184325
Sum of electronic and zero-point Energies= -924.671516
Sum of electronic and thermal Energies= -924.657679
Sum of electronic and thermal Enthalpies= -924.656735
Sum of electronic and thermal Free Energies= -924.711491
CBS-DLPNO-CCSD(T) Single Point Energy = -923.607553837993

MeSOBcat
H 1.1846710000 -0.2018260000 2.4626850000
C 0.1153490000 -0.3917700000 2.3705790000
H -0.1578310000 -1.3323060000 2.8476310000
S -0.3950090000 -0.3672370000 0.6440300000
H -0.4346090000 0.4251550000 2.8439620000
O 0.5858950000 -1.5876430000 0.0166540000
B 0.3237690000 -2.8983510000 0.2444990000
O -0.6147250000 -3.4174960000 1.1318310000
C -0.4778750000 -4.7872930000 1.0264110000
O 1.0362550000 -3.9027570000 -0.4001670000
C 0.5206840000 -5.0782140000 0.1018120000
C 0.8738360000 -6.3734840000 -0.2045590000
C -1.1716910000 -5.7747030000 1.6886040000
C 0.1772670000 -7.3872030000 0.4615220000
C -0.8221490000 -7.0951160000 1.3866120000
H 1.6507060000 -6.5876610000 -0.9252570000
H 0.4219090000 -8.4200330000 0.2513020000
H -1.3412140000 -7.9044230000 1.8828960000
H -1.9468910000 -5.5345350000 2.4029870000
Zero-point correction= 0.136034 (Hartree/Particle)
Thermal correction to Energy= 0.146566
Thermal correction to Enthalpy= 0.147510
Thermal correction to Gibbs Free Energy= 0.098487
Sum of electronic and zero-point Energies= -919.905820
Sum of electronic and thermal Energies= -919.895289
Sum of electronic and thermal Enthalpies= -919.894345
Sum of electronic and thermal Free Energies= -919.943368
CBS-DLPNO-CCSD(T) Single Point Energy = -918.756945143813

MeSOBMIDA

H 2.6645770000 -0.1497080000 -0.2549130000
C 2.1124050000 -1.0886620000 -0.2787100000
H 1.9627900000 -1.4240530000 -1.3028380000
S 0.5388800000 -0.9011200000 0.5817850000
H 2.6640210000 -1.8465430000 0.2822840000
O -0.1680340000 0.3361990000 -0.2871530000
B -0.9049510000 0.0467920000 -1.4562460000
O -0.3495110000 -0.9736310000 -2.3510760000
C -0.9428970000 -2.1644060000 -2.3017080000
O -1.2892260000 1.2732700000 -2.1258120000
C -2.5357840000 1.2798680000 -2.5885520000
O -3.0496770000 2.1616330000 -3.2123360000
C -3.2389780000 -0.0309870000 -2.2281330000
C -2.1679730000 -2.1098390000 -1.3860320000
O -0.5788000000 -3.1492580000 -2.8760010000
N -2.4262630000 -0.6689560000 -1.1532800000
H -3.2424420000 -0.6637080000 -3.1154990000
H -4.2666210000 0.1410380000 -1.9160350000
C -2.9698740000 -0.3578140000 0.1890250000
H -1.9006220000 -2.5855320000 -0.4441210000
H -3.0203170000 -2.6259340000 -1.8239540000
H -3.0327940000 0.7227980000 0.3011440000
H -2.2981650000 -0.7483480000 0.9476490000
H -3.9594310000 -0.8016640000 0.3029230000
Zero-point correction= 0.178983 (Hartree/Particle)
Thermal correction to Energy= 0.192537
Thermal correction to Enthalpy= 0.193481
Thermal correction to Gibbs Free Energy= 0.138637
Sum of electronic and zero-point Energies= -1088.878328
Sum of electronic and thermal Energies= -1088.864774
Sum of electronic and thermal Enthalpies= -1088.863829
Sum of electronic and thermal Free Energies= -1088.918673
CBS-DLPNO-CCSD(T) Single Point Energy = -1087.586691231292