A Theoretical Investigation on the Mechanism and Stereochemical Course of the Addition of (*E*)-2-Butenyltrimethylsilane to Acetaldehyde by Electrophilic and Nucleophilic Activation

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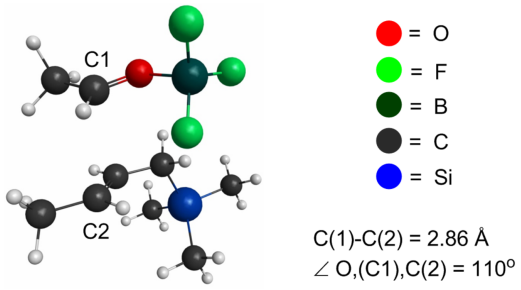
SUPPORTING INFORMATION

Table of Contents[1]

Analysis of Pre-transition State Complex 3. The physical nature of complex **3** (T-Figure 1) was probed through an energy decomposition analysis of the reactants (SI-Figure 1). The primary intermolecular NBO donor-acceptor stabilization interaction is the $\pi_{C=C} \rightarrow \pi^*_{C=O}$ and amounts to 9.3 kcal/mol. No other intermolecular NBO donor-acceptor interactions were found that are greater than 0.5 kcal/mol. The NBO charge transfer (Δq), which is likely exclusively associated with the $\pi_{C=C} \rightarrow \pi^*_{C=O}$ interaction, amounts to 0.06 *e*. The angle of approach of the aldehyde (110^o) is close to that for optimal frontier orbital overlap (107^o, Burgi-Dunitz approach).[2] Complex **3** is sterically and electrostatically unfavorable, however, through orbital interactions and dispersion forces, an overall favorable electronic interaction energy results (ΔE_{int} = –8.1 kcal/mol). A low level of distortion (ΔE_d = 1.42 kcal/mol) is necessary to form complex **3** from the isolated optimized reactants. Thus, orbital interactions and dispersion forces more than compensate for the unfavorable electrostatic, steric, and distortion components of the overall energy. Complex **3** can best be described as a charge transfer / van der Waals complex since both favorable energetic components (ΔE_{pol} and ΔE_{disp}) are nearly equal. However, the overall enthalpy of association ($\Delta H = \Delta E + \Delta H_{corr}$ = –5.2 kcal/mol) is not sufficient to offset the entropic penalty of $-T\Delta S$ = 8.7 kcal/mol which causes the overall Gibbs free energy of association to be positive ($\Delta G = \Delta E + \Delta H_{corr} - T\Delta S$ = 3.5 kcal/mol). Similar pre-transition state complexes have been invoked in the structurally similar Mukaiyama aldol reaction in gas phase computational studies,[3] but should also exist in solution of moderate polarity in view of the smaller frontier orbital energy difference in the reactants relative to crotylation examined in this study (ε_{HOMO}(silyl enol ether) > ε_{HOMO}(crotylsilane)).

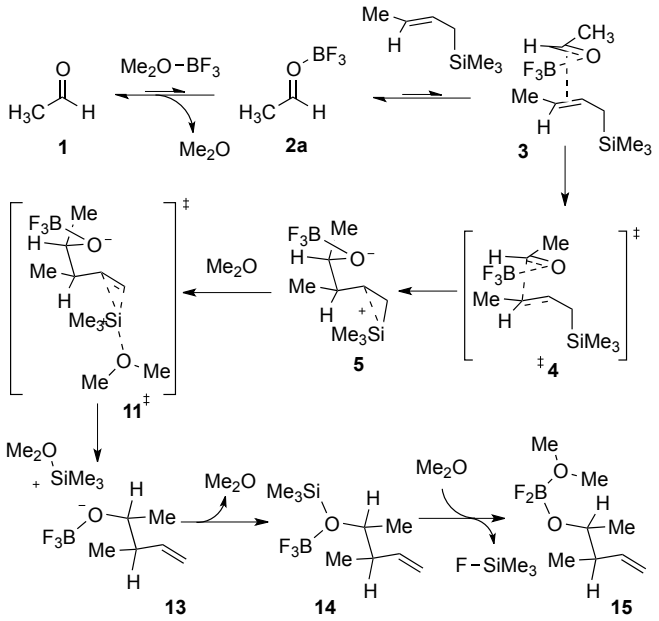


ΔE_{es}	ΔE_{exrep}	ΔE_{pol}	ΔE_{disp}	ΔE_{int}	ΔE_{d}	ΔE^{a}	$\Delta H_{corr}{}^{b}$	$-T\Delta S$	$\pi\rightarrow\pi^{*c}$	Δq
2.9	26.5	-19.3	-18.2	-8.1	1.4	-6.7	1.5	8.7	9.3	0.06

SI-Figure 1. Geometry of complex **3** and an energy decomposition analysis. Energy values are in units of kcal/mol. [a] $\Delta E = \Delta E_{int} + \Delta E_{d}$. [b] Enthalpic correction including zero point energy. [c] NBO donor-acceptor stabilization energy.

Minimum Energy Pathway. The lowest energy pathway from the diagram in T-Figure 1 is reproduced in SI-Scheme 1. After initial coordination of acetaldehyde to BF_3 to generate complex **2a**, crotylsilane associates to form pre-transition state complex **3**. Complex **3** proceeds through the C-C bond forming transition state **4**‡ to form intermediate **5**. Although a number of pathways are accessible to intermediate **5**, the lowest energy is desilylation promoted by dimethyl ether via transition state **11**‡ to form intermediate ion pair **13** which quickly transfers the silyl group to the oxygen atom to form intermediate **14**.

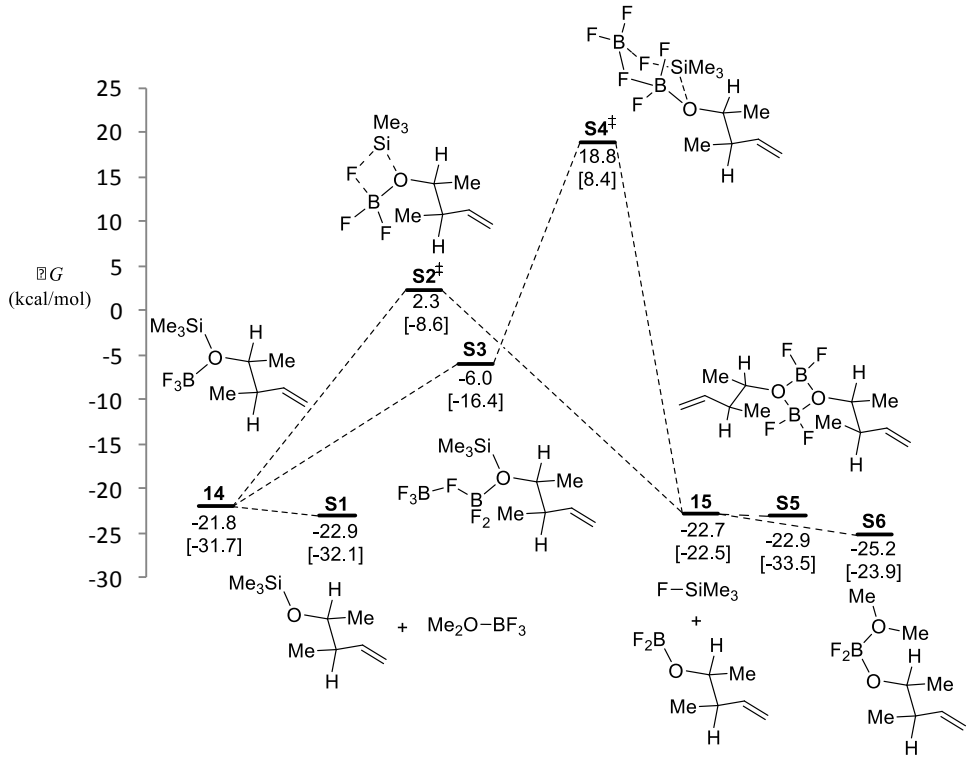
SI-Scheme 1



Pathways Torward Active BF_3 Consumption. Experimental evidence for the formation of fluorotrimethylsilane and the requirement for a stoichiometric amount of BF_3•OEt_2 for full conversion of the aldehyde requires the consumption of product **14**. The transfer of the BF_3 group from **14** to **S1** is more preferred ($\Delta G_{\mathbf{14}\text{–}\mathbf{S1}}$ = −1.1 kcal/mol) which is consistent with the stronger lewis basicity of dialkyl ethers relative to silyl thers.[4] Two pathways for consumption of product **14** have been considered and investigated here (SI-Figure 2). The first involves progression via a 4-membered σ-bond metathesis transition state **S2‡** to generate product **15**. Similar transition states have been invoked in the deprotection of *t*-butyldimethylsilyl ethers with BF_3•OEt_2.[5] However, this is a high barrier process ($\Delta G^{\ddagger}_{\mathbf{14}\text{–}\mathbf{S2}}$ = 24.0 kcal/mol) and is only mildly exergonic ($\Delta G_{\mathbf{14}\text{–}\mathbf{15}}$ = −0.9 kcal/mol). An alternative pathway involves first association of BF_3 with one of the fluorine atoms on **14** to generate **S3** which then can undergo fluorine transfer to the silicon group via a six membered transition state **S4‡**. This pathway is also high in energy ($\Delta G_{\mathbf{14}\text{–}\mathbf{S3}}$ = 15.8 kcal/mol and $\Delta G^{\ddagger}_{\mathbf{S3}\text{–}\mathbf{S4}}$ = 24.8 kcal/mol) and is not expected to occur at low

temperatures. Decomposition through a bimolecular process may provide a lower energy pathway but was not investigated.

There is not a strong thermodynamic driving force for the formation of fluorotrimethylsilane and product **15** ($\Delta G_{\mathbf{14}\rightarrow\mathbf{15}}$ = -0.9 and $\Delta G_{\mathbf{S1}\rightarrow\mathbf{15}}$ = 0.2 kcal/mol). The potential of the tricoordinate boron atom in **15** can be quenched by either dimerization to form **S5** ($\Delta G_{\mathbf{15}\rightarrow\mathbf{S5}}$ = -0.2 kcal/mol) or coordination with dimethylether ($\Delta G_{\mathbf{15}\rightarrow\mathbf{S6}}$ = -2.5 kcal/mol). Dimerization is highly enthalpically favorable ($\Delta G_{\mathbf{15}\rightarrow\mathbf{S5}}$ = −11.0 kcal/mol) but a low driving force due to the high entropic cost ($-T\Delta S_{\mathbf{15}\rightarrow\mathbf{S5}}$ = 10.8 kcal/mol). Hence, coordination with dimethylether is probably the most viable pathway for deactivation of any source of active BF_3.



SI-Figure 2. Energy diagram for consumption of active BF_3 continued from T-Figure 1 of manuscript.

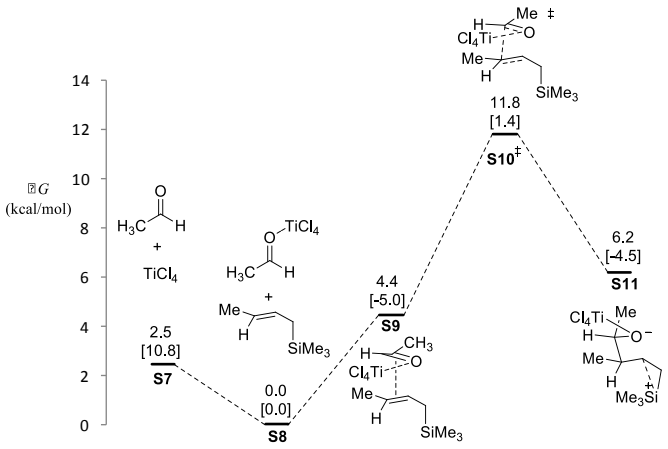
$TiCl_4$-Promoted Addition. The broad energy landscape accessible to intermediate **5** equates to a complex dependence of the diastereoselectivity on the energies of multiple

stationary points including transition state energies to C-C bond formation that lead to **5** and the transition state energies of desilylation. To address the impact of these factors on the diastereoselectivity of addition, a different Lewis acid was evaluated in the hope that the energy landscape would be more favorable (less likely to revert).

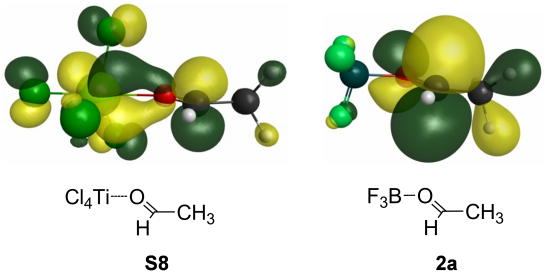
Titanium (IV) tetrachloride is another commonly used Lewis acid for this reaction which furnishes higher diastereoselectivities than BF_3•OEt_2.[6]**Error! Bookmark not defined.** The $TiCl_4$-mediated crotylation reaction was also modeled to understand the origins of the higher diastereoselectivity with $TiCl_4$ relative to BF_3•OEt_2.

Titanium (IV) chloride carbonyl complexes can exist in various titanium/carbonyl stoichiometries including 1:1, 1:2, 2:1, and 2:2.[7] The 1:1 complex is chosen for this study on the basis of likely greater reactivity as well as computational efficiency. The $TiCl_4$ promoted pathway begins with an exergonic ($\Delta G_{\mathbf{S7}\rightarrow\mathbf{S8}}$ = −2.5 kcal/mol) association with acetaldehyde which translates to a near stoichiometric complexation consistent with experimental observation[7] (SI-Figure 3). The effective concentration of the activated aldehyde is thus greater in the $TiCl_4$ pathway compared to the BF_3•OEt_2 pathway. However, the barrier to C-C bond formation ($\Delta G^{\ddagger}_{\mathbf{S8}\rightarrow\mathbf{S10}}$ = 11.8 kcal/mol) is not much different than that for the BF_3•OEt_2 pathway ($\Delta G^{\ddagger}_{\mathbf{2a}\rightarrow\mathbf{4}}$ = 10.8 kcal/mol, T-Figure 1). This difference is seemingly contradictory with the lower LUMO of the activated aldehyde•$TiCl_4$ complex **S8** (−3.46 eV) compared with the aldehyde•BF_3 complex **2a** (−2.54 eV) (SI-Figure 4). However, the LUMO of aldehyde•$TiCl_4$ complex **S8** is considerably more delocalized through mixing of the $\pi^*_{C=O}$ with an empty *d* orbital on the titanium metal center. Additionally, the NBO and electrostatic potential fitted charges on the carbon atom of the aldehyde are both more positive for the aldehyde•BF_3 complex ($q(C)_{NBO}$ =

0.587, $q(C)_{ESP}$ = 0.601) compared to the aldehyde•$TiCl_4$ complex ($q(C)_{NBO}$ = 0.560, $q(C)_{ESP}$ = 0.539).



SI-Figure 3. Energy diagram illustrating reaction pathways investigated for the $TiCl_4$-promoted crotylation of acetaldehyde. Relative energy values are represented as free energies *G* (kcal/mol) and are calculated at the CPCM(CH_2Cl_2)-M06/TZV(2f),6-311+G(2d,2p)//CPCM(CH_2Cl_2)-M06/TZV(2f),6-31+G(d,p) level. Energies in brackets represent enthalpies *H* (kcal/mol). Thermodynamic quantities are determined at 195 K.



	LUMO[a]	$q(C)_{NBO}$[b]	$q(C)_{ESP}$[c]
$TiCl_4$	-3.46	0.560	0.539
BF_3	-2.54	0.587	0.601

SI-Figure 4. LUMO for **S8** and **2a** [a] LUMO energy in eV [b] NBO partial atomic charges at C(1) [c] electrostatic potential fitted charges according to the CHelpG scheme.

It is important to note that the barrier to reversion is significantly greater in the $TiCl_4$-promoted pathway ($\Delta G^{\ddagger}_{\mathbf{S11\text{-}S10}}$ = 5.6 kcal/mol) compared to the BF_3 pathway ($\Delta G^{\ddagger}_{\mathbf{5\text{-}4}}$ = 1.8

kcal/mol, T-Figure 1). Moreover, the ground state energy difference is less unfavorable for $TiCl_4$ ($\Delta G_{\mathbf{S8}\rightarrow\mathbf{S11}}$ = 6.2 kcal/mol) than for BF_3 ($\Delta G_{\mathbf{2a}\rightarrow\mathbf{5}}$ = 9.0 kcal/mol, T-Figure 1). The difference in barrier energies ($\Delta\Delta G^{\ddagger}$ = 3.8 kcal/mol) may have important consequences for diastereoselectivity. The barrier to desilylation of intermediate **S11** in the $TiCl_4$ pathway is likely to be similar to the barrier for desilylation of **5** since the lability of the silyl group is unlikely to be dependent on the group bound to the oxygen atom. Intermediate **S11** is likely to be consumed by chloride-promoted desilylation.[8]

Solvation Energies. The current implementation of the LMO-EDA method is not capable of isolating the contribution from solvation which is subsumed in the other interaction energy components (mostly electrostatic). Thus, it is important to independently check if the solvation energies correlate with the transition state energies. The solvation energies $\Delta E^{\ddagger}$(solv) of the transition states ($E^{\ddagger}$(solv) - $E^{\ddagger}$(gas)) for the Lewis acid promoted pathways are provided in SI-Table 1. The variation in the solvation energy is minimal and there is no clear relationship with the variation in the transition sate energies overall.

SI-Table 1. Solvation energies (kcal/mol) for Lewis acid promoted transition states

	$\Delta E^{\ddagger}$(solv)		$\Delta E^{\ddagger}$(solv)
syn-T1-H	-40.1	syn-T1-L	-19.0
syn-T2-H	-40.7	syn-T2-L	-14.9
syn-T3-H	-41.4	syn-T3-L	-16.6
anti-T1-H	-40.8	anti-T1-L	-18.2
anti-T2-H	-40.3	anti-T2-L	-18.7
anti-T2-H	-40.7	anti-T3-L	-15.2

Energy Components Along the Intrinsic Reaction Coordinate.

SI-Table 2. Energy components at varying bond lengths along the intrinsic reaction coordinate for all three activation. Units are in kcal/mol.

$d_{C\text{-}C}$	ΔE_{es}	ΔE_{ex}	ΔE_{rep}	ΔE_{ste}	ΔE_{orb}	ΔE_{disp}	ΔE_{int}	ΔE_{d}
syn-T1-L								
1.92	-41.97	-73.62	213.30	139.68	-102.59	-30.63	-35.50	39.54
1.97	-36.50	-66.35	192.48	126.13	-89.85	-29.95	-30.17	34.26
2.02	-31.70	-59.87	174.03	114.16	-78.71	-29.29	-25.54	29.50
2.15	-21.80	-46.15	135.24	89.09	-56.41	-27.60	-16.73	19.78
2.28	-14.64	-35.97	106.44	70.47	-41.45	-25.89	-11.51	13.29
2.54	-4.97	-22.37	68.05	45.68	-25.47	-22.52	-7.28	6.31
2.80	1.73	-13.22	42.64	29.42	-19.39	-18.44	-6.68	3.64
syn-T2-L								
1.92	-48.32	-80.60	233.95	153.35	-106.96	-33.67	-35.60	35.43
1.97	-42.95	-73.47	213.35	139.88	-94.75	-33.01	-30.83	30.61
2.02	-38.17	-67.04	194.86	127.82	-83.98	-32.35	-26.68	26.27
2.15	-27.86	-52.97	154.77	101.80	-61.86	-30.60	-18.53	17.29
2.28	-19.55	-41.73	123.12	81.39	-46.36	-28.79	-13.31	11.01
2.54	-7.72	-25.56	77.93	52.37	-28.31	-25.03	-8.68	4.18
2.80	0.14	-14.49	47.19	32.70	-20.45	-20.41	-8.02	1.59
syn-T3-L								
1.92	-44.94	-76.69	221.98	145.29	-103.42	-31.16	-34.24	33.40
1.97	-39.78	-69.75	201.95	132.20	-91.43	-30.48	-29.48	28.52
2.02	-35.16	-63.49	183.96	120.47	-80.98	-29.79	-25.46	24.28
2.15	-25.11	-49.75	144.76	95.01	-59.92	-27.96	-17.98	15.98
2.28	-16.90	-38.60	113.35	74.75	-45.16	-26.05	-13.36	10.49
2.54	-4.95	-22.24	67.84	45.60	-27.34	-22.07	-8.77	4.35
2.80	1.91	-12.29	40.22	27.93	-19.61	-18.01	-7.77	2.12
anti-T1-L								
1.92	-43.08	-74.09	213.64	139.55	-100.34	-29.29	-33.17	34.37
1.97	-37.72	-66.92	193.12	126.20	-88.24	-28.60	-28.36	29.48
2.02	-32.96	-60.46	174.78	114.32	-77.67	-27.92	-24.23	25.14
2.15	-22.88	-46.61	135.69	89.08	-56.47	-26.17	-16.44	16.48
2.28	-15.26	-36.02	105.95	69.93	-42.01	-24.42	-11.75	10.74
2.54	-4.59	-21.42	64.99	43.57	-25.86	-20.88	-7.77	4.63
2.80	2.42	-11.62	37.65	26.03	-19.00	-16.56	-7.11	2.39
anti-T2-L								
1.92	-47.15	-78.49	228.51	150.02	-105.29	-31.81	-34.23	36.72
1.97	-41.67	-71.43	208.02	136.59	-93.18	-31.14	-29.40	31.80
2.02	-36.76	-65.04	189.60	124.56	-82.62	-30.48	-25.31	27.50
2.15	-26.20	-51.05	149.60	98.55	-61.09	-28.73	-17.46	18.82

2.28	-17.84	-39.95	118.15	78.20	-45.87	-26.90	-12.40	12.73
2.54	-6.11	-24.11	73.62	49.51	-27.58	-23.27	-7.45	5.52
2.80	1.29	-13.67	44.39	30.72	-19.96	-19.04	-6.99	2.80
anti-T3-L								
1.92	-42.27	-75.57	220.48	144.91	-107.07	-32.45	-36.88	27.15
1.97	-36.74	-68.40	199.74	131.34	-94.26	-31.77	-31.42	23.66
2.02	-31.87	-61.98	181.30	119.32	-83.06	-31.09	-26.70	20.47
2.15	-21.80	-48.28	142.15	93.87	-60.43	-29.33	-17.69	13.76
2.28	-14.38	-37.87	112.61	74.74	-44.96	-27.53	-12.14	8.94
2.54	-4.05	-23.35	71.65	48.30	-27.71	-23.92	-7.37	3.33
2.80	2.60	-13.58	44.27	30.69	-20.76	-19.60	-7.06	1.48

$d_{C\text{-}C}$	ΔE_{es}	ΔE_{ex}	ΔE_{rep}	ΔE_{ste}	ΔE_{orb}	ΔE_{disp}	ΔE_{int}	ΔE_{d}
syn-T1-H								
2.10	6.73	-48.02	142.65	94.63	-101.12	-25.77	-25.53	23.63
2.16	11.36	-42.46	126.78	84.32	-92.15	-25.01	-21.49	19.61
2.22	15.40	-37.62	112.92	75.30	-84.58	-24.25	-18.13	16.16
2.31	20.60	-31.48	95.33	63.85	-75.45	-23.14	-14.14	11.90
2.40	24.98	-26.44	80.82	54.38	-68.55	-22.04	-11.23	8.61
2.58	32.05	-18.56	58.18	39.62	-60.04	-19.80	-8.17	4.53
2.76	37.24	-12.55	41.10	28.55	-55.65	-17.23	-7.10	2.55
syn-T2-H								
2.10	-1.98	-59.63	174.64	115.01	-113.60	-27.38	-27.94	23.91
2.16	3.14	-53.45	156.90	103.45	-104.38	-26.56	-24.35	20.25
2.22	7.95	-47.65	140.37	92.72	-96.29	-25.68	-21.30	17.12
2.31	14.65	-39.65	117.63	77.98	-85.76	-24.25	-17.38	13.06
2.40	20.47	-32.75	98.01	65.26	-77.03	-22.83	-14.14	9.66
2.58	29.74	-21.96	67.38	45.42	-64.79	-20.10	-9.73	4.84
2.76	36.66	-13.49	43.27	29.78	-57.62	-16.71	-7.88	2.52
syn-T3-H								
2.10	4.69	-52.39	154.09	101.70	-105.51	-26.12	-25.24	20.20
2.16	9.46	-46.59	137.37	90.78	-96.65	-25.25	-21.66	16.64
2.22	13.84	-41.30	122.16	80.86	-89.04	-24.33	-18.68	13.64
2.31	19.76	-34.24	101.95	67.71	-79.63	-22.90	-15.06	9.98
2.40	24.99	-28.11	84.53	56.42	-72.17	-21.46	-12.22	7.09
2.58	33.22	-18.41	57.11	38.70	-62.17	-18.58	-8.82	3.46
2.76	38.67	-11.82	38.40	26.58	-57.03	-15.82	-7.60	1.93
anti-T1-H								
2.10	7.30	-48.88	144.16	95.28	-101.25	-25.28	-23.94	20.34
2.16	11.93	-43.24	128.09	84.85	-92.62	-24.50	-20.34	16.69
2.22	16.05	-38.25	113.84	75.59	-85.35	-23.68	-17.39	13.62
2.31	21.44	-31.74	95.33	63.59	-76.51	-22.45	-13.93	9.94

2.40	26.07	-26.24	79.67	53.43	-69.67	-21.20	-11.36	7.10
2.58	33.42	-17.49	54.79	37.30	-60.78	-18.55	-8.61	3.74
2.76	38.95	-10.70	35.38	24.68	-55.98	-15.27	-7.62	2.26
anti-T2-H								
2.10	2.61	-53.42	158.08	104.66	-105.83	-27.63	-26.19	22.52
2.16	7.57	-47.58	141.34	93.76	-96.91	-26.82	-22.39	18.74
2.22	12.11	-42.30	126.22	83.92	-89.12	-25.98	-19.07	15.36
2.31	18.19	-35.22	105.94	70.72	-79.51	-24.67	-15.27	11.43
2.40	23.28	-29.33	89.05	59.72	-71.87	-23.42	-12.29	8.27
2.58	31.20	-20.22	63.10	42.88	-61.76	-20.97	-8.65	4.02
2.76	36.89	-13.37	43.70	30.33	-56.42	-18.14	-7.34	2.12
anti-T3-H								
2.10	-2.00	-58.68	172.16	113.48	-111.96	-28.42	-28.90	25.89
2.16	3.15	-52.53	154.57	102.04	-102.81	-27.61	-25.22	22.19
2.22	7.82	-46.94	138.64	91.70	-94.83	-26.77	-22.08	18.98
2.31	14.12	-39.46	117.34	77.88	-84.55	-25.47	-18.02	14.77
2.40	19.65	-32.99	98.98	65.99	-76.12	-24.16	-14.64	11.16
2.58	28.62	-22.89	70.34	47.45	-64.32	-21.65	-9.90	5.65
2.76	35.10	-15.39	49.09	33.70	-58.13	-18.88	-8.20	3.10

$d_{C\text{-}C}$	ΔE_{es}	ΔE_{ex}	ΔE_{rep}	ΔE_{ste}	ΔE_{orb}	ΔE_{disp}	ΔE_{int}	ΔE_{d}
syn-T1-F								
2.18	-7.67	-61.82	160.64	98.82	-88.65	-21.91	-19.41	23.91
2.23	-1.69	-54.90	143.02	88.12	-80.95	-21.33	-15.84	20.66
2.28	3.58	-48.78	127.49	78.71	-74.38	-20.74	-12.82	17.75
2.38	12.64	-38.50	101.53	63.03	-63.80	-19.57	-7.70	12.35
2.48	19.74	-30.62	81.65	51.03	-56.91	-18.42	-4.57	8.09
2.68	30.77	-19.02	52.27	33.25	-51.12	-15.76	-2.86	2.56
2.88	37.47	-11.69	33.53	21.84	-49.67	-13.00	-3.35	0.56
syn-T2-F								
2.18	-6.82	-62.12	161.17	99.05	-88.06	-21.04	-16.87	22.77
2.23	-0.66	-55.01	143.11	88.10	-80.64	-20.49	-13.68	19.82
2.28	4.89	-48.60	126.95	78.35	-74.22	-19.94	-10.93	17.13
2.38	14.44	-37.68	99.63	61.95	-63.93	-18.90	-6.44	12.08
2.48	22.14	-29.23	78.53	49.30	-57.40	-17.88	-3.85	7.95
2.68	33.27	-17.55	49.02	31.47	-52.35	-15.50	-3.11	2.86
2.88	39.18	-10.48	30.83	20.35	-50.51	-12.85	-3.84	1.43
syn-T3-F								
2.18	3.64	-55.45	146.93	91.48	-86.57	-22.13	-13.58	18.77
2.23	9.18	-49.11	130.62	81.51	-79.65	-21.54	-10.50	15.68
2.28	14.10	-43.47	116.14	72.67	-73.75	-20.95	-7.93	12.90

2.38	22.52	-33.95	91.86	57.91	-64.84	-19.79	-4.20	8.06
2.48	29.04	-26.68	73.18	46.50	-59.69	-18.56	-2.71	4.86
2.68	38.15	-16.25	46.13	29.88	-55.22	-15.71	-2.89	1.82
2.88	42.28	-9.87	29.23	19.36	-52.80	-12.62	-3.77	1.28
anti-T1-F								
2.18	-2.22	-55.31	146.05	90.74	-81.91	-22.18	-15.56	19.55
2.23	3.38	-48.91	129.69	80.78	-74.89	-21.64	-12.37	16.42
2.28	8.32	-43.29	115.35	72.06	-69.04	-21.10	-9.76	13.66
2.38	16.82	-33.84	91.31	57.47	-60.18	-19.99	-5.89	8.85
2.48	23.60	-26.56	72.70	46.14	-55.17	-18.85	-4.27	5.47
2.68	33.50	-16.11	45.77	29.66	-51.43	-16.04	-4.30	2.02
2.88	38.60	-9.06	27.34	18.28	-49.32	-12.57	-4.99	1.51
anti-T2-F								
2.18	-3.11	-59.25	155.28	96.03	-84.67	-21.85	-13.59	20.12
2.23	3.00	-52.35	137.62	85.27	-77.22	-21.29	-10.23	16.81
2.28	8.60	-46.00	121.57	75.57	-70.83	-20.73	-7.40	13.75
2.38	18.38	-35.32	94.92	59.60	-62.89	-19.63	-4.53	8.57
2.48	24.78	-27.84	75.63	47.79	-56.58	-18.46	-2.47	5.59
2.68	34.43	-16.98	47.80	30.82	-52.27	-15.86	-2.88	2.37
2.88	39.38	-10.46	30.90	20.44	-50.35	-13.13	-3.67	1.15
anti-T3-F								
2.18	-0.08	-60.67	157.58	96.91	-93.17	-20.84	-17.18	24.03
2.23	5.16	-53.25	139.19	85.94	-85.42	-20.39	-14.71	21.98
2.28	10.56	-47.07	123.48	76.41	-78.95	-19.82	-11.80	19.16
2.38	20.50	-36.66	97.02	60.36	-68.48	-18.55	-6.17	13.16
2.48	27.18	-28.13	75.89	47.76	-60.73	-17.51	-3.29	9.01
2.68	37.70	-16.70	46.80	30.10	-55.08	-14.86	-2.14	3.28
2.88	42.84	-9.85	28.96	19.11	-53.15	-12.04	-3.25	1.92

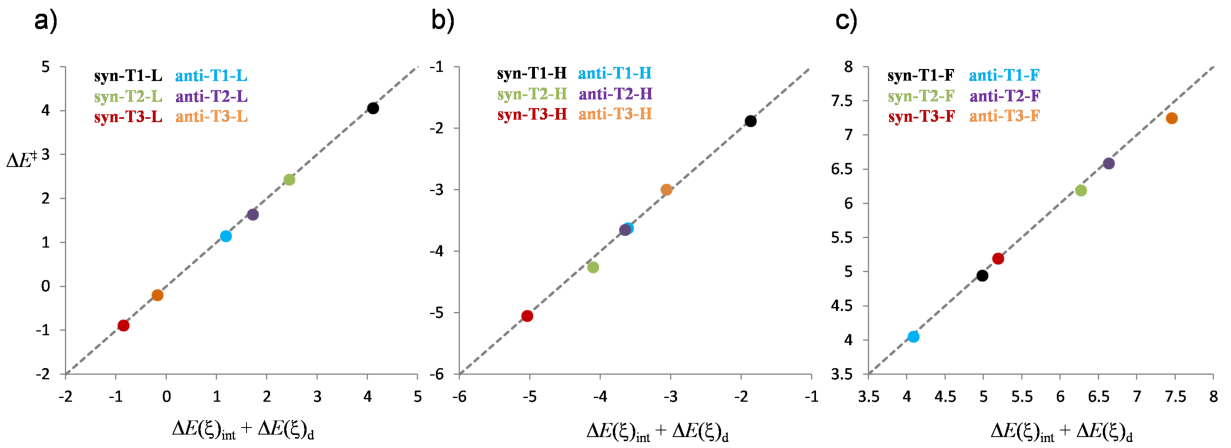
Energy Components at Constant Levels of Distortion.

SI-Table 3. Energetic Components at Constant Levels of Distortion.[a, b, c]

TS	$\Delta E_{es,d}‡$	$\Delta E_{ste,d}‡$	$\Delta E_{orb,d}‡$	$\Delta E_{disp,d}‡$	$\Delta E_{int,d}‡$
syn-T1-L[a]	-35.3	123.2	-87.1	-29.5	-28.9
syn-T2-L	-45.7	146.7	-101.0	-33.4	-33.2
syn-T3-L	-44.4	144.1	-102.4	-31.1	-33.9
anti-T1-L	-41.6	135.8	-97.0	-29.1	-31.8
anti-T2-L	-43.1	140.1	-96.2	-31.4	-30.6
anti-T3-L	-36.7	131.3	-94.1	-31.8	-31.3
syn-T1-H[b]	13.5	79.4	-87.9	-24.6	-19.6
syn-T2-H	7.0	94.7	-97.8	-25.9	-21.9
syn-T3-H	8.0	94.2	-99.3	-25.6	-22.7
anti-T1-H	10.6	87.9	-95.0	-24.8	-21.3
anti-T2-H	8.9	90.9	-94.5	-26.6	-21.4
anti-T3-H	9.7	87.6	-91.7	-26.4	-20.8
syn-T1-F[c]	2.9	80.0	-75.1	-20.8	-13.1
syn-T2-F	2.8	81.9	-76.4	-20.2	-11.8
syn-T3-F	4.9	89.2	-85.0	-22.0	-12.9
anti-T1-F	0.4	86.1	-78.6	-21.9	-14.0
anti-T2-F	0.5	89.6	-80.1	-21.5	-11.5
anti-T3-F	12.4	73.6	-77.0	-19.6	-10.6

[a] Values for BF_3 pathway are interpolated at $\Delta E_d(\xi)$ = 33.0 kcal/mol. [b] Values for Brønsted acid pathway are interpolated at $\Delta E_d(\xi)$ = 17.7 kcal/mol. [c] Values for fluoride pathway are interpolated at $\Delta E_d(\xi)$ = 18.1 kcal/mol.

The linear trends between $\Delta E‡$ and $\Delta E_{int,d}(\xi)+\Delta E_d(\xi)$ are provided in SI-Figure 5. The good correlations justify comparison of the components of the interaction energy (ΔE_{int}) at constant levels of distortion.



SI-Figure 5. Plots of $\Delta E^{\ddagger}$ versus $\Delta E(\xi)_{int,d}$. (a) BF_3 with $\Delta E_d(\xi)$ = 33.0 kcal/mol; R^2=0.9999 (b) H^+ with $\Delta E_d(\xi)$=17.7; R^2=0.996 (c) F^- with $\Delta E_d(\xi)$=18.1; R^2=0.998.

Calculation of Values in SI-Table 3. For each transition state, a plot of each component of the interaction energy as a function of the total distortion energy is constructed. From these plots, each interaction energy component is interpolated at a total distortion energy that leads to the optimum correlation coefficient between the electronic activation energy ($\Delta E^{\ddagger}$) and the sum of the interaction energy (the sum of the interapolated interaction energy components) and the chosen total distortion energy. This procedure is performed for each activation manifold. SI-Table 2 contains all the interpolated interaction energy components at the indicated distortion energy.

BF_3-mediated transition states. Interpolated at $\Delta E_d^{\ddagger}$= 33.0 kcal/mol.

syn-T1-L

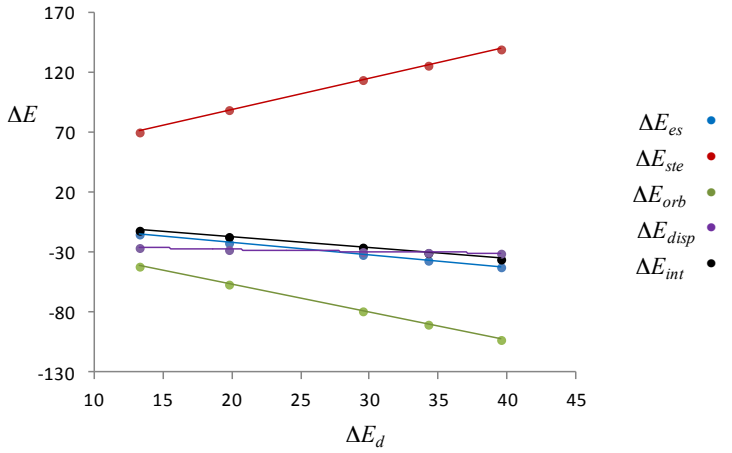
$\Delta E_{es,d} = -1.071 - 1.036\Delta E_d$ $R^2 = 0.9997$

$\Delta E_{ste,d} = 36.391 + 2.622\Delta E_d$ $R^2 = 0.9993$

$\Delta E_{orb,d} = -10.458 - 2.322\Delta E_d$ $R^2 = 0.9999$

$\Delta E_{disp,d} = -21.899 - 0.347\Delta E_d + 3.21E\text{-}3(\Delta E_d)^2$ $R^2 = 0.9974$

$\Delta E_{int,d}$ $= -1.939 - 0.652\Delta E_d - 5.00\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9974$



syn-T2-L

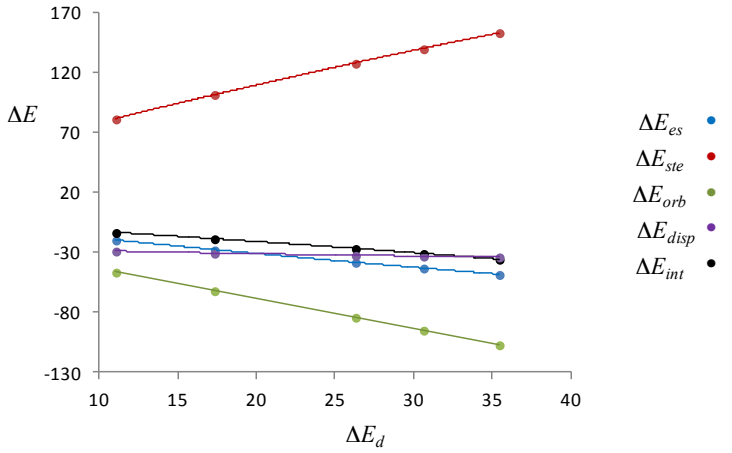
$\Delta E_{es,d}$ $= -4.656 - 1.423\Delta E_d + 5.46\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9996$

$\Delta E_{ste,d}$ $= 44.647 + 3.488\Delta E_d - 1.20\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9998$

$\Delta E_{orb,d}$ $= -19.01 - 2.478\Delta E_d$ $R^2 = 0.9999$

$\Delta E_{disp,d} =$ $-25.11 - 0.381\Delta E_d - 3.97\text{E-}3(\Delta E_d)^2$ $R^2 = 0.999$

$\Delta E_{int,d}$ $= -4.854 - 0.721\Delta E_d - 4.20\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0$



syn-T3-L

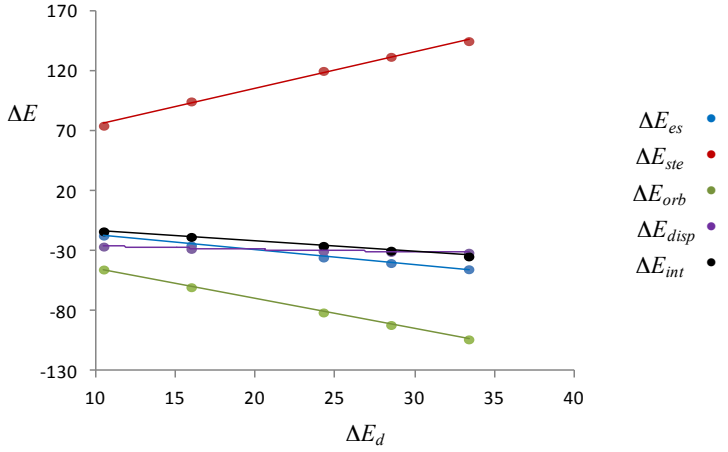
$\Delta E_{es,d}$ $= -0.170 - 1.733\Delta E_d + 1.19\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9994$

$\Delta E_{ste,d}$ $= 33.329 + 4.265\Delta E_d - 2.76\text{E-}2(\Delta E_d)^2$ $R^2 = 1.0$

$\Delta E_{\text{orb},d} = -16.414 - 2.814\Delta E_d + 6.30\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0$

$\Delta E_{\text{disp},d} = -21.83 - 0.467\Delta E_d + 5.65\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9973$

$\Delta E_{\text{int},d} = -5.112 - 0.746\Delta E_d - 3.89\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0$



anti-T1-L

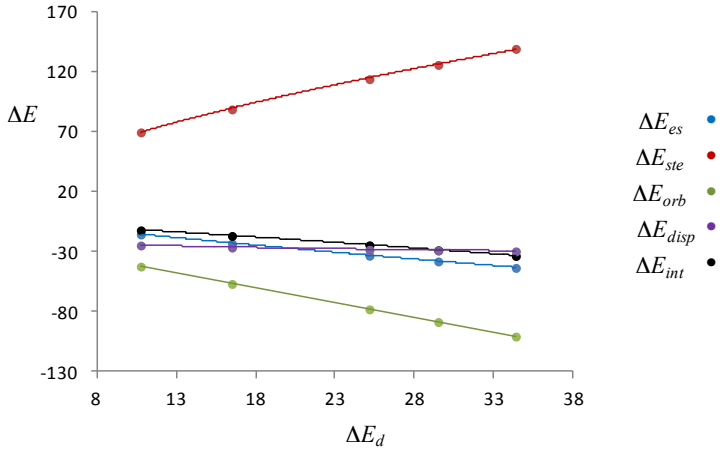
$\Delta E_{\text{es},d} = -0.516 - 1.447\Delta E_d + 6.14\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9998$

$\Delta E_{\text{ste},d} = 32.77 + 3.655\Delta E_d - 1.61\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9997$

$\Delta E_{\text{orb},d} = -15.69 - 2.464\Delta E_d$ $R^2 = 1.0$

$\Delta E_{\text{disp},d} = -20.70 - 0.398\Delta E_d + 4.33\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9977$

$\Delta E_{\text{int},d} = -3.635 - 0.705\Delta E_d - 4.50\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0$



anti-T2-L

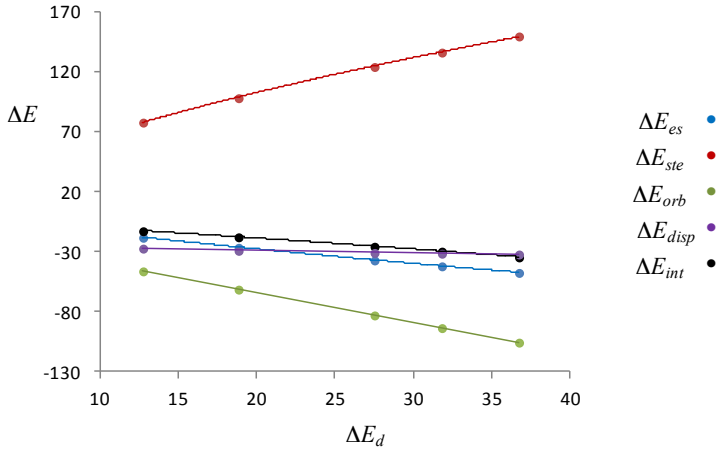
$\Delta E_{es,d} = 0.823 - 1.559\Delta E_d + 6.92\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta E_{ste,d} = 32.577 + 3.804\Delta E_d - 1.66\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta E_{orb,d} = -14.410 - 2.477\Delta E_d$ $R^2 = 1.0000$

$\Delta E_{disp,d} = -22.32 - 0.419\Delta E_d + 4.39\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9982$

$\Delta E_{int,d} = -2.659 - 0.713\Delta E_d - 4.02\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$



anti-T3-L

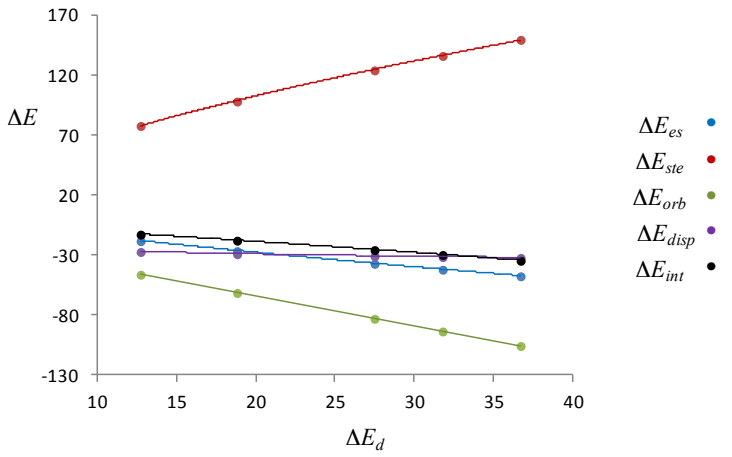
$\Delta E_{es,d} = -2.072 - 1.048\Delta E_d$ $R^2 = 0.9996$

$\Delta E_{ste,d} = 39.273 + 3.085\Delta E_d - 8.94\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta E_{orb,d} = -16.93 - 2.339\Delta E_d$ $R^2 = 1.0000$

$\Delta E_{disp,d} = -23.8 - 0.357\Delta E_d + 3.46\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9980$

$\Delta E_{int,d} = -2.894 - 0.719\Delta E_d - 4.27\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$



Brønsted acid-mediated transition states interpolated at $\Delta E_d^{\ddagger}$= 17.7 kcal/mol.

syn-T1-H

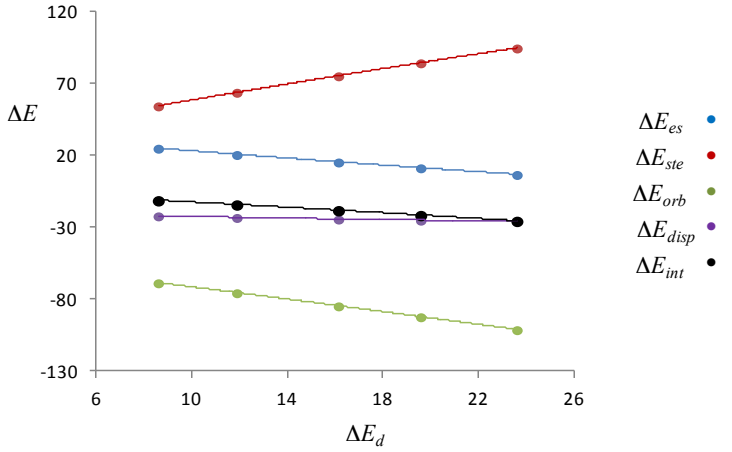
$\Delta E_{es,d} = 36.87 - 1.448\Delta E_d - 7.36\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{ste,d} = 28.82 + 3.083\Delta E_d - 1.27\text{E-}2(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{orb,d} = -51.03 - 1.983\Delta E_d - 6.04\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{disp,d} = -18.71 - 0.441\Delta E_d - 5.78\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9997$

$\Delta E_{int,d} = -4.033 - 0.791\Delta E_d - 5.05\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$



syn-T2-H

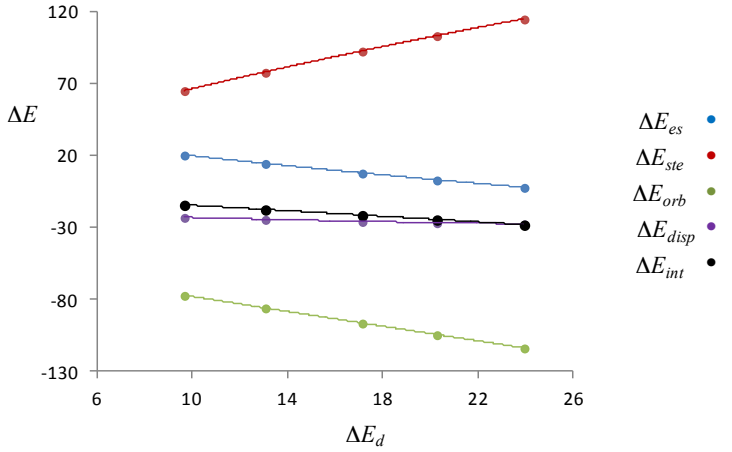
$\Delta E_{es,d} = 39.24 - 2.085\Delta E_d + 1.51\text{E-}2(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{ste,d} = 24.49 + 4.437\Delta E_d - 2.79\text{E-}2(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{orb,d} = -51.60 - 2.653\Delta E_d + 2.48\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{disp,d} = -17.63 - 0.627\Delta E_d + 9.16\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{int,d} = -5.069 - 0.927\Delta E_d - 1.23\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$



syn-T3-H

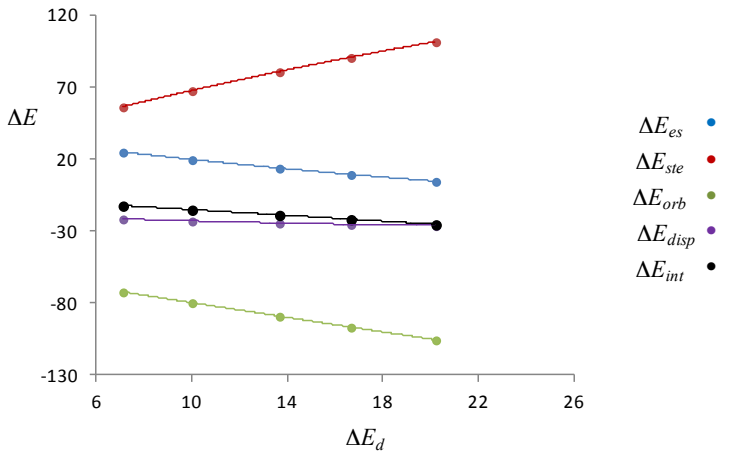
$\Delta E_{es,d} = 39.23 - 2.176\Delta E_d + 2.31\text{E-}2(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{ste,d} = 26.03 + 4.587\Delta E_d - 4.16\text{E-}2(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{orb,d} = -53.46 - 2.671\Delta E_d + 4.61\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{disp,d} = -17.18 - 0.695\Delta E_d + 1.25\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta E_{int,d} = -5.363 - 0.959\Delta E_d - 1.25\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$



anti-T1-H

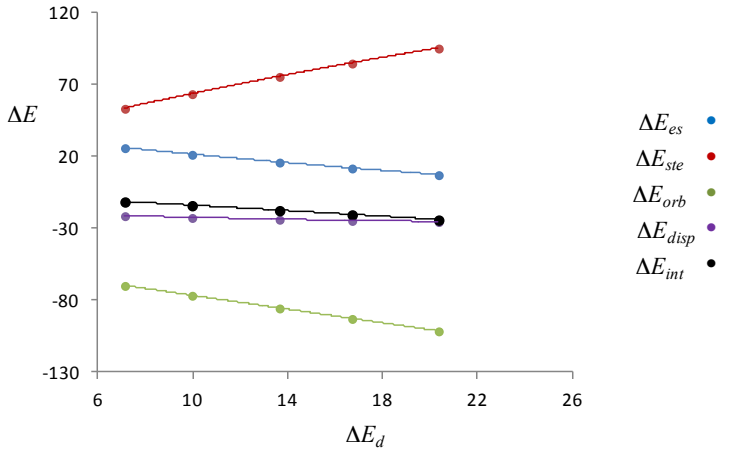
$\Delta E_{es,d} = 36.87 - 1.448\Delta E_d + 7.36\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{ste,d} = 28.82 + 3.084\Delta E_d - 1.\text{E-}227(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{orb,d} = -51.03 - 1.983\Delta E_d - 5.78\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{disp,d} = -18.71 - 0.441\Delta E_d + 6.04\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9997$

$\Delta E_{int,d} = -4.033 - 0.791\Delta E_d - 5.05\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$



anti-T2-H

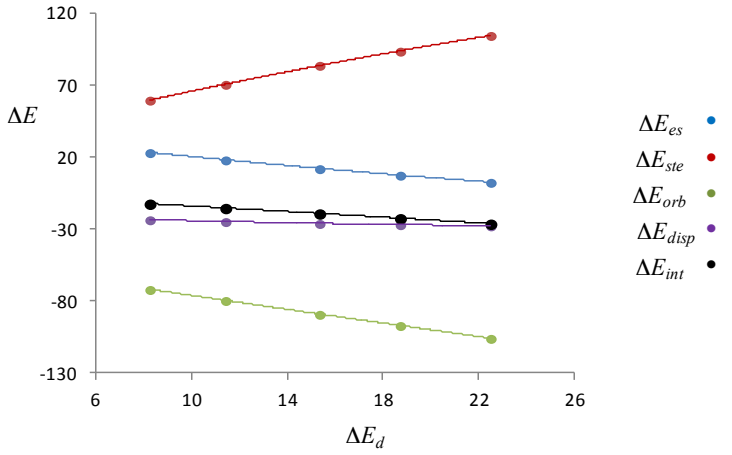
$\Delta E_{es,d} = 38.21 - 1.935\Delta E_d + 0.0158(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta E_{ste,d} = 27.66 + 4.143\Delta E_d - 3.23\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta E_{orb,d} = -51.24 - 2.535\Delta E_d - 4.97\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{disp,d} = -19.36 - 0.564\Delta E_d + 8.76\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9998$

$\Delta E_{int,d} = -4.749 - 0.888\Delta E_d - 2.83\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$



anti-T3-H

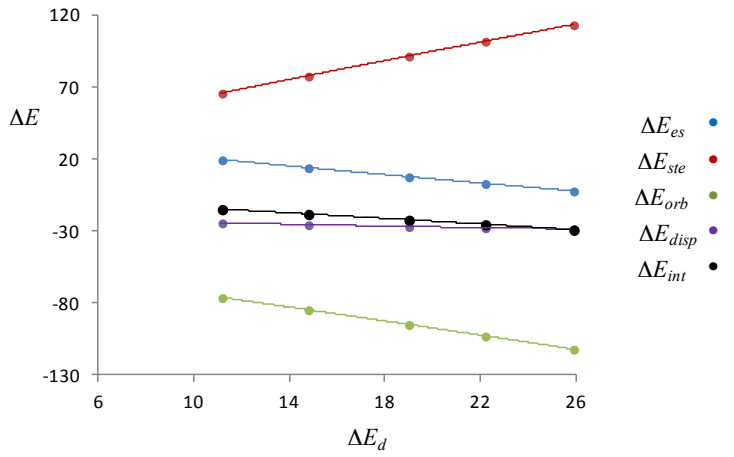
$\Delta E_{es,d} = 37.87 - 1.701\Delta E_d + 6.19\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{ste,d} = 27.29 + 3.564\Delta E_d - 9.02\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{orb,d} = -50.63 - 2.212\Delta E_d - 6.13\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{disp,d} = -19.07 - 0.528\Delta E_d + 6.45\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{int,d} = -4.564 - 0.874\Delta E_d - 2.55\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$



Fluoride-mediated transition states interpolated at $\Delta E_d^{\ddagger}$= 18.1 kcal/mol.

syn-T1-F

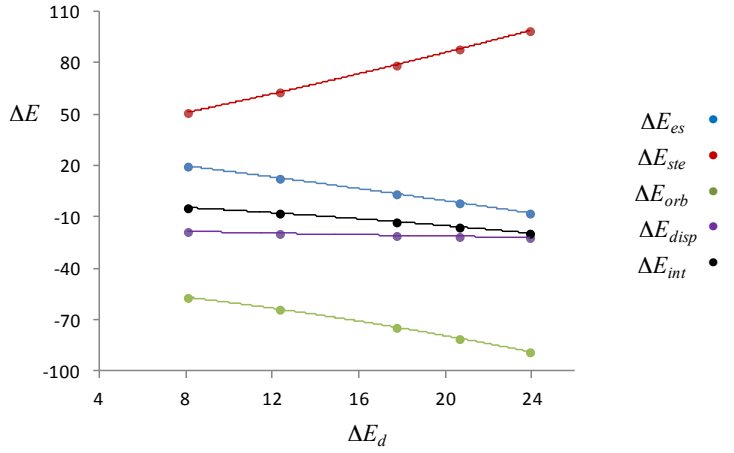
$\Delta E_{es,d} = 32.13 - 1.471\Delta E_d - 8.06\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{ste,d} = 30.95 + 2.312\Delta E_d + 2.20\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta E_{orb,d} = -46.77 - 0.991\Delta E_d - 3.19\text{E-}2(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{disp,d} = -15.97 - 0.334\Delta E_d + 3.57\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9998$

$\Delta E_{int,d} = 0.292 - 0.476\Delta E_d - 1.46\text{E-}2(\Delta E_d)^2$ $R^2 = 1.0000$



syn-T2-F

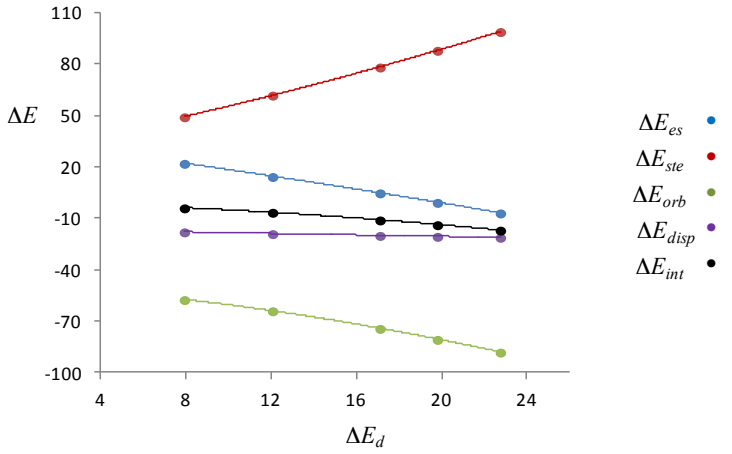
$\Delta E_{es,d} = 35.54 - 1.601\Delta E_d - 1.14\text{E-}2(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{ste,d} = 28.37 + 2.391\Delta E_d + 3.13\text{E-}2(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{orb,d} = -48.55 - 0.768\Delta E_d - 4.26\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta E_{disp,d} = -15.77 - 0.286\Delta E_d + 2.41\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9998$

$\Delta E_{int,d} = -0.428 - 0.263\Delta E_d - 2.03\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9997$



syn-T3-F

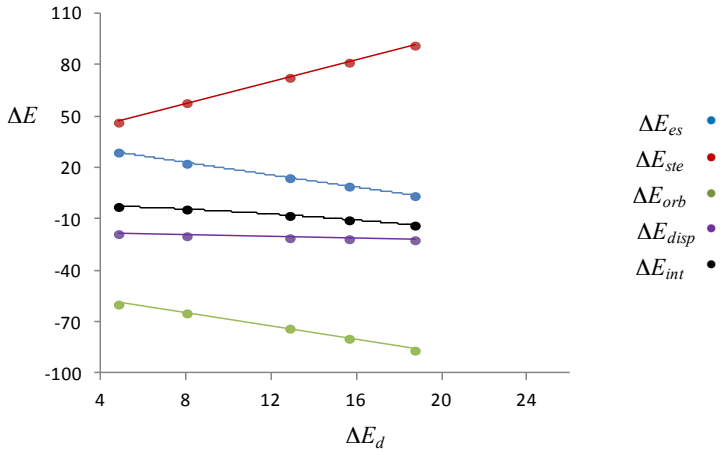
$\Delta E_{es,d} = 38.41 - 2.000\Delta E_d + 8.10\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9996$

$\Delta E_{ste,d} = 30.41 + 3.413\Delta E_d - 8.96\text{E-}3(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta E_{orb,d} = -53.09 - 1.210\Delta E_d - 3.07\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta E_{disp,d} = -16.68 - 0.436\Delta E_d + 7.86\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9977$

$\Delta E_{int,d} = -0.941 - 0.233\Delta E_d - 2.37\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9994$



anti-T1-F

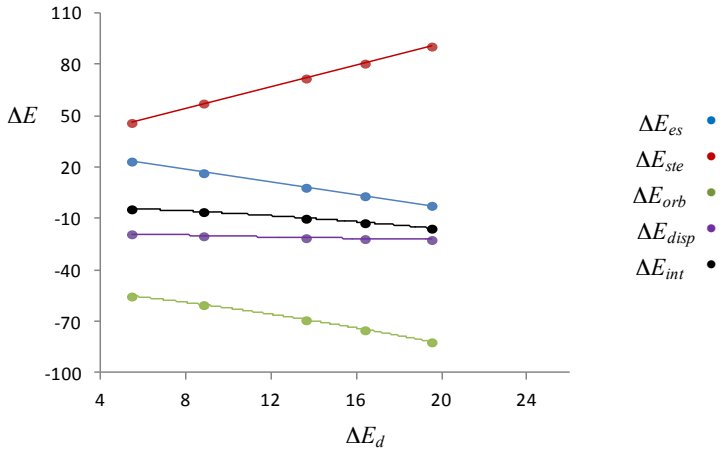
$\Delta E_{es,d} = 34.30 - 2.019\Delta E_d + 7.96\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9998$

$\Delta E_{ste,d} = 28.68 + 3.246\Delta E_d - 4.00\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9998$

$\Delta E_{orb,d} = -48.43 - 1.030\Delta E_d - 3.50\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta E_{disp,d} = -16.85 - 0.410\Delta E_d + 7.11\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9989$

$\Delta E_{int,d} = -2.265 - 0.221\Delta E_d - 2.37\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9993$



anti-T2-F

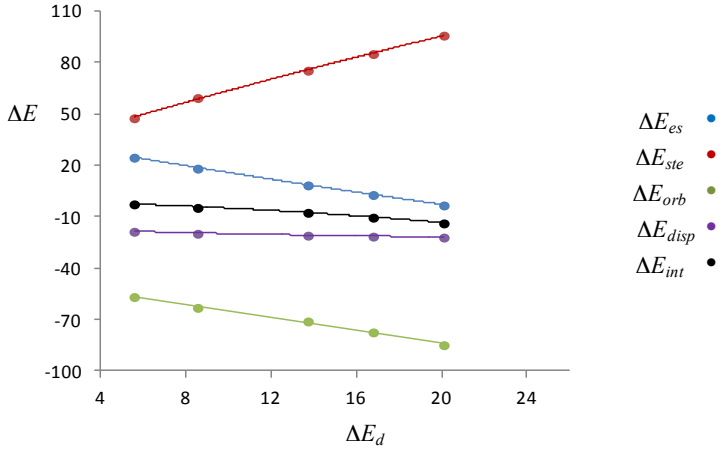
$\Delta E_{es,d} = 36.55 - 2.190\Delta E_d + 1.11\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9998$

$\Delta E_{ste,d} = 27.87 + 3.759\Delta E_d - 1.92\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9990$

$\Delta E_{orb,d} = -48.95 - 1.333\Delta E_d - 2.14\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9971$

$\Delta E_{\text{disp},d} = -16.39 - 0.428\Delta E_d + 7.93\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9949$

$\Delta E_{\text{int},d} = -0.904 - 0.195\Delta E_d - 2.15\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9969$



anti-T3-F

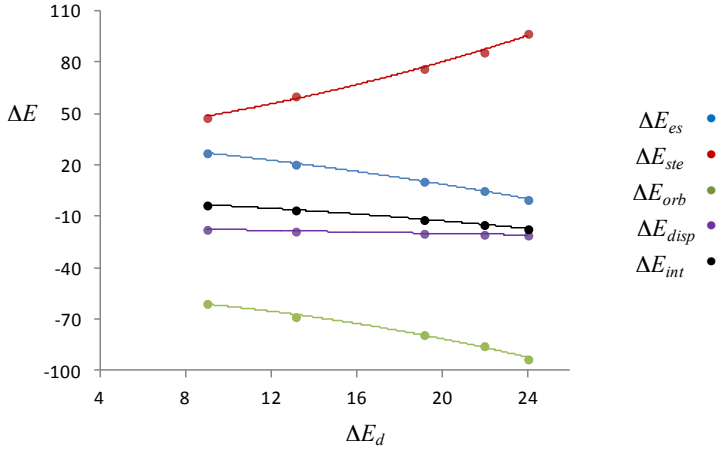
$\Delta E_{\text{es},d} = 36.58 - 0.801\Delta E_d - 2.95\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9988$

$\Delta E_{\text{ste},d} = 34.23 + 1.012\Delta E_d + 6.41\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9947$

$\Delta E_{\text{orb},d} = -54.28 - 0.216\Delta E_d - 5.58\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9941$

$\Delta E_{\text{disp},d} = -15.16 - 0.278\Delta E_d + 1.79\text{E-}3(\Delta E_d)^2$ $R^2 = 0.9996$

$\Delta E_{\text{int},d} = -0.897 - 0.288\Delta E_d - 1.93\text{E-}2(\Delta E_d)^2$ $R^2 = 0.9999$



Orbital Energies and Charge Transfer for T-Table 3.

SI-Table 4. Orbital energies and charge transfer at C-C separation. Orbital energies are listed in hartrees

$d_{C\text{-}C}$	$\varepsilon_{HOMO}^{\ddagger}$	ε_{HOMO}	ε_{LUMO}	Δq
syn-T1-L				
1.92	-0.318	-0.266	-0.116	0.502
1.97	-0.315	-0.267	-0.110	0.479
2.02	-0.313	-0.269	-0.105	0.453
2.15	-0.306	-0.271	-0.092	0.341
2.28	-0.302	-0.272	-0.082	0.249
2.54	-0.294	-0.275	-0.068	0.116
2.80	-0.290	-0.276	-0.061	0.055
syn-T2-L				
1.92	-0.322	-0.265	-0.114	0.549
1.97	-0.319	-0.266	-0.109	0.505
2.02	-0.316	-0.268	-0.104	0.463
2.15	-0.310	-0.271	-0.092	0.360
2.28	-0.304	-0.273	-0.082	0.271
2.54	-0.295	-0.276	-0.067	0.129
2.80	-0.290	-0.278	-0.059	0.057
syn-T3-L				
1.92	-0.323	-0.264	-0.115	0.545
1.97	-0.320	-0.265	-0.110	0.500
2.02	-0.317	-0.267	-0.104	0.457
2.15	-0.311	-0.270	-0.093	0.358
2.28	-0.306	-0.272	-0.083	0.273
2.54	-0.297	-0.276	-0.069	0.133
2.80	-0.291	-0.278	-0.061	0.061
anti-T1-L				
1.92	-0.321	-0.264	-0.116	0.535
1.97	-0.318	-0.265	-0.110	0.488
2.02	-0.316	-0.266	-0.105	0.442
2.15	-0.309	-0.269	-0.093	0.338
2.28	-0.304	-0.272	-0.083	0.251
2.54	-0.295	-0.275	-0.069	0.117
2.80	-0.290	-0.277	-0.062	0.054
anti-T2-L				
1.92	-0.320	-0.263	-0.115	0.560
1.97	-0.317	-0.265	-0.109	0.514
2.02	-0.315	-0.266	-0.104	0.470
2.15	-0.309	-0.269	-0.092	0.367
2.28	-0.304	-0.271	-0.082	0.278
2.54	-0.296	-0.275	-0.066	0.132
2.80	-0.291	-0.277	-0.059	0.060
anti-T3-L				
1.92	-0.323	-0.263	-0.117	0.563
1.97	-0.320	-0.265	-0.111	0.515
2.02	-0.316	-0.266	-0.106	0.468
2.15	-0.309	-0.269	-0.093	0.359
2.28	-0.304	-0.272	-0.082	0.267
2.54	-0.295	-0.276	-0.067	0.126
2.80	-0.291	-0.278	-0.061	0.060

$d_{C\text{-}C}$	$\varepsilon_{HOMO}^{\ddagger}$	ε_{HOMO}	ε_{LUMO}	$1-\Delta q$
syn-T1-H				
2.10	-0.331	-0.266	-0.126	0.565
2.16	-0.328	-0.267	-0.121	0.613
2.22	-0.325	-0.269	-0.116	0.658
2.31	-0.321	-0.271	-0.109	0.720
2.40	-0.318	-0.272	-0.102	0.776
2.58	-0.312	-0.275	-0.092	0.866
2.76	-0.308	-0.276	-0.086	0.917
syn-T2-H				
2.10	-0.339	-0.268	-0.132	0.532
2.16	-0.335	-0.269	-0.127	0.574
2.22	-0.332	-0.270	-0.122	0.613
2.31	-0.328	-0.271	-0.115	0.672
2.40	-0.324	-0.273	-0.108	0.731
2.58	-0.316	-0.275	-0.096	0.836
2.76	-0.310	-0.276	-0.089	0.910
syn-T3-H				
2.10	-0.335	-0.268	-0.124	0.564
2.16	-0.332	-0.269	-0.119	0.609
2.22	-0.329	-0.270	-0.115	0.651
2.31	-0.325	-0.272	-0.108	0.710
2.40	-0.321	-0.274	-0.102	0.766

2.58	-0.314	-0.276	-0.092	0.860
2.76	-0.310	-0.278	-0.086	0.916
anti-T1-H				
2.10	-0.332	-0.267	-0.124	0.579
2.16	-0.328	-0.268	-0.119	0.626
2.22	-0.326	-0.269	-0.114	0.669
2.31	-0.322	-0.271	-0.107	0.729
2.40	-0.318	-0.273	-0.101	0.786
2.58	-0.311	-0.275	-0.092	0.876
2.76	-0.307	-0.276	-0.086	0.929
anti-T2-H				
2.10	-0.334	-0.267	-0.126	0.550
2.16	-0.331	-0.269	-0.121	0.596
2.22	-0.328	-0.270	-0.115	0.639
2.31	-0.324	-0.271	-0.108	0.700
2.40	-0.320	-0.273	-0.102	0.758
2.58	-0.313	-0.275	-0.091	0.856
2.76	-0.309	-0.277	-0.085	0.916
anti-T3-H				
2.10	-0.337	-0.267	-0.131	0.528
2.16	-0.334	-0.268	-0.126	0.570
2.22	-0.331	-0.269	-0.121	0.610
2.31	-0.328	-0.271	-0.114	0.668
2.40	-0.322	-0.272	-0.108	0.726
2.58	-0.314	-0.274	-0.095	0.832
2.76	-0.308	-0.275	-0.087	0.901

$d_{C\text{-}C}$	$\varepsilon_{HOMO}^{\ddagger}$	ε_{HOMO}	ε_{LUMO}	Δq
syn-T1-F				
2.18	-0.183	-0.153	-0.023	0.403
2.23	-0.180	-0.154	-0.019	0.355
2.28	-0.179	-0.156	-0.015	0.310
2.38	-0.178	-0.162	-0.008	0.224
2.48	-0.180	-0.169	-0.002	0.148
2.68	-0.196	-0.191	0.004	
2.88	-0.208	-0.204	0.006	
syn-T2-F				
2.18	-0.182	-0.155	-0.023	0.392
2.23	-0.180	-0.156	-0.019	0.344
2.28	-0.179	-0.158	-0.016	0.298
2.38	-0.179	-0.164	-0.009	0.208
2.48	-0.184	-0.174	-0.004	0.132
2.68	-0.200	-0.195	0.002	0.054
2.88	-0.208	-0.204	0.004	0.028
syn-T3-F				
2.18	-0.185	-0.159	-0.019	0.340
2.23	-0.184	-0.162	-0.015	0.293
2.28	-0.184	-0.165	-0.011	0.248
2.38	-0.187	-0.174	-0.005	0.166
2.48	-0.192	-0.183	0.000	0.106
2.68	-0.205	-0.199	0.004	0.047
2.88	-0.208	-0.204	0.005	0.028
anti-T1-F				
2.18	-0.184	-0.156	-0.020	0.340
2.23	-0.183	-0.159	-0.016	0.292
2.28	-0.182	-0.161	-0.012	0.247
2.38	-0.185	-0.170	-0.006	0.162
2.48	-0.190	-0.180	-0.002	0.100
2.68	-0.205	-0.199	0.002	0.042
2.88	-0.209	-0.204	0.003	0.023
anti-T2-F				
2.18	-0.184	-0.163	-0.020	0.357
2.23	-0.183	-0.166	-0.016	0.305
2.28	-0.184	-0.169	-0.013	0.253
2.38	-0.189	-0.178	-0.009	0.165
2.48	-0.192	-0.186	-0.001	0.103
2.68	-0.204	-0.200	0.003	0.045
2.88	-0.208	-0.205	0.005	0.026
anti-T3-F				
2.18	-0.183	-0.154	-0.023	0.400
2.23	-0.180	-0.152	-0.020	0.353
2.28	-0.178	-0.154	-0.016	0.309
2.38	-0.177	-0.162	-0.009	0.221
2.48	-0.182	-0.170	-0.003	0.136
2.68	-0.200	-0.193	0.003	0.052
2.88	-0.209	-0.203	0.005	0.027

Parabolic Fits for Calulation of Values in T-Table 3

BF_3-mediated transition states. Interpolated at $\Delta E_d^{\ddagger}$= 33.0 kcal/mol.

syn-T1-L

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.291 - 8.90\text{E-}4\Delta E_d + 4.96\text{E-}6(\Delta E_d)^2$ $R^2 = 0.9998$

$\varepsilon_{\text{HOMO}} = -0.277 - 5.34\text{E-}4\Delta E_d - 3.88\text{E-}6(\Delta E_d)^2$ $R^2 = 0.9999$

$\varepsilon_{\text{LUMO}} = -5.79\text{E-}2 - 1.99\text{E-}3\Delta E_d + 1.35\text{E-}5(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta q = 2.32\text{E-}2 + 2.395\text{E-}2\Delta E_d - 2.698\text{E-}4(\Delta E_d)^2$ $R^2 = 0.9991$

syn-T2-L

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.293 - 9.85\text{E-}4\Delta E_d + 4.97\text{E-}6(\Delta E_d)^2$ $R^2 = 1.0000$

$\varepsilon_{\text{HOMO}} = -0.278 - 5.49\text{E-}4\Delta E_d - 4.20\text{E-}6(\Delta E_d)^2$ $R^2 = 0.9998$

$\varepsilon_{\text{LUMO}} = -6.09\text{E-}2 - 1.96\text{E-}3\Delta E_d + 1.31\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta q = 9.55\text{E-}2 + 1.75\text{E-}2\Delta E_d - 1.34\text{E-}4(\Delta E_d)^2$ $R^2 = 0.9999$

syn-T3-L

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.294 - 1.08\text{E-}3\Delta E_d + 8.05\text{E-}6(\Delta E_d)^2$ $R^2 = 1.0000$

$\varepsilon_{\text{HOMO}} = -0.276 - 4.73\text{E-}4\Delta E_d - 2.90\text{E-}6(\Delta E_d)^2$ $R^2 = 1.0000$

$\varepsilon_{\text{LUMO}} = -6.16\text{E-}2 - 2.19\text{E-}3\Delta E_d + 1.82\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta q = 9.31\text{E-}2 + 1.91\text{E-}2\Delta E_d - 1.67\text{E-}4(\Delta E_d)^2$ $R^2 = 0.9997$

anti-T1-L

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.294 - 1.08\text{E-}3\Delta E_d + 8.05\text{E-}6(\Delta E_d)^2$ $R^2 = 0.9997$

$\varepsilon_{\text{HOMO}} = -0.276 - 4.73\text{E-}4\Delta E_d - 2.90\text{E-}6(\Delta E_d)^2$ $R^2 = 1.0000$

$\varepsilon_{\text{LUMO}} = -6.16\text{E-}2 - 2.19\text{E-}3\Delta E_d + 1.815\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta q = 7.04\text{E-}2 + 1.845\text{E-}2\Delta E_d - 1.445\text{E-}4(\Delta E_d)^2$ $R^2 = 0.9998$

anti-T2-L

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.293 - 1.03\text{E-}3\Delta E_d + 7.84\text{E-}6(\Delta E_d)^2$ $R^2 = 0.9997$

$\varepsilon_{\text{HOMO}} = -0.277 - 4.63\text{E-}4\Delta E_d - 2.82\text{E-}6(\Delta E_d)^2$ $R^2 = 0.9999$

$\varepsilon_{\text{LUMO}} = -5.69\text{E-}2 - 2.18\text{E-}3\Delta E_d + 1.66\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9998$

$\Delta q = 6.25\text{E-}2 + 1.88\text{E-}2\Delta E_d - 1.43\text{E-}4(\Delta E_d)^2$ $R^2 = 0.9999$

anti-T3-L

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.295 - 1.13\text{E-}3\Delta E_d + 9.14\text{E-}6(\Delta E_d)^2$ $R^2 = 0.9998$

$\varepsilon_{\text{HOMO}} = -0.278 - 5.62\text{E-}4\Delta E_d - 4.05\text{E-}6(\Delta E_d)^2$ $R^2 = 1.0000$

$\varepsilon_{\text{LUMO}} = -6.20\text{E-}2 - 2.19\text{E-}3\Delta E_d + 1.83\text{E-}5(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta q = 7.97\text{E-}2 + 1.71\text{E-}2\Delta E_d - 1.195\text{E-}4(\Delta E_d)^2$ $R^2 = 0.9999$

Brønsted acid-mediated transition states interpolated at $\Delta E_d^{\ddagger} = 17.7$ kcal/mol.

syn-T1-H

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.308 - 1.26\text{E-}3\Delta E_d + 1.24\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9997$

$\varepsilon_{\text{HOMO}} = -0.277 + 6.53\text{E-}4\Delta E_d - 7.05\text{E-}6(\Delta E_d)^2$ $R^2 = 1.0000$

$\varepsilon_{\text{LUMO}} = -8.32\text{E-}2 - 2.44\text{E-}3\Delta E_d + 2.63\text{E-}5(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta q = 1 - 0.939 + 2.09\text{E-}2\Delta E_d - 2.14\text{E-}4(\Delta E_d)^2$ $R^2 = 0.9999$

syn-T2-H

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.310 - 1.62\text{E-}3\Delta E_d + 1.79\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9992$

$\varepsilon_{\text{HOMO}} = -0.276 + 3.70\text{E-}4\Delta E_d - 3.27\text{E-}7(\Delta E_d)^2$ $R^2 = 0.9999$

$\varepsilon_{\text{LUMO}} = -8.61\text{E-}2 - 2.50\text{E-}3\Delta E_d + 2.44\text{E-}5(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta q = 1 - 0.926 + 2.29\text{E-}2\Delta E_d - 2.69\text{E-}4(\Delta E_d)^2$ $R^2 = 1.0000$

syn-T3-H

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.309 - 1.76\text{E-}3\Delta E_d + 2.47\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9999$

$\varepsilon_{\text{HOMO}} = -0.278 + 6.12\text{E-}4\Delta E_d - 5.97\text{E-}6(\Delta E_d)^2$ $R^2 = 1.0000$

$\varepsilon_{\text{LUMO}} = -8.39\text{E-}2 - 2.76\text{E-}3\Delta E_d + 3.80\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta q = 1 - 0.921 + 2.43\text{E-}2\Delta E_d - 3.30\text{E-}4(\Delta E_d)^2$ $R^2 = 0.9999$

anti-T1-H

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.308 - 1.64\text{E-}3\Delta E_d + 2.27\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9995$

$\varepsilon_{\text{HOMO}} = -0.276 + 6.07\text{E-}4\Delta E_d - 6.58\text{E-}6(\Delta E_d)^2$ $R^2 = 0.9996$

$\varepsilon_{\text{LUMO}} = -8.41\text{E-}2 - 2.68\text{E-}3\Delta E_d + 3.64\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9999$

$\Delta q = 1 - 0.945 + 2.50\text{E-}2\Delta E_d - 3.44\text{E-}4(\Delta E_d)^2$ $R^2 = 0.9998$

anti-T2-H

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.308 - 1.53\text{E-}3\Delta E_d + 1.73\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9999$

$\varepsilon_{\text{HOMO}} = -0.276 + 4.74\text{E-}4\Delta E_d - 3.61\text{E-}6(\Delta E_d)^2$ $R^2 = 0.9997$

$\varepsilon_{\text{LUMO}} = -8.22\text{E-}2 - 2.58\text{E-}3\Delta E_d + 2.76\text{E-}5(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta q = 1 - 0.930 + 2.33\text{E-}2\Delta E_d - 2.86\text{E-}4(\Delta E_d)^2$ $R^2 = 0.9998$

anti-T3-H

$\varepsilon_{\text{HOMO}}^{\ddagger} = -0.305 - 1.83\text{E-}3\Delta E_d + 2.24\text{E-}5(\Delta E_d)^2$ $R^2 = 0.9839$

$\varepsilon_{\text{HOMO}} = -0.276 + 3.51\text{E-}4\Delta E_d - 6.86\text{E-}6(\Delta E_d)^2$ $R^2 = 1.0000$

$\varepsilon_{\text{LUMO}} = -8.33\text{E-}2 - 2.43\text{E-}3\Delta E_d + 2.20\text{E-}5(\Delta E_d)^2$ $R^2 = 1.0000$

$\Delta q = 1 - 0.936 + 2.125\text{E-}2\Delta E_d - 2.13\text{E-}4(\Delta E_d)^2$ $R^2 = 1.0000$

Fluoride-mediated transition states interpolated at $\Delta E_d^{\ddagger}$= 18.1 kcal/mol.

syn-T1-F

$\varepsilon_{HOMO}^{\ddagger} = -0.1883 + 1.44E\text{-}3\Delta E_d - 5.08E\text{-}5(\Delta E_d)^2$ $R^2 = 0.9934$

$\varepsilon_{HOMO} = -0.189 + 2.86E\text{-}3\Delta E_d - 5.70E\text{-}5(\Delta E_d)^2$ $R^2 = 0.9996$

$\varepsilon_{LUMO} = 2.23E\text{-}2 - 2.63E\text{-}4\Delta E_d + 2.19E\text{-}6(\Delta E_d)^2$ $R^2 = 0.9992$

$\Delta q = -4.69E\text{-}3 + 1.99E\text{-}2\Delta E_d - 1.215E\text{-}4(\Delta E_d)^2$ $R^2 = 1.0000$

syn-T2-F

$\varepsilon_{HOMO}^{\ddagger} = -0.200 + 2.71E\text{-}3\Delta E_d - 8.49E\text{-}5(\Delta E_d)^2$ $R^2 = 0.9882$

$\varepsilon_{HOMO} = -0.199 + 3.93E\text{-}3\Delta E_d - 8.76E\text{-}5(\Delta E_d)^2$ $R^2 = 0.9993$

$\varepsilon_{LUMO} = 2.17E\text{-}2 - 1.852E\text{-}4\Delta E_d + 1.19E\text{-}8(\Delta E_d)^2$ $R^2 = 0.9992$

$\Delta q = -2.53E\text{-}2 + 2.06E\text{-}2\Delta E_d - 9.91E\text{-}5(\Delta E_d)^2$ $R^2 = 1.0000$

syn-T3-F

$\varepsilon_{HOMO}^{\ddagger} = -0.203 + 2.66E\text{-}3\Delta E_d - 9.12E\text{-}5(\Delta E_d)^2$ $R^2 = 0.9974$

$\varepsilon_{HOMO} = -0.199 + 3.88E\text{-}3\Delta E_d - 9.28E\text{-}5(\Delta E_d)^2$ $R^2 = 0.9996$

$\varepsilon_{LUMO} = 2.18E\text{-}2 - 1.03E\text{-}4\Delta E_d - 1.26E\text{-}6(\Delta E_d)^2$ $R^2 = 0.9975$

$\Delta q = -1.04E\text{-}2 + 2.06E\text{-}2\Delta E_d - 1.60E\text{-}4(\Delta E_d)^2$ $R^2 = 1.0000$

anti-T1-F

$\varepsilon_{HOMO}^{\ddagger} = -0.202 + 2.74E\text{-}3\Delta E_d - 9.31E\text{-}5(\Delta E_d)^2$ $R^2 = 0.9831$

$\varepsilon_{HOMO} = -0.199 + 4.05E\text{-}3\Delta E_d - 9.67E\text{-}5(\Delta E_d)^2$ $R^2 = 0.9983$

$\varepsilon_{LUMO} = 2.14E\text{-}2 - 1.52E\text{-}4\Delta E_d - 7.635E\text{-}7(\Delta E_d)^2$ $R^2 = 0.9986$

$\Delta q = -9.48E\text{-}3 - 2.07E\text{-}2\Delta E_d + 1.46E\text{-}4(\Delta E_d)^2$ $R^2 = 1.0000$

anti-T2-F

$\varepsilon_{HOMO}^{\ddagger} = -0.204 + 2.415E\text{-}3\Delta E_d - 7.16E\text{-}5(\Delta E_d)^2$ $R^2 = 0.9974$

ε_{HOMO}= –0.202 + 3.42E-3ΔE_d – 7.40E-5$(\Delta E_d)^2$ R^2 = 0.9978

ε_{LUMO}= 2.17E-2 – 1.81E-4ΔE_d –2.67E-7$(\Delta E_d)^2$ R^2 = 0.9992

Δq = – 1.06E-2 – 2.155E-2ΔE_d + 1.64E-4$(\Delta E_d)^2$ R^2 = 0.9996

anti-T3-F

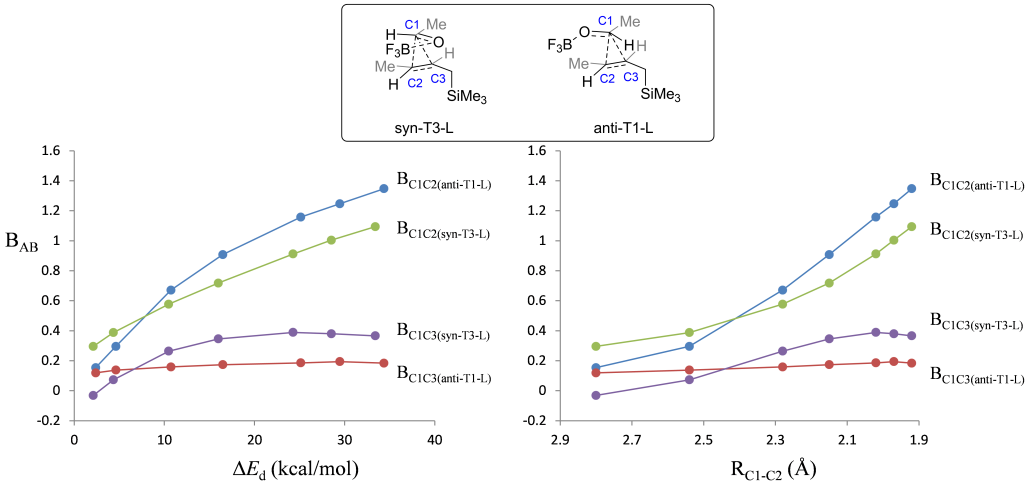
$\varepsilon_{HOMO}^{\ddagger}$= –0.203 + 3.18E-3$\Delta E_d$ – 9.73E-5$(\Delta E_d)^2$ R^2 = 0.9784

ε_{HOMO}= –0.205 + 4.78E-3ΔE_d – 1.10E-4$(\Delta E_d)^2$ R^2 = 0.9924

ε_{LUMO}= 2.22E-2 – 1.89E-4ΔE_d –1.13E-6$(\Delta E_d)^2$ R^2 = 0.9999

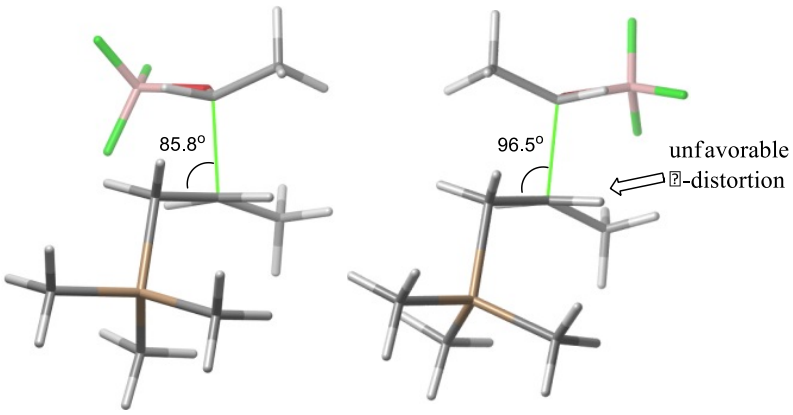
Δq = 1.93E-2 – 1.80E-2ΔE_d + 2.65E-5$(\Delta E_d)^2$ R^2 = 0.9956

Mayer Bond Orders. The determination of Mayer bond orders along the reaction coordinate as a function of both the total distortion energy and the C1-C2 bond distance is consistent with additional overlap for **syn-T3-L** between atoms C1 and C3 (SI-Figure 6). While the overlap between C1 and C2 in **syn-T3-L** is slightly lower than that in **anti-T1-L**, the gain in overlap between C1 and C3 is important for producing a greater π→π* interaction as illustrated in the main text (T-Figure 10).



SI-Figure 6. Mayer bond orders (B_{AB}) for pathways **syn-T3-L** and **anti-T1-L** as a function of the total distortion energy ΔE_d and the C1-C2 bond distance along the reaction coordinate.

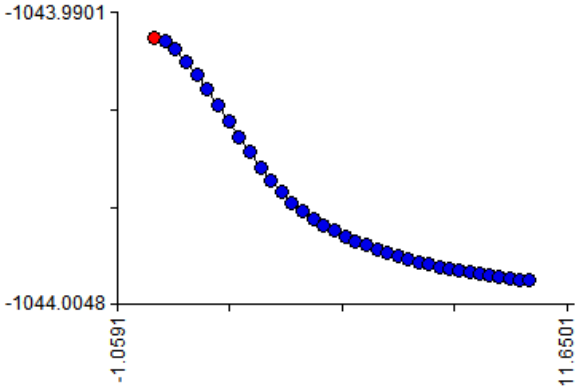
The Distortion Difference Between Antiperiplanar Transition States. The greater distortion in transition state **syn-T1-L** arises from the attempted avoidance of steric interactions between the aldehyde methyl group and the silylmethylene group. However, this causes a tilt that leads to an unfavorable compression between the methyl group of the crotylsilane and the BF_3 unit. Because of this second compression, a favorable orbital alignment cannot be achieved thus accounting for the considerable orbital interaction and electrostatic energy difference. In transition state **anti-T1-L**, the distortion arises from avoidance of the steric interactions between the aldehyde and crotylsilane methyl groups. However, in this case, that interaction causes a tilt that compresses the two gauche hydrogens and the BF_3 unit thus requiring less distortion to achieve transition state. This tilt is easily seen in the acute dihedral angle between the silylmethylene (C-C) bond and the forming sigma bond (SI-Figure 7).



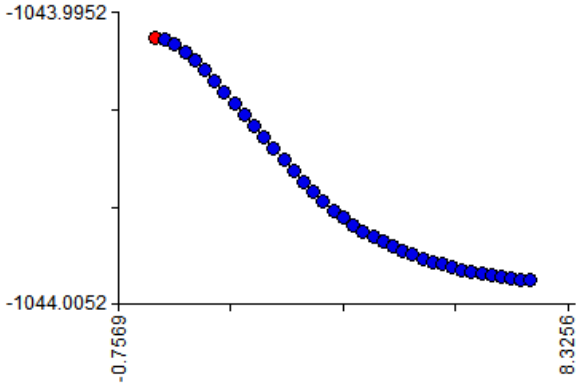
SI-Figure 7 Transition states for **anti-T1-L** and **syn-T1-L** from the perspective of the internuclear axis of the C-C bond of the alkene from the silylmethylene bound carbon.

Intrinsic Reaction Coordinate Diagrams From Transition State to Reactants.

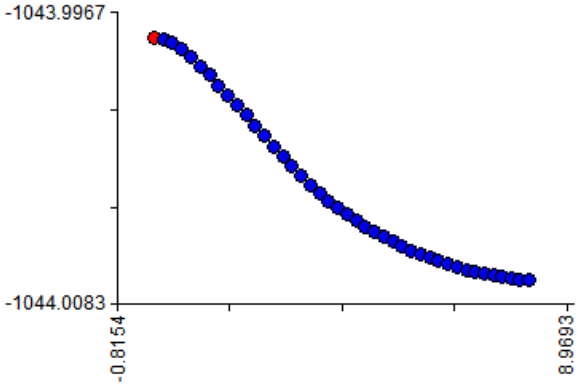
syn-T1-L



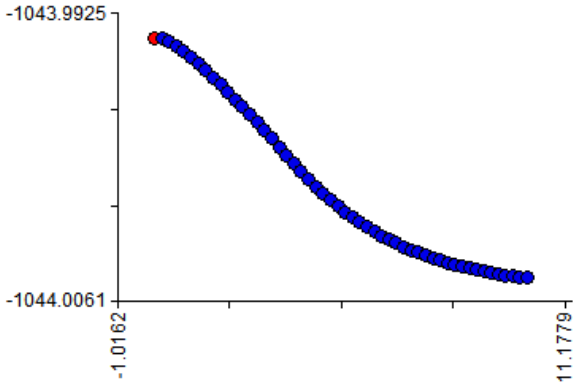
anti-T1-L



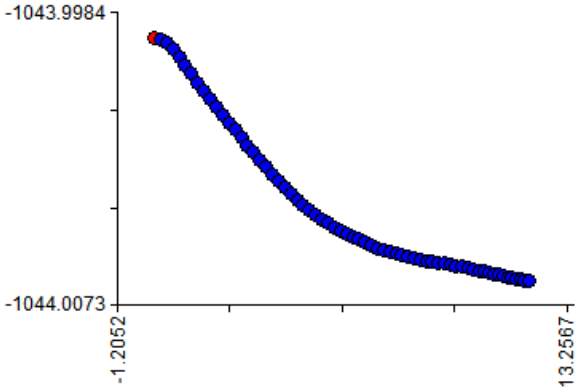
syn-T2-L



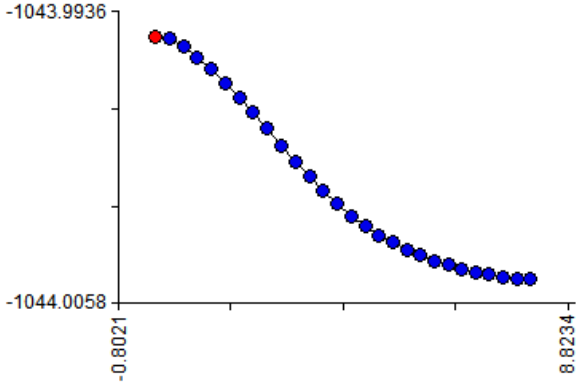
anti-T2-L



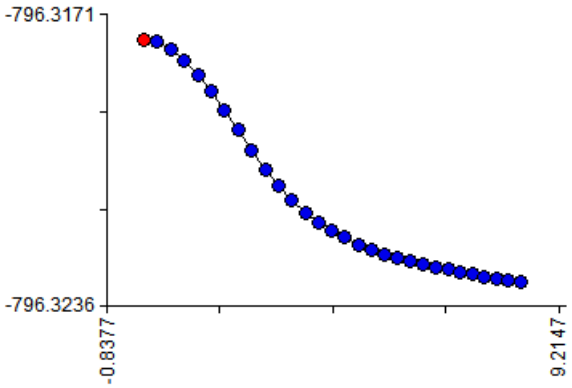
syn-T3-L



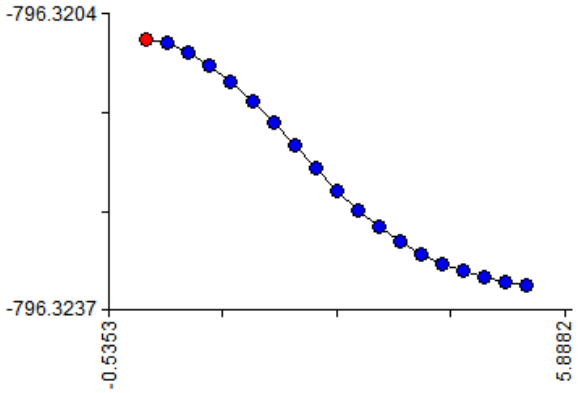
anti-T3-L



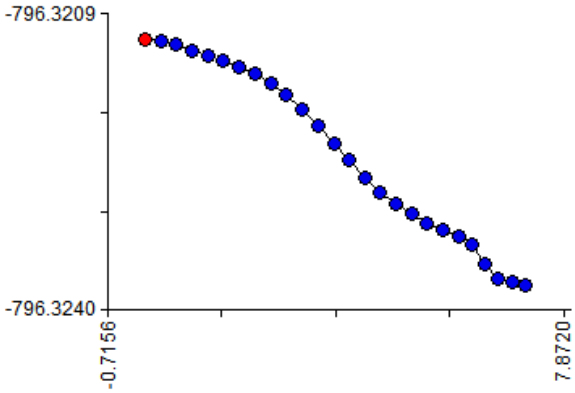
syn-T1-H



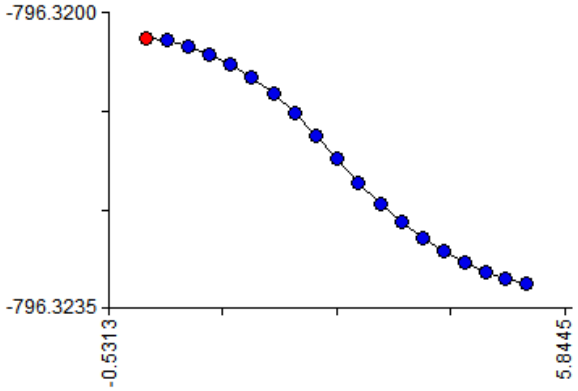
anti-T1-H



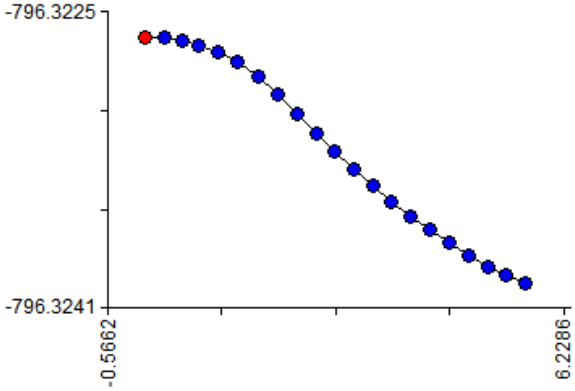
syn-T2-H



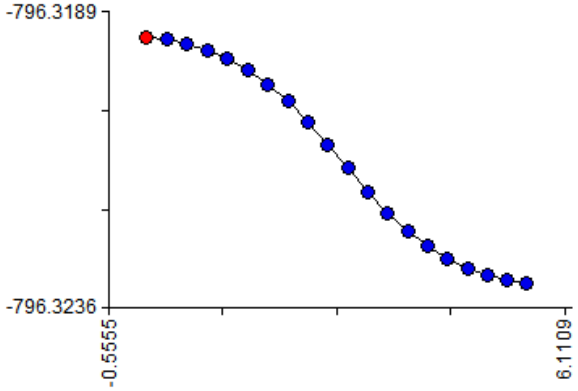
anti-T2-H



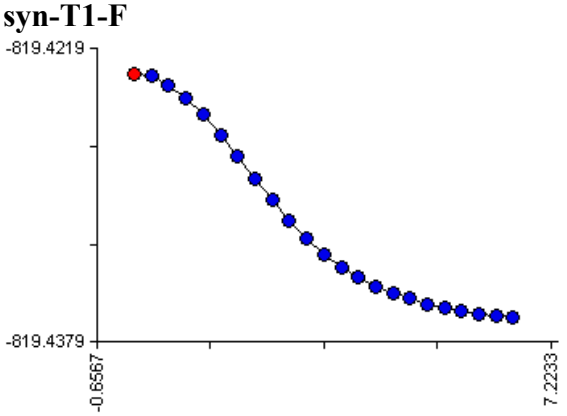
synT3-H



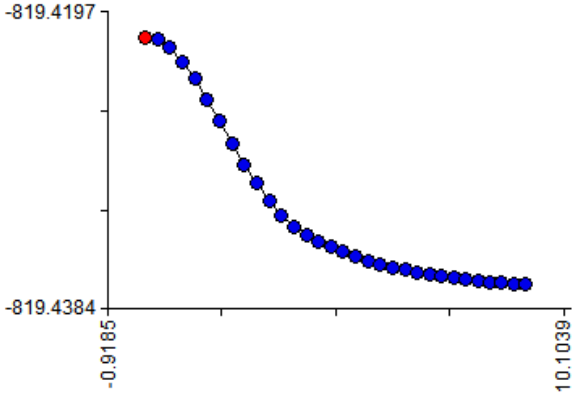
anti-T3-H



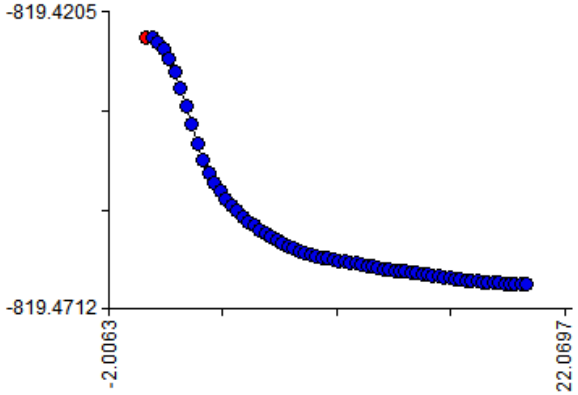
syn-T1-F



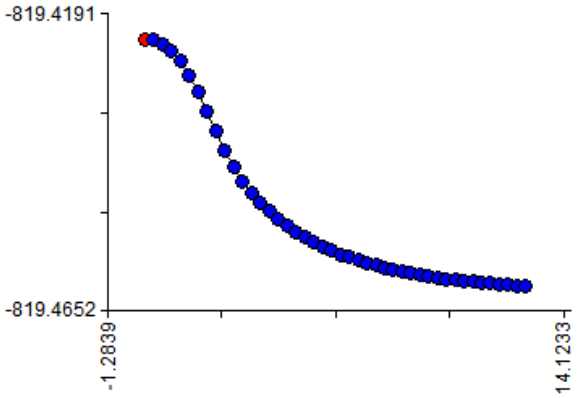
syn-T2-F



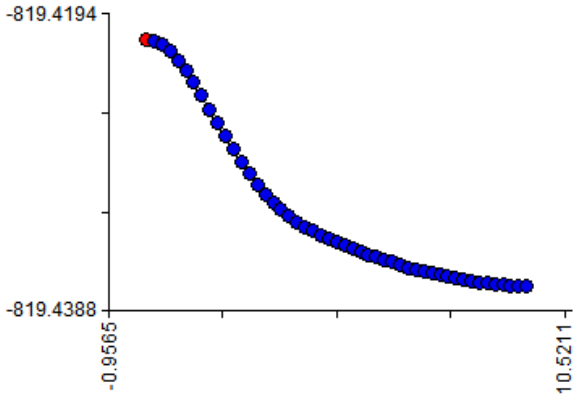
anti-T1-F



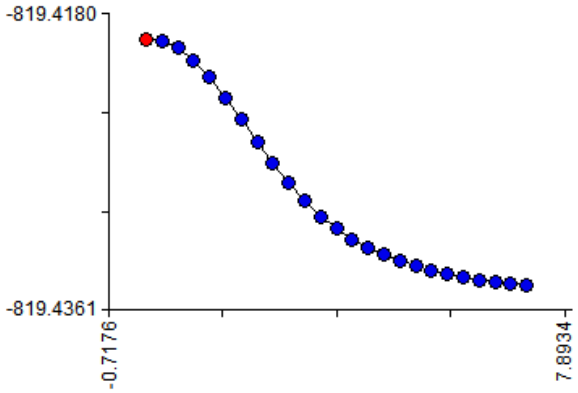
syn-T3-F



anti-T2-F



anti-T3-F



Geometries and Energies

1-CH_3CHO

C	0.23287	-0.40467	0.00051
H	0.30915	-1.50849	-0.00183
C	-1.15316	0.16091	0.00011
H	-1.69277	-0.20745	0.87931
H	-1.68965	-0.20724	-0.88096
H	-1.12898	1.25109	-0.00002
O	1.24450	0.26617	-0.00025

E(0 K) = -153.770052
E(0 K) + ZPE = -153.715731
H (195 K) = -153.712858
G (195 K) = -153.730761

1-BF_3•OEt_2

B	-0.75702	0.00257	0.00187
O	0.78354	-0.37268	-0.00092
C	1.49277	0.00884	-1.20801
H	2.47927	-0.44931	-1.16253
H	1.56193	1.09782	-1.25137
H	0.92071	-0.38285	-2.04470
C	1.49870	-0.00698	1.20690
H	0.88844	-0.33325	2.04467
H	1.64427	1.07522	1.21998
H	2.45214	-0.53264	1.19200
F	-1.26624	-0.55353	-1.14632
F	-1.26412	-0.55895	1.14844
F	-0.79498	1.38131	-0.00000

E(0 K) = -479.618168
E(0 K) + ZPE = -479.523899
H (195 K) = -479.519407
G (195 K) = -479.542547

2-a

C	3.41041	1.00202	1.01771
H	4.48874	0.80217	1.04498
H	3.20709	2.03561	1.29199
C	2.94577	0.70721	-0.34549
H	3.01740	-0.31117	-0.74551
O	2.48545	1.59761	-1.07308
H	2.94331	0.30163	1.71713
B	2.10236	1.32073	-2.59194
F	3.27695	1.50529	-3.27981
F	1.13716	2.25279	-2.86439
F	1.64365	0.02057	-2.64773

E(0 K) = -478.423414
E(0 K) + ZPE = -478.353511
H (195 K) = -478.349099
G (195 K) = -478.372262

2-b

C	-0.86187	0.03403	0.68575
H	-1.74684	0.02941	1.32786
O	-1.09076	0.03644	-0.53221
C	0.46513	0.02503	1.32491
H	0.56712	-0.93947	1.83914
H	0.46601	0.79082	2.10702
H	1.28512	0.16770	0.62659
B	0.04091	-0.02474	-1.65624
F	0.73425	-1.18921	-1.40906
F	0.80556	1.10514	-1.48525
F	-0.66463	-0.03515	-2.82851

E(0 K) = -478.422059
E(0 K) + ZPE = -478.351673
H (195 K) = -478.347503
G (195 K) = -478.370019

***E*-crotylsilane**

C	0.40795	-0.40440	0.66445
C	-0.56523	0.51416	-0.00946
H	-0.38442	0.54947	-1.09138
H	-0.46621	1.53707	0.37430
Si	-2.36174	-0.05915	0.24876
C	-2.58847	-1.68504	-0.67562
H	-1.92151	-2.45411	-0.27270
H	-2.35544	-1.55743	-1.73837
H	-3.61864	-2.04585	-0.59181
C	-3.52741	1.24848	-0.44786
H	-3.40473	2.19898	0.08149
H	-4.57101	0.93349	-0.34608
H	-3.32617	1.42217	-1.51006
C	-2.69633	-0.30718	2.08676
H	-2.52383	0.61829	2.64611
H	-2.04516	-1.08390	2.50046
H	-3.73479	-0.61393	2.24942
C	1.09793	-1.38184	0.06673
H	0.98915	-1.51392	-1.01172
H	0.51725	-0.28386	1.74472
C	2.02612	-2.32737	0.77316
H	3.04178	-2.26586	0.36733
H	1.69879	-3.36640	0.65580

H	2.07201	-2.10354	1.84298

E(0 K) = -565.832123
E(0 K) + ZPE -565.628236
H (195 K) = -565.621278
G (195 K) = -565.649705

3

C	3.27174	1.07217	0.94194
H	4.27604	1.50992	0.85480
H	2.63208	1.77062	1.48207
C	2.78483	0.86875	-0.43657
H	3.07103	-0.02028	-1.00624
O	2.13687	1.76001	-1.01611
H	3.36705	0.12158	1.46764
B	1.78295	1.61856	-2.54251
F	2.93900	1.95095	-3.21953
F	0.75158	2.50136	-2.74278
F	1.42392	0.29927	-2.74595
C	0.40271	-0.40389	0.66327
C	-0.56652	0.51101	-0.00549
H	-0.39094	0.54340	-1.08761
H	-0.46769	1.53402	0.38031
Si	-2.36644	-0.06183	0.25265
C	-2.58355	-1.68751	-0.67224
H	-1.92027	-2.45806	-0.26582
H	-2.34572	-1.55921	-1.73369
H	-3.61412	-2.04835	-0.59377
C	-3.51454	1.25302	-0.45419
H	-3.38921	2.20284	0.07549
H	-4.56098	0.94536	-0.36033
H	-3.30275	1.42334	-1.51471
C	-2.70226	-0.30618	2.08995
H	-2.52876	0.61909	2.64916
H	-2.05571	-1.08581	2.50576
H	-3.74203	-0.60953	2.25045
C	1.09820	-1.38180	0.06032
H	0.98006	-1.51531	-1.01646
H	0.52118	-0.28197	1.74328
C	2.02817	-2.32240	0.76911
H	3.04562	-2.26609	0.36117
H	1.70352	-3.36132	0.64821
H	2.07328	-2.10247	1.83998

E(0 K) = -1044.266175
E(0 K) + ZPE = -1043.989710
H (195 K) = -1043.978604
G (195 K) = -1044.016383

4‡ (syn-T3-L)

C	3.06882	1.01002	0.94746
H	3.99107	1.54945	0.70848
H	2.40923	1.68931	1.49125
C	2.44735	0.59659	-0.35972
H	3.04982	-0.09608	-0.95826
O	1.88363	1.57782	-1.02967
H	3.32678	0.15269	1.57130
B	1.82851	1.51756	-2.51900
F	3.12533	1.68475	-3.02314
F	0.97784	2.53732	-2.92971
F	1.33980	0.26352	-2.92929
C	0.40742	-0.09172	0.74318
C	-0.60772	0.82289	0.28927
H	-0.49264	1.08488	-0.76881
H	-0.70579	1.71186	0.91935
Si	-2.32815	-0.09677	0.36732
C	-2.21454	-1.57039	-0.78967
H	-1.51703	-2.32278	-0.40731
H	-1.88300	-1.26871	-1.78817
H	-3.19699	-2.04309	-0.88768
C	-3.59712	1.15845	-0.20496
H	-3.62198	2.02452	0.46249
H	-4.59131	0.69987	-0.20756
H	-3.37812	1.50634	-1.21867
C	-2.64765	-0.64943	2.13280
H	-2.61863	0.19394	2.82909
H	-1.90970	-1.39080	2.45560
H	-3.63782	-1.11098	2.20281
C	1.19345	-0.86929	-0.08893
H	0.89080	-0.91882	-1.13402
H	0.59859	-0.14681	1.81795
C	1.98849	-2.03905	0.43538
H	2.92225	-2.16919	-0.12025
H	1.40952	-2.95981	0.31838
H	2.22565	-1.92524	1.49655

E(0 K) = -1044.256951
E(0 K) + ZPE = -1043.979477
H (195 K) = -1043.969449
G (195 K) = -1044.004813

5

C	0.26147	0.63714	0.77449
C	3.03811	1.46763	-0.17584
H	3.66012	1.10252	0.64525
H	3.69278	1.87152	-0.95157
C	-0.79170	1.12291	0.03277
H	-0.81801	0.90261	-1.03624
H	-1.28655	2.03295	0.37333
Si	-2.19875	-0.28551	0.71533
C	-1.67949	-1.95506	0.07824
H	-0.93634	-2.43283	0.72247
H	-1.27861	-1.88640	-0.93856
H	-2.56580	-2.59777	0.05050
C	-3.67121	0.41654	-0.19280
H	-3.87530	1.44895	0.10034

H	-4.54638	-0.19329	0.05676
H	-3.51884	0.37422	-1.27443
C	-2.31133	-0.13790	2.57030
H	-2.41377	0.90505	2.88360
H	-1.44033	-0.57425	3.06750
H	-3.20037	-0.67859	2.91088
O	1.42073	0.88378	-1.81258
H	0.38319	1.02312	1.78990
H	2.40508	2.28265	0.19130
B	1.02044	0.03232	-2.91064
F	2.06411	-0.14427	-3.84760
F	-0.07876	0.64203	-3.54747
F	0.61855	-1.26321	-2.46852
C	2.02737	-1.02539	1.41508
H	2.82306	-1.65064	1.00061
H	1.37743	-1.67002	2.01456
H	2.48414	-0.29289	2.08703
C	1.24620	-0.34935	0.29161
H	0.73130	-1.09221	-0.32282
C	2.18500	0.35949	-0.77620
H	2.83546	-0.45524	-1.13025

E(0 K) = -1044.262065
E(0 K) + ZPE = -1043.982422
H (195 K) = -1043.972469
G (195 K) = -1044.007596

6‡

C	1.93993	2.57444	1.50279
H	2.38365	3.17764	0.70658
H	1.95975	3.15332	2.42914
C	-0.77767	-0.95736	0.64998
H	-1.76745	-0.52461	0.49092
H	-0.73443	-1.74304	1.40546
Si	-0.48700	-1.98671	-1.06560
C	-1.43440	-3.55569	-0.69791
H	-2.47003	-3.33586	-0.42428
H	-0.96625	-4.11531	0.11658
H	-1.44074	-4.18947	-1.59077
C	1.33608	-2.32368	-1.31794
H	1.91991	-1.41853	-1.50470
H	1.45232	-2.97900	-2.18755
H	1.75899	-2.84091	-0.45127
C	-1.28515	-0.98712	-2.42815
H	-0.81157	-0.01549	-2.58592
H	-2.34464	-0.82410	-2.21021
H	-1.21488	-1.54999	-3.36497
H	2.55157	1.67831	1.65001
B	-1.37537	1.69149	2.69876
F	-2.28374	1.50918	1.62406
F	-1.50041	3.02424	3.14614
F	-1.68749	0.80613	3.74014
C	1.36012	1.38448	-1.12360
H	1.40372	2.41264	-1.49273
H	1.13136	0.74105	-1.97589
H	2.35088	1.11574	-0.74584
C	0.29270	1.28373	-0.03077
H	-0.70303	1.46381	-0.44882
C	0.49806	2.21332	1.19346
H	-0.09198	3.12914	1.07543
O	-0.00708	1.42154	2.27291
C	0.27559	-0.03877	0.67700
H	1.22496	-0.36335	1.10665

E(0 K) = -1044.257775
E(0 K) + ZPE = -1043.978259
H (195 K) = -1043.968729
G (195 K) = -1044.003007

7‡

C	0.10020	0.86614	1.75425
H	0.08092	1.55621	0.89707
O	-1.12800	0.16510	1.82548
B	-2.12759	0.54031	0.90795
F	-3.19221	-0.34806	0.91181
F	-1.55741	0.47102	-0.51063
F	-2.56121	1.86163	1.01774
C	1.25178	-0.12839	1.51773
H	2.16248	0.46977	1.39511
C	1.10162	-0.97875	0.27847
H	2.01525	-1.10591	-0.30177
C	0.02730	-1.71436	-0.08770
H	-0.89156	-1.70625	0.48574
H	0.12315	-2.45138	-0.88003
Si	-0.31089	-0.07530	-2.03174
C	-1.79127	-0.92824	-2.77695
H	-2.68287	-0.30446	-2.69643
H	-1.98761	-1.87549	-2.26690
H	-1.58307	-1.14503	-3.82927
C	1.24537	-0.83205	-2.78623
H	2.15193	-0.31950	-2.45389
H	1.14487	-0.65309	-3.86537
H	1.35996	-1.90786	-2.63602
C	-0.04723	1.76522	-2.19864
H	0.42430	1.96618	-3.16568
H	0.63467	2.12206	-1.41930
H	-0.98405	2.31783	-2.11771
C	1.45674	-1.08523	2.70662
H	2.20949	-1.84304	2.47212
H	0.51567	-1.59198	2.93788
H	1.79496	-0.53912	3.59027
C	0.29607	1.69307	3.01816
H	1.27932	2.17409	3.02796
H	0.20175	1.06205	3.90563
H	-0.47385	2.46674	3.06575

E(0 K) = -1044.244049
E(0 K) + ZPE = -1043.964141

H (195 K) = -1043.954595
G (195 K) = -1043.988757

8‡

C	0.89062	2.72791	-1.44472
H	0.41702	3.63327	-1.83446
H	1.78311	3.02153	-0.89064
C	0.57341	-0.47827	-1.89450
H	1.41625	0.18858	-1.75327
H	0.78898	-1.45441	-2.31522
H	1.18512	2.11933	-2.30146
B	0.99484	1.78069	1.70061
F	-0.12886	2.38926	2.28933
F	1.96607	2.75832	1.45215
F	1.49541	0.79716	2.55397
C	-1.86389	1.98801	-2.31986
H	-2.21950	2.95906	-1.96259
H	-2.72295	1.43227	-2.70366
H	-1.16514	2.15329	-3.14386
C	-1.19227	1.22345	-1.17113
H	-1.95955	1.02928	-0.40928
C	-0.07850	2.02196	-0.49416
H	-0.56140	2.78729	0.12116
O	0.60075	1.12474	0.41069
C	-0.70694	-0.11363	-1.65514
H	-1.48793	-0.84334	-1.87242
Si	0.33414	-1.02178	0.50190
C	-0.97072	-0.73296	1.81846
H	-0.92220	-1.59686	2.49194
H	-1.95887	-0.75768	1.34586
H	-0.86783	0.18672	2.38921
C	2.18197	-1.20957	0.74192
H	2.71986	-0.26434	0.69385
H	2.57183	-1.90633	-0.00534
H	2.34248	-1.64543	1.73415
C	-0.20059	-2.75259	-0.09406
H	-1.25498	-2.80013	-0.38392
H	-0.06885	-3.42319	0.76550
H	0.40921	-3.14583	-0.91132

E(0 K) = -1044.258176
E(0 K) + ZPE = -1043.977131
H (195 K) = -1043.967962
G (195 K) = -1044.001218

9‡

Si	-1.16435	-0.33403	1.03095
C	-2.52826	-1.59023	1.25163
H	-2.69279	-1.72882	2.32313
H	-2.24997	-2.55024	0.80992
H	-3.45989	-1.24613	0.79597
C	0.56705	-0.95257	1.35077
H	0.56042	-1.51897	2.28532
H	1.29281	-0.13866	1.43782
H	0.89075	-1.62845	0.55396
C	-1.67334	1.46176	1.14739
H	-2.41014	1.69670	0.37431
H	-0.81714	2.13201	1.02558
H	-2.12673	1.64793	2.12252
C	-1.26636	-0.70271	-1.25811
H	-2.34819	-0.64655	-1.35516
H	-0.79023	-1.68107	-1.27624
C	-0.51324	0.41344	-1.43504
H	-1.03093	1.36981	-1.53647
O	-1.24737	-0.12875	3.51686
C	0.63257	1.09639	-4.06959
H	0.84423	2.14606	-3.84704
H	0.98642	0.88203	-5.08065
O	1.00682	-1.15409	-3.43265
H	-0.45079	0.93950	-4.05289
B	1.71674	-2.24739	-2.81466
F	3.02567	-1.86814	-2.41617
F	1.79323	-3.32447	-3.71607
F	1.04112	-2.69925	-1.63482
C	1.56561	1.77169	-1.09987
H	2.63608	1.80973	-1.31993
H	1.44692	1.88416	-0.01744
H	1.08727	2.63282	-1.57782
C	0.96923	0.45228	-1.59017
H	1.41760	-0.38268	-1.04651
C	1.32548	0.16270	-3.08731
H	2.41302	0.31623	-3.14509
C	-0.36881	0.04191	4.34632
H	0.68634	0.08260	4.02207
C	-0.63020	0.19845	5.80356
H	-0.09988	-0.59433	6.34228
H	-1.69800	0.15539	6.01658
H	-0.20747	1.14978	6.14262

E(0 K) = -1198.089145
E(0 K) + ZPE = -1197.752674
H (195 K) = -1197.740563
G (195 K) = -1197.780258

10

C	1.09769	3.39764	1.18186
H	1.13320	4.14486	0.38341
H	0.75100	3.88286	2.09623
C	-0.89153	-0.71737	0.45490
H	-1.78929	-0.11417	0.27725
H	-1.06651	-1.31508	1.35727
Si	-0.67282	-1.93897	-1.00052
C	-2.08591	-3.17545	-0.90860
H	-3.05176	-2.66363	-0.96701
H	-2.05561	-3.74414	0.02579
H	-2.02427	-3.88235	-1.74214

C	0.98865	-2.80603	-0.82350
H	1.82358	-2.11420	-0.97783
H	1.07732	-3.60530	-1.56643
H	1.09511	-3.25376	0.17013
C	-0.76134	-1.03700	-2.65351
H	0.09596	-0.37793	-2.82156
H	-1.67552	-0.43859	-2.72722
H	-0.77544	-1.77257	-3.46510
H	2.10521	3.00946	1.34518
B	-0.80676	1.11102	2.95407
F	-2.09858	1.14838	2.45858
F	-0.51741	2.23500	3.70603
F	-0.50782	-0.07582	3.58968
C	1.91293	1.41792	-0.94205
H	2.04550	2.35103	-1.49649
H	2.08501	0.58905	-1.63592
H	2.68090	1.36470	-0.16492
C	0.51408	1.32045	-0.35467
H	-0.23839	1.32103	-1.14737
C	0.14925	2.29952	0.78273
H	-0.88229	2.65522	0.71260
O	0.17295	1.18162	1.75308
C	0.30416	0.16648	0.64683
H	1.20893	-0.40178	0.87969

E(0 K) = -1044.281226
E(0 K) + ZPE = -1044.000768
H (195 K) = -1043.990797
G (195 K) = -1044.026120

11‡

Si	-1.17817	-0.38459	1.11895
C	-2.64165	-1.52087	1.35543
H	-3.06457	-1.32600	2.34430
H	-2.34631	-2.57129	1.28846
H	-3.42095	-1.32575	0.61673
C	0.52992	-1.07092	1.44027
H	0.52059	-1.61593	2.38698
H	1.27524	-0.27307	1.51359
H	0.83566	-1.76351	0.65100
C	-1.59656	1.43442	1.26492
H	-2.34152	1.70802	0.51292
H	-0.72474	2.08064	1.12824
H	-2.03120	1.62198	2.24945
C	-1.24069	-0.76797	-1.16164
H	-2.31689	-0.72337	-1.30402
H	-0.75369	-1.74172	-1.16113
C	-0.49669	0.35825	-1.32138
H	-1.02691	1.30473	-1.44899
O	-1.14170	-0.21438	3.65717
C	-0.12952	0.65999	4.14257
H	-0.08374	1.52488	3.47965
H	0.84332	0.15312	4.15326
H	-0.37568	0.99280	5.15658
C	-1.24505	-1.36915	4.47971
H	-2.02190	-2.01392	4.06924
H	-1.51732	-1.07872	5.50027
H	-0.29293	-1.91496	4.50512
C	0.70929	1.09772	-3.91065
H	0.89258	2.14572	-3.65681
H	1.10268	0.91383	-4.91299
O	1.08728	-1.15931	-3.29751
H	-0.37058	0.92011	-3.93673
B	1.80108	-2.25372	-2.68571
F	3.10607	-1.86991	-2.27956
F	1.88657	-3.32263	-3.59689
F	1.12337	-2.72099	-1.51361
C	1.56015	1.73527	-0.90898
H	2.63080	1.79437	-1.12357
H	1.43730	1.82117	0.17534
H	1.07087	2.59967	-1.36957
C	0.98829	0.41783	-1.43142
H	1.43037	-0.42159	-0.88969
C	1.38476	0.15422	-2.92555
H	2.47183	0.31830	-2.95085

E(0 K) = -1199.279589
E(0 K) + ZPE = -1198.918917
H (195 K) = -1198.906721
G (195 K) = -1198.946473

12

Si	-1.20437	-0.30914	1.69436
C	-2.44433	-1.67269	1.46571
H	-2.22198	-2.49255	2.15563
H	-2.40153	-2.06652	0.44750
H	-3.45856	-1.31478	1.66134
C	0.55979	-0.83393	1.44003
H	0.83572	-1.62073	2.15043
H	1.27271	-0.00835	1.52063
H	0.65084	-1.27272	0.44000
C	-1.73322	1.42522	1.26666
H	-2.48611	1.40535	0.47575
H	-0.88534	2.01751	0.91268
H	-2.16581	1.91320	2.14469
C	-1.32560	-0.47579	-1.59680
H	-2.40989	-0.38994	-1.58175
H	-0.88388	-1.46555	-1.50740
C	-0.54895	0.59664	-1.77942
H	-1.02293	1.57354	-1.90423
O	-1.34146	-0.16989	3.54506
C	0.86709	0.99804	-4.40441
H	1.11236	2.05586	-4.27001
H	1.28022	0.66749	-5.36099
O	1.10448	-1.19559	-3.54800
H	-0.22138	0.89035	-4.44487
B	1.73582	-2.25676	-2.81677
F	3.08281	-1.93444	-2.48301

F	1.71953	-3.43178	-3.60252
F	1.06960	-2.55831	-1.58640
C	1.55402	1.91537	-1.44939
H	2.64343	1.91026	-1.55560
H	1.32061	2.13629	-0.40228
H	1.15634	2.73727	-2.05438
C	0.95449	0.57257	-1.87152
H	1.33667	-0.20479	-1.20185
C	1.43855	0.14359	-3.28137
H	2.53403	0.25290	-3.27178
C	-0.44757	-0.16185	4.40749
H	0.59988	-0.25119	4.09222
C	-0.76533	-0.02383	5.83323
H	-0.30457	-0.85961	6.37199
H	-1.84013	0.01066	6.00247
H	-0.28078	0.88855	6.20165

E(0 K) = -1198.101607
E(0 K) + ZPE = -1197.764181
H (195 K) = -1197.751870
G (195 K) = -1197.792040

13

Si	-1.24153	-0.42830	1.81395
C	-2.57862	-1.69328	1.57925
H	-3.48656	-1.41500	2.12295
H	-2.26260	-2.69543	1.88038
H	-2.82504	-1.72891	0.51379
C	0.49182	-1.00146	1.45843
H	0.83609	-1.67502	2.25140
H	1.19058	-0.16157	1.39245
H	0.53430	-1.55509	0.51484
C	-1.73489	1.32426	1.41629
H	-2.48046	1.31522	0.61733
H	-0.88721	1.92198	1.07068
H	-2.18161	1.80427	2.29239
C	-1.32052	-0.49995	-1.53975
H	-2.40249	-0.39621	-1.58048
H	-0.90050	-1.49880	-1.44421
C	-0.52253	0.56451	-1.67034
H	-0.97976	1.54842	-1.80343
O	-1.16865	-0.28575	3.67482
C	-0.14385	0.59961	4.21017
H	0.00871	1.39815	3.48626
H	0.77461	0.02849	4.35853
H	-0.52005	1.00399	5.14848
C	-1.36625	-1.46479	4.50252
H	-2.28254	-1.94547	4.17135
H	-1.47149	-1.12317	5.53159
H	-0.50398	-2.12684	4.39616
C	0.97719	1.04636	-4.21705
H	1.21496	2.09912	-4.03653
H	1.42006	0.75246	-5.17223
O	1.21114	-1.17736	-3.43709
H	-0.10914	0.93881	-4.29442
B	1.81715	-2.25153	-2.70403
F	3.13846	-1.92833	-2.28935
F	1.85179	-3.40718	-3.52211
F	1.08858	-2.60209	-1.51932
C	1.58105	1.84099	-1.19927
H	2.67405	1.81930	-1.25345
H	1.30192	2.02883	-0.15663
H	1.22779	2.69304	-1.79035
C	0.98275	0.52518	-1.70055
H	1.32747	-0.28620	-1.05198
C	1.51895	0.15440	-3.10863
H	2.61232	0.27398	-3.05852

E(0 K) = -1199.293641
E(0 K) + ZPE = -1198.932479
H (195 K) = -1198.919879
G (195 K) = -1198.960580

14

C	-0.30470	2.29567	2.66693
C	-2.13784	-0.05615	1.77928
H	-2.61989	0.79945	2.25768
H	-2.80122	-0.44660	1.00355
C	-0.63547	2.58554	3.92483
H	-0.58356	1.83342	4.70884
H	-0.96478	3.57996	4.20955
O	-0.23180	-0.70796	0.39871
H	-0.36561	3.07409	1.90259
H	-1.97732	-0.83188	2.53161
B	-0.05899	-2.10594	1.06522
F	-1.24020	-2.80391	0.89146
F	0.24798	-1.92673	2.39721
F	0.98865	-2.69876	0.37038
C	1.58410	1.08508	1.58323
H	1.98305	0.11119	1.28781
H	2.27026	1.53947	2.30171
H	1.55316	1.72877	0.69475
C	0.18751	0.94985	2.19833
H	0.22765	0.27276	3.05656
C	-0.82148	0.39740	1.17793
H	-1.00910	1.18135	0.43999
Si	0.00259	-0.61722	-1.37861
C	-0.92607	0.89207	-1.96693
H	-1.98143	0.87374	-1.67818
H	-0.88319	0.87458	-3.06198
H	-0.47993	1.83470	-1.63800
C	1.83506	-0.46709	-1.67382
H	2.03367	-0.57668	-2.74522
H	2.37737	-1.25047	-1.13952
H	2.21422	0.50843	-1.35782
C	-0.76189	-2.17012	-2.06288
H	-0.75928	-2.10705	-3.15600
H	-1.79632	-2.27159	-1.72399

H	-0.20448	-3.05806	-1.75941

E(0 K) = -1044.316487
E(0 K) + ZPE = -1044.036788
H (195 K) = -1044.026622
G (195 K) = -1044.062069

15

C	-2.93577	1.75040	1.46812
C	-0.06188	1.19261	2.23526
H	-0.63033	1.84197	2.90420
H	0.70029	0.66896	2.81779
C	-3.08380	3.05899	1.26336
H	-2.53084	3.57286	0.48012
H	-3.76065	3.65514	1.86757
O	-0.18169	-0.65948	0.72326
H	-3.50713	1.26258	2.26113
H	0.43385	1.81379	1.48272
B	0.01178	-1.95397	0.97895
F	-0.48671	-2.57503	2.05214
F	0.72553	-2.68849	0.12423
C	-2.88189	-0.21227	-0.06440
H	-2.25748	-0.84421	-0.70063
H	-3.63969	0.26133	-0.69346
H	-3.39718	-0.85217	0.66193
C	-2.04327	0.85060	0.65566
H	-1.50928	1.45771	-0.08805
C	-0.98650	0.19759	1.55843
H	-1.49209	-0.42168	2.31142

E(0 K) = -535.152439
E(0 K) + ZPE = -534.986215
H (195 K) = -534.979937
G (195 K) = -535.007643

$(CH_3)_3SiF$

F	-0.06520	-1.08007	0.20261
Si	0.04022	-0.77595	-1.42232
C	-1.09551	0.66686	-1.75926
H	-2.12698	0.42386	-1.48751
H	-1.07531	0.92378	-2.82314
H	-0.78445	1.54782	-1.18990
C	1.82875	-0.36124	-1.75968
H	1.97476	-0.14324	-2.82241
H	2.48121	-1.19716	-1.49071
H	2.13692	0.51799	-1.18608
C	-0.51012	-2.33600	-2.28675
H	-0.46446	-2.20352	-3.37240
H	-1.54014	-2.58736	-2.01688
H	0.13395	-3.17851	-2.01808

E(0 K) = -509.147042
E(0 K) + ZPE = -509.037093
H (195 K) = -509.032061
G (195 K) = -509.055800

CH_3CHO

C	0.22928	-0.40071	0.00055
H	0.29561	-1.51085	-0.00170
C	-1.14977	0.15884	0.00017
H	-1.69480	-0.21302	0.87702
H	-1.69089	-0.21235	-0.87928
H	-1.13557	1.25163	0.00002
O	1.24613	0.26554	-0.00030

E(0 K) = -153.787774
E(0 K) + ZPE = -153.734326
H (195 K) = -153.731440
G (195 K) = -153.749366

$TiCl_4$

Cl	1.02614	1.77141	-0.72328
Cl	1.02614	-1.77141	-0.72328
Cl	-2.04867	0.00000	-0.71926
Cl	-0.00258	0.00000	2.16828
Ti	-0.00075	0.00000	-0.00180

E(0 K) = -2690.508679
E(0 K) + ZPE = -2690.503149
H (195 K) = -2690.498445
G (195 K) = -2690.523568

S8

C	0.25374	-0.91430	0.47770
O	-0.25395	0.16768	0.18866
Cl	2.16800	0.85535	-1.39084
Cl	-1.52981	1.33040	-2.15360
Cl	0.75729	3.71682	-2.17461
Cl	0.04019	2.94351	0.95958
H	1.25322	-1.16209	0.07489
C	-0.40872	-1.89847	1.34654
H	0.26836	-2.15736	2.16955
H	-0.55644	-2.82672	0.77947
H	-1.36246	-1.52733	1.72549
Ti	0.25504	1.90454	-0.98246

E(0 K) = -2844.315750
E(0 K) + ZPE = -2844.254045
H (195 K) = -2844.247077
G (195 K) = -2844.276845

***E*-crotylsilane**

C	0.41036	-0.39751	0.66774
C	-0.56064	0.52240	0.00901
H	-0.38541	0.57048	-1.07669
H	-0.47340	1.54609	0.40093
Si	-2.35392	-0.06112	0.25173
C	-2.57521	-1.69200	-0.66207
H	-1.95835	-2.48093	-0.21498
H	-2.28169	-1.58720	-1.71474
H	-3.62216	-2.01797	-0.63136
C	-3.52046	1.23679	-0.45766
H	-3.39371	2.19674	0.05808
H	-4.56584	0.92472	-0.34238
H	-3.32990	1.39665	-1.52609
C	-2.71557	-0.29872	2.08509
H	-2.54566	0.62984	2.64445
H	-2.07980	-1.08087	2.51765
H	-3.76166	-0.59425	2.23303
C	1.09049	-1.37875	0.06128
H	0.96861	-1.50356	-1.02002
H	0.52888	-0.28216	1.75094
C	2.01399	-2.32957	0.74991
H	3.03038	-2.27926	0.33731
H	1.68281	-3.37077	0.63664
H	2.07526	-2.11174	1.82317

E(0 K) = -565.746788
E(0 K) + ZPE = -565.545850
H (195 K) = -565.538857
G (195 K) = -565.567357

S9

C	0.71992	-0.00536	1.03915
C	1.41667	3.01648	0.28651
H	1.81881	4.00183	0.00723
H	0.35962	3.13893	0.53682
C	-0.71251	0.19047	0.69430
H	-0.83950	0.35693	-0.38677
H	-1.13550	1.06304	1.21369
Si	-1.78140	-1.31880	1.14939
C	-1.24544	-2.78576	0.10242
H	-0.19564	-3.04220	0.28974
H	-1.35623	-2.56064	-0.96639
H	-1.85701	-3.66740	0.33004
C	-3.57190	-0.88181	0.76704
H	-3.91216	-0.03463	1.37466
H	-4.23761	-1.73105	0.96261
H	-3.67561	-0.60507	-0.29031
C	-1.54994	-1.70409	2.97636
H	-1.82922	-0.84479	3.59853
H	-0.50213	-1.95255	3.18759
H	-2.16802	-2.55796	3.27890
C	1.65289	-0.54012	0.23398
H	1.35180	-0.85634	-0.77113
C	1.59741	2.14141	-0.88659
H	2.57863	1.66084	-1.04717
O	0.72791	2.02339	-1.75700
H	1.02447	0.28006	2.05233
H	1.99468	2.66161	1.14372
C	3.07627	-0.77708	0.61809
H	3.77477	-0.29946	-0.08391
H	3.32221	-1.84712	0.60969
H	3.28861	-0.39099	1.62291
Cl	0.57411	0.71426	-5.92531
Cl	0.54949	3.52384	-4.22090
Cl	2.66069	0.46445	-3.40227
Cl	-1.11781	0.20262	-3.12954
Ti	0.66081	1.35166	-3.78817

E(0 K) = -3410.072102
E(0 K) + ZPE = -3409.807459
H (195 K) = -3409.793829
G (195 K) = -3409.837140

S10‡

C	0.62278	0.28152	0.93518
C	1.62161	2.84684	0.19306
H	1.93396	3.75262	-0.34453
H	0.60109	3.01020	0.55207
C	-0.77816	0.36911	0.57800
H	-0.91917	0.46663	-0.50933
H	-1.29703	1.18031	1.10507
Si	-1.73746	-1.25479	1.00616
C	-1.03393	-2.63192	-0.05401
H	0.01600	-2.83280	0.19235
H	-1.09867	-2.37897	-1.11975
H	-1.59905	-3.55716	0.10992
C	-3.51804	-0.88139	0.55291
H	-3.90450	-0.03540	1.13311
H	-4.16215	-1.74795	0.74195
H	-3.59047	-0.62855	-0.51266
C	-1.51737	-1.62399	2.83170
H	-1.83489	-0.77520	3.44901
H	-0.46627	-1.84181	3.05969
H	-2.11257	-2.49718	3.12382
C	1.63480	-0.17177	0.12462
H	1.35347	-0.65047	-0.81751
C	1.69240	1.72482	-0.78883
H	2.70382	1.39834	-1.07806
O	0.79394	1.67707	-1.70658
H	0.91180	0.63255	1.93214
H	2.30507	2.69941	1.03479
C	3.01451	-0.45173	0.63407
H	3.77474	-0.27542	-0.13657
H	3.10684	-1.50304	0.93336
H	3.25495	0.16456	1.50878
Cl	0.52586	0.76208	-5.83900

Cl	0.49161	3.49609	-4.00751
Cl	2.67937	0.36886	-3.46130
Cl	-1.21583	0.12226	-3.14934
Ti	0.63488	1.30347	-3.62755

E(0 K) = -3410.061886
E(0 K) + ZPE = -3409.796492
H (195 K) = -3409.783648
G (195 K) = -3409.825363

S11

C	0.14639	0.63629	0.25657
C	2.17075	2.67174	-0.49626
H	2.65645	3.36385	-1.19157
H	1.18490	3.08303	-0.24602
C	-1.01907	0.58102	-0.46497
H	-0.95567	0.31871	-1.52600
H	-1.86603	1.19147	-0.14022
Si	-1.71528	-1.24479	0.33476
C	-0.51183	-2.58964	-0.10851
H	0.41459	-2.54927	0.47473
H	-0.26608	-2.56798	-1.17731
H	-0.99483	-3.55146	0.10457
C	-3.27256	-1.31271	-0.68238
H	-3.93456	-0.46274	-0.49197
H	-3.80979	-2.23596	-0.43199
H	-3.02419	-1.34009	-1.74931
C	-1.92211	-0.94285	2.15946
H	-2.36796	0.03826	2.35884
H	-0.95732	-1.00289	2.67755
H	-2.57965	-1.70409	2.59347
C	1.46291	0.18306	-0.23777
H	1.31307	-0.66216	-0.92652
C	2.04277	1.31277	-1.15669
H	3.04229	0.94893	-1.45839
O	1.24249	1.41739	-2.28986
H	0.11002	1.06170	1.26697
H	2.77832	2.62361	0.41377
C	2.42209	-0.19550	0.88114
H	3.37943	-0.53186	0.46938
H	2.01998	-1.01207	1.49285
H	2.62032	0.65085	1.54909
Cl	1.17348	0.50639	-6.32083
Cl	3.27605	1.75072	-4.23811
Cl	0.22144	-0.98745	-3.60064
Cl	-0.53474	2.64918	-4.38014
Ti	1.07050	1.11811	-4.05343

E(0 K) = -3410.074424
E(0 K) + ZPE = -3409.805758
H (195 K) = -3409.793057
G (195 K) = -3409.834347

S1

C	0.18525	0.28514	0.74531
H	0.82652	0.84143	0.03738
C	-0.35935	1.25090	1.78973
H	-0.99850	2.00159	1.31713
H	0.45139	1.76137	2.31606
H	-0.95672	0.69951	2.52365
C	1.04469	-0.82952	1.36457
H	0.41662	-1.35870	2.09501
C	1.51388	-1.81903	0.29142
H	2.14926	-1.31352	-0.44631
H	0.65831	-2.25036	-0.23320
H	2.09659	-2.62607	0.74347
C	2.23425	-0.24758	2.07807
H	2.89709	0.36887	1.46540
C	2.53806	-0.45566	3.35921
H	1.90153	-1.06582	3.99635
H	3.42767	-0.02615	3.80980
O	-0.90220	-0.31043	0.04562
Si	-1.32357	0.21399	-1.50032
C	0.04232	-0.24810	-2.70573
H	0.98981	0.23227	-2.43866
H	-0.22103	0.06984	-3.71998
H	0.20138	-1.33107	-2.71515
C	-1.55427	2.07890	-1.50547
H	-1.80037	2.42104	-2.51639
H	-0.63966	2.59436	-1.19248
H	-2.36568	2.38092	-0.83579
C	-2.91621	-0.67233	-1.92033
H	-3.26376	-0.37209	-2.91410
H	-3.69893	-0.43149	-1.19503
H	-2.76829	-1.75643	-1.92356

E(0 K) = -719.704914
E(0 K) + ZPE = -719.440443
H (195 K) = -719.432030
G (195 K) = -719.463765

S2‡

C	3.50341	0.69086	-1.98077
H	3.35864	0.44828	-3.03784
H	4.22737	-0.01137	-1.55832
H	3.92253	1.70160	-1.91715
C	0.79247	1.90058	-1.94508
H	-0.07376	2.22719	-1.36608
H	0.43715	1.45179	-2.87908
H	1.39648	2.77504	-2.20630
C	2.28912	0.98586	0.76196
H	3.08967	1.72709	0.84038
H	2.63998	0.05351	1.21759
H	1.41875	1.32942	1.32598
B	0.56864	-1.70763	-0.94904
F	0.75104	-2.65968	0.02483

F	1.90490	-1.27494	-1.45091
F	-0.18750	-2.16828	-1.99659
C	-1.06463	0.04529	0.02497
H	-0.89999	1.06871	0.38750
Si	1.87667	0.67884	-1.03088
O	0.22345	-0.37986	-0.46370
C	-2.08391	0.04548	-1.10446
H	-1.68824	0.56766	-1.97784
H	-2.99781	0.54697	-0.77868
H	-2.33455	-0.97830	-1.39562
C	-1.48349	-0.82933	1.21828
H	-1.61250	-1.85800	0.85357
C	-0.42841	-0.81366	2.33022
H	0.53883	-1.15776	1.95899
H	-0.73813	-1.46822	3.14900
H	-0.31077	0.19894	2.73397
C	-2.80287	-0.34561	1.76032
H	-2.82397	0.69425	2.09533
C	-3.89667	-1.09618	1.88534
H	-4.81193	-0.69746	2.31170
H	-3.90783	-2.13543	1.56428

E(0 K) = -1044.278845
E(0 K) + ZPE = -1043.999193
H (195 K) = -1043.989735
G (195 K) = -1044.023659

S3

C	-0.79190	-0.64487	-0.14748
H	-0.54415	-1.03713	-1.14001
C	-0.60497	-1.73427	0.89339
H	0.45367	-1.96504	1.03014
H	-1.11172	-2.63793	0.54817
H	-1.02749	-1.44382	1.85617
C	-2.20079	-0.04316	-0.21240
H	-2.47832	0.29570	0.79110
C	-2.27439	1.13183	-1.19372
H	-2.03672	0.80252	-2.21169
H	-1.58026	1.93053	-0.91771
H	-3.28602	1.54394	-1.20215
C	-3.15602	-1.13323	-0.62970
H	-2.99352	-1.55740	-1.62302
C	-4.16714	-1.57409	0.11716
H	-4.35261	-1.16941	1.10937
H	-4.83785	-2.34939	-0.23930
O	0.21397	0.44118	0.05031
Si	1.63264	0.40204	-1.07685
B	0.29355	1.17540	1.36713
F	1.57441	0.67388	1.95214
B	1.88242	0.13530	3.49874
F	1.27065	1.06367	4.27037
F	3.23873	0.16123	3.49714
F	1.32421	-1.09787	3.50402
F	-0.72233	0.83836	2.19906
F	0.43299	2.50781	1.13824
C	2.46164	-1.23430	-0.75544
H	2.75766	-1.32412	0.29388
H	3.36796	-1.29027	-1.36717
H	1.83150	-2.08751	-1.02239
C	2.67875	1.87357	-0.64772
H	3.54739	1.85560	-1.31539
H	3.03630	1.85697	0.38307
H	2.13525	2.80543	-0.81997
C	0.91056	0.55990	-2.78566
H	1.74921	0.62534	-3.48804
H	0.32513	1.47920	-2.87797
H	0.29482	-0.28987	-3.09060

E(0 K) = -1368.903620
E(0 K) + ZPE = -1368.609465
H (195 K) = -1368.597402
G (195 K) = -1368.636842

S4‡

B	2.06141	-0.18833	2.72728
F	0.70857	0.10081	2.97989
F	2.17295	-0.26909	1.23916
Si	2.05165	0.63749	-0.57913
B	-0.28095	1.26922	1.43154
F	-1.42811	1.29761	2.09369
F	0.59582	2.26632	1.57482
F	2.40987	-1.42700	3.20114
F	2.88812	0.81801	3.15292
O	-0.04678	0.42451	0.38393
C	-0.90729	-0.69945	0.01528
H	-0.50405	-1.00941	-0.95578
C	2.13883	-1.03349	-1.39673
H	3.18514	-1.23659	-1.64695
H	1.55245	-1.05765	-2.31835
H	1.80203	-1.83034	-0.72974
C	3.63412	1.46119	-0.03656
H	4.05123	2.03599	-0.86873
H	4.36623	0.73150	0.31439
H	3.42110	2.15361	0.78402
C	1.11185	1.90274	-1.58248
H	0.86206	2.78489	-0.98681
H	0.20030	1.49622	-2.02345
H	1.78518	2.22100	-2.38833
C	-0.73946	-1.80989	1.03682
H	0.31801	-2.03414	1.19436
H	-1.24361	-2.71163	0.68381
H	-1.17919	-1.51871	1.99533
C	-2.36830	-0.26439	-0.19301
H	-2.81746	-0.06503	0.78618
C	-2.47763	0.98382	-1.07488
H	-2.05769	0.79296	-2.06921
H	-1.95336	1.84092	-0.64307
H	-3.52687	1.26048	-1.20078

C	-3.11929	-1.40716	-0.82854
H	-2.79398	-1.69368	-1.83095
C	-4.13679	-2.05075	-0.25763
H	-4.48225	-1.78731	0.73947
H	-4.65439	-2.85665	-0.76829

E(0 K) = -1368.862810
E(0 K) + ZPE = -1368.569957
H (195 K) = -1368.557918
G (195 K) = -1368.597312

S5

C	-0.35139	2.41740	0.52276
H	-1.41128	2.34580	0.25092
O	0.18220	1.04713	0.46258
B	-0.05131	-0.02225	1.52752
B	0.01276	0.01125	-0.64229
O	-0.22216	-1.05983	0.42261
F	-1.09329	0.24246	-1.40101
F	1.16680	-0.21212	-1.33190
F	1.05973	-0.19281	2.29415
F	-1.20715	0.13642	2.23045
C	0.32592	-2.42495	0.46740
H	1.39502	-2.33499	0.24033
C	0.09436	-2.96283	1.86960
H	0.58355	-2.35437	2.62873
H	0.49717	-3.97440	1.93227
H	-0.97941	-3.01016	2.07798
C	-0.37941	-3.28891	-0.59029
H	-1.44616	-3.31042	-0.32990
C	-0.16974	2.91149	1.94822
H	-0.57089	3.92274	2.02640
H	0.89574	2.94597	2.19724
H	-0.69050	2.28309	2.66953
C	0.40743	3.29955	-0.48132
H	1.46344	3.29525	-0.17986
C	-0.21854	-2.78121	-2.02970
H	0.83935	-2.67199	-2.28977
H	-0.71617	-1.82476	-2.19007
H	-0.66617	-3.50494	-2.71545
C	0.16421	-4.69448	-0.51433
H	1.23249	-4.80128	-0.71431
C	-0.57176	-5.77759	-0.26978
H	-0.13363	-6.77070	-0.26282
H	-1.63846	-5.70132	-0.07118
C	0.29301	2.83461	-1.93944
H	0.77314	3.57121	-2.58829
H	-0.75606	2.74565	-2.23915
H	0.78581	1.87707	-2.10898
C	-0.11431	4.71222	-0.38700
H	-1.16941	4.84598	-0.63470
C	0.63020	5.77249	-0.07734
H	0.21174	6.77399	-0.06221
H	1.68454	5.66845	0.16877

E(0 K) = -1070.324322
E(0 K) + ZPE = -1069.988662
H (195 K) = -1069.977389
G (195 K) = -1070.015662

S6

C	-2.72997	1.55971	-0.16791
C	-0.16491	0.88764	1.35825
H	-0.84897	1.61833	1.79647
H	0.31775	0.33366	2.16852
C	-2.81793	2.87916	-0.33912
H	-2.05410	3.42704	-0.88681
H	-3.64984	3.45116	0.06042
O	-0.11361	-1.12362	-0.03384
H	-3.51657	1.04051	0.38579
H	0.60436	1.42738	0.79700
C	-2.20984	-0.29911	-1.73561
H	-1.42170	-0.92188	-2.16466
H	-2.71025	0.24052	-2.54429
H	-2.94503	-0.96138	-1.26246
C	-1.63223	0.68643	-0.71365
H	-0.89072	1.32471	-1.21015
C	-0.93305	-0.05931	0.44291
H	-1.71651	-0.55853	1.03011
B	1.10117	-0.91603	-0.68075
F	1.52412	-2.02895	-1.38993
F	1.27417	0.25823	-1.39356
O	2.25837	-0.76433	0.48564
C	3.57315	-0.39302	0.02235
H	4.17836	-0.14667	0.89517
H	3.44763	0.47781	-0.61518
H	4.01172	-1.22623	-0.53277
C	2.29623	-1.83999	1.44501
H	2.83754	-1.48554	2.32262
H	2.79586	-2.70507	1.00154
H	1.26345	-2.07477	1.69178

E(0 K) = -690.176774
E(0 K) + ZPE = -689.929229
H (195 K) = -689.920968
G (195 K) = -689.952681

syn-T1-L

C	-2.67067	-0.94863	-1.36248
H	-2.92463	-1.35089	-0.37847
H	-3.53895	-1.08222	-2.01592
C	-2.40485	0.52667	-1.29981
H	-1.91942	0.97475	-2.16840
O	-3.37997	1.23409	-0.77944
H	-1.83071	-1.49611	-1.78801
C	0.05147	0.14004	-0.64364

C	0.47582	-1.23089	-0.50083
H	0.87389	-1.67649	-1.41647
H	-0.26182	-1.87641	-0.01347
Si	1.97288	-1.19006	0.76578
C	3.25580	0.02952	0.14486
H	2.90482	1.06319	0.22640
H	3.51429	-0.16786	-0.90025
H	4.16934	-0.06174	0.74114
C	2.64822	-2.93920	0.78887
H	1.88824	-3.65922	1.10496
H	3.48817	-2.99945	1.48855
H	3.00886	-3.22689	-0.20316
C	1.27959	-0.67296	2.42939
H	0.45120	-1.31995	2.73445
H	0.92418	0.36221	2.41463
H	2.06327	-0.74600	3.19043
C	-0.96643	0.76162	0.05903
H	-1.44369	0.17131	0.84433
H	0.60704	0.75765	-1.35493
B	-3.73544	2.60040	-1.28080
F	-2.72856	3.06808	-2.13160
F	-3.89465	3.44850	-0.18390
F	-4.94843	2.49712	-1.97197
C	-0.92311	2.25324	0.28739
H	-0.23555	2.47981	1.10853
H	-1.90918	2.63083	0.55887
H	-0.58046	2.78356	-0.60583

E(0 K) = -1044.249076
E(0 K) + ZPE = -1043.972308
H (195 K) = -1043.962023
G (195 K) = -1043.998071

syn-T2-L

C	-3.56981	0.83241	-0.07775
H	-3.60301	1.91143	0.08243
H	-4.46679	0.54137	-0.63487
C	-2.39504	0.43151	-0.93510
H	-2.23044	-0.64599	-0.98657
O	-2.32756	1.07602	-2.08331
H	-3.56927	0.30750	0.87769
C	-0.09650	0.10768	-0.35038
C	0.14835	-1.22876	0.14336
H	0.24425	-1.95788	-0.66742
H	-0.57374	-1.55820	0.89809
Si	1.89043	-1.22306	1.02945
C	3.14972	-0.53522	-0.17908
H	2.98161	0.52925	-0.37101
H	3.10965	-1.06840	-1.13455
H	4.16008	-0.64763	0.22626
C	2.25080	-3.01067	1.46189
H	1.45645	-3.43518	2.08243
H	3.19155	-3.07475	2.01836
H	2.34883	-3.61843	0.55736
C	1.70859	-0.13912	2.54854
H	0.96913	-0.55662	3.23894
H	1.38706	0.86945	2.26831
H	2.66163	-0.05471	3.07956
C	-0.94048	1.05045	0.21610
H	-1.34940	0.80180	1.19637
H	0.41218	0.39580	-1.27267
B	-1.45471	0.57709	-3.18309
F	-1.02901	-0.72998	-2.88954
F	-0.33325	1.41957	-3.26461
F	-2.18218	0.59775	-4.36622
C	-0.79439	2.51665	-0.10767
H	-0.07429	2.97544	0.57632
H	-1.74251	3.04809	0.00571
H	-0.44244	2.64672	-1.13282

E(0 K) = -1044.255851
E(0 K) + ZPE = -1043.978159
H (195 K) = -1043.968079
G (195 K) = -1044.003588

anti-T1-L

C	-0.69565	0.01315	0.06863
C	-1.98013	2.60978	-0.43867
H	-2.34990	2.79414	0.57268
H	-2.20286	3.49457	-1.04307
C	-0.12082	-0.72137	-1.03291
H	0.82049	-0.29370	-1.39351
H	-0.82264	-0.90774	-1.85197
Si	0.33719	-2.50658	-0.36261
C	1.41068	-2.27957	1.15813
H	0.83972	-1.84312	1.98414
H	2.26100	-1.62422	0.94465
H	1.80209	-3.24580	1.49160
C	1.26524	-3.32586	-1.76835
H	0.66460	-3.33569	-2.68253
H	1.50538	-4.36084	-1.50484
H	2.20118	-2.79733	-1.97187
C	-1.26612	-3.38906	0.04946
H	-1.93167	-3.42034	-0.81846
H	-1.79258	-2.89938	0.87468
H	-1.05475	-4.41961	0.35196
C	-0.03777	0.98596	0.80045
H	1.03452	1.07398	0.62498
C	-0.48811	2.43464	-0.44328
H	-0.05318	2.01023	-1.35318
O	0.16688	3.45300	0.07075
H	-1.73527	-0.20012	0.32942
H	-2.49000	1.74721	-0.87151
B	1.56470	3.71566	-0.38582
F	1.57663	3.72380	-1.78770
F	2.42021	2.70200	0.07909
F	1.93579	4.94699	0.13816
C	-0.52517	1.43869	2.15189

H	-1.59839	1.26722	2.27382
H	-0.31276	2.50215	2.29556
H	-0.00339	0.88503	2.93792

E(0 K) = -1044.253716
E(0 K) + ZPE = -1043.976119
H (195 K) = -1043.966090
G (195 K) = -1044.001628

anti-T2-L

C	2.37598	1.88849	-0.07874
H	3.12646	2.62746	-0.37867
H	1.64295	2.38754	0.55753
C	1.75523	1.37383	-1.34524
H	2.45246	0.85538	-2.01097
O	0.93269	2.21322	-1.94202
H	2.88149	1.09754	0.47866
C	-0.00090	0.23260	-0.18735
C	0.05134	0.25674	1.25434
H	-0.29587	1.19674	1.69523
H	1.01870	-0.05216	1.66125
Si	-1.23401	-1.08596	1.88057
C	-2.95799	-0.40613	1.59517
H	-3.15630	-0.23152	0.53349
H	-3.10185	0.53613	2.13285
H	-3.70136	-1.12148	1.96158
C	-0.86720	-1.30182	3.70571
H	0.14080	-1.69718	3.86121
H	-1.58278	-2.00296	4.14730
H	-0.95276	-0.34775	4.23414
C	-0.94376	-2.66078	0.90258
H	0.10948	-2.95844	0.93233
H	-1.23506	-2.53220	-0.14492
H	-1.53863	-3.47882	1.32029
C	0.92270	-0.36889	-1.02293
H	1.74523	-0.89230	-0.53111
H	-0.83688	0.74499	-0.66941
B	0.78099	2.30963	-3.41974
F	1.78121	1.55098	-4.04694
F	0.91160	3.65751	-3.75862
F	-0.48661	1.84407	-3.78642
C	0.55666	-0.85921	-2.40245
H	1.42864	-0.86864	-3.06059
H	-0.21116	-0.22926	-2.85660
H	0.17519	-1.88225	-2.33040

E(0 K) = -1044.251666
E(0 K) + ZPE = -1043.974577
H (195 K) = -1043.964530
G (195 K) = -1043.999981

anti-T3-L

C	-0.16914	-0.15851	-0.58182
C	0.81658	0.63577	-1.13858
C	2.13769	-0.85989	-1.32784
H	1.69620	-1.27771	-2.23691
O	2.18244	-1.64675	-0.28138
B	1.49162	-2.96915	-0.29523
F	1.31419	-3.34500	1.03097
F	0.25879	-2.85540	-0.96585
F	2.29722	-3.88854	-0.97419
C	3.39201	-0.04046	-1.48470
H	4.16995	-0.73852	-1.81433
H	3.68895	0.36889	-0.51735
H	3.31109	0.75465	-2.22256
H	-0.89865	-0.60233	-1.26151
C	-0.28356	-0.48875	0.81441
H	0.63785	-0.30358	1.37617
H	-0.65005	-1.50687	0.97269
Si	-1.63475	0.68270	1.59416
C	-3.19925	0.56468	0.56425
H	-3.05444	0.98677	-0.43534
H	-4.00634	1.12218	1.05037
H	-3.52444	-0.47503	0.45693
C	-0.93592	2.42428	1.59905
H	-0.72171	2.77107	0.58319
H	-0.01149	2.47265	2.18294
H	-1.65660	3.11659	2.04595
C	-1.91605	0.03598	3.33200
H	-2.30531	-0.98616	3.30533
H	-2.64590	0.66650	3.84996
H	-0.98823	0.03874	3.91147
H	1.42047	1.21579	-0.43876
C	0.62361	1.20631	-2.52561
H	1.56659	1.35350	-3.05515
H	0.13123	2.18137	-2.46415
H	-0.00755	0.54760	-3.12906

E(0 K) = -1044.252924
E(0 K) + ZPE = -1043.977111
H (195 K) = -1043.966562
G (195 K) = -1044.003233

syn-T1-H

C	-2.66964	-0.99510	-1.12003
H	-2.95569	-1.34382	-0.12518
H	-3.52557	-1.14223	-1.78900
C	-2.38941	0.46685	-1.12421
H	-1.83658	0.89871	-1.95920
O	-3.31749	1.22048	-0.60611
H	-3.24647	2.17083	-0.94618
H	-1.83034	-1.57101	-1.50406
H	-2.85252	4.31721	-1.15466
O	-3.01402	3.51775	-1.67354

H	-3.70039	3.74737	-2.31546
C	0.08339	0.13296	-0.38123
C	0.47425	-1.26745	-0.28601
H	0.73512	-1.70520	-1.25507
H	-0.26748	-1.88265	0.23508
Si	2.07787	-1.38884	0.81089
C	3.40651	-0.28938	0.06787
H	3.12634	0.76734	0.12358
H	3.59743	-0.54271	-0.97939
H	4.34280	-0.41582	0.62094
C	2.58245	-3.19477	0.79982
H	1.78558	-3.82843	1.20035
H	3.47347	-3.33497	1.42016
H	2.81721	-3.53045	-0.21456
C	1.60922	-0.80317	2.53154
H	0.84207	-1.44540	2.97552
H	1.22688	0.22252	2.50688
H	2.48556	-0.81888	3.18727
C	-0.86724	0.75760	0.38311
H	-1.36622	0.16439	1.15163
H	0.62934	0.74878	-1.10098
C	-0.90755	2.25147	0.55251
H	-0.23661	2.54965	1.36405
H	-1.91009	2.58763	0.82884
H	-0.58541	2.76878	-0.35715

E(0 K) = -796.4989445
E(0 K) + ZPE = -796.200629
H (195 K) = -796.190480
G (195 K) = -796.225902

syn-T2-H

C	1.57186	1.59597	-0.95941
O	1.15702	2.41135	-1.91013
H	0.55934	3.09917	-1.50811
H	0.11273	4.64209	0.05939
O	-0.34342	3.93917	-0.42286
H	-1.16477	4.33469	-0.74594
C	-0.20633	0.58367	0.04071
C	0.13939	0.26446	1.42412
H	0.17119	1.15671	2.05843
H	1.08203	-0.28871	1.50292
Si	-1.22316	-0.88487	2.19805
C	-2.89150	-0.05357	1.97905
H	-3.17357	0.00275	0.92294
H	-2.88676	0.95969	2.39294
H	-3.66482	-0.62659	2.50058
C	-0.77048	-1.05198	4.01092
H	0.24328	-1.44523	4.13236
H	-1.46322	-1.73546	4.51175
H	-0.82817	-0.08148	4.51304
C	-1.15691	-2.53024	1.29804
H	-0.18839	-3.01952	1.44056
H	-1.32574	-2.40219	0.22393
H	-1.93347	-3.19941	1.68221
C	0.30338	-0.04232	-1.07181
H	0.99849	-0.86386	-0.90261
H	-0.94537	1.37267	-0.11994
C	-0.28969	0.06521	-2.44250
H	0.48987	0.14443	-3.20552
H	-0.95448	0.92674	-2.52759
H	-0.86538	-0.84242	-2.64918
C	2.83198	0.84184	-1.26782
H	3.63475	1.58700	-1.28896
H	2.78086	0.35828	-2.24521
H	3.06099	0.11018	-0.49271
H	1.50687	1.99106	0.05504

E(0 K) = -796.5023165
E(0 K) + ZPE = -796.202799
H (195 K) = -796.192753
G (195 K) = -796.228001

syn-T2-H (*Z*-CH_3CHOH^+)

C	1.42526	1.61445	-0.93207
O	0.92451	2.41139	-1.84939
H	1.25028	2.19191	-2.77221
H	1.21747	1.95491	-4.97572
O	1.81509	1.80383	-4.23079
H	2.65905	2.20056	-4.48658
C	-0.32900	0.52261	0.08264
C	0.01107	0.26994	1.48173
H	-0.05636	1.17376	2.09613
H	0.99934	-0.19154	1.59316
Si	-1.22898	-1.01683	2.23878
C	-2.98194	-0.37967	2.02443
H	-3.26673	-0.33551	0.96836
H	-3.09985	0.61881	2.45688
H	-3.68324	-1.05098	2.53044
C	-0.75654	-1.16292	4.04808
H	0.28545	-1.47891	4.15620
H	-1.39083	-1.90049	4.54922
H	-0.88102	-0.20297	4.55825
C	-0.98423	-2.62575	1.30249
H	0.05416	-2.96719	1.36193
H	-1.25055	-2.50917	0.24669
H	-1.62136	-3.41003	1.72304
C	0.23658	-0.11072	-0.99654
H	0.97122	-0.88855	-0.79020
H	-1.11150	1.25740	-0.12174
C	-0.33376	-0.08331	-2.38142
H	0.45964	-0.05766	-3.13513
H	-0.99674	0.77255	-2.52484
H	-0.90891	-0.99967	-2.54762
C	2.72423	0.90696	-1.20294
H	3.50086	1.67981	-1.22318
H	2.71508	0.38500	-2.16222
H	2.96707	0.20985	-0.40044
H	1.32210	2.02416	0.06932

E(0 K) = -796.5027299
E(0 K) + ZPE = -796.203743
H (195 K) = -796.193766
G (195 K) = -796.228748

syn-T3-H

C	0.44494	-0.16671	0.69417
C	2.91384	1.27474	1.03042
H	3.81686	1.88064	0.88815
H	2.14539	1.90837	1.47561
C	-0.58628	0.80369	0.31723
H	-0.49744	1.11651	-0.72948
H	-0.57059	1.68615	0.96708
Si	-2.33787	0.00533	0.48695
C	-2.45020	-1.38438	-0.77151
H	-1.70445	-2.16028	-0.57082
H	-2.29397	-1.01118	-1.78877
H	-3.44002	-1.84987	-0.73025
C	-3.58087	1.36507	0.12444
H	-3.48708	2.18043	0.84837
H	-4.60080	0.97238	0.18474
H	-3.43245	1.77593	-0.87893
C	-2.53758	-0.64972	2.23615
H	-2.41627	0.15072	2.97285
H	-1.80440	-1.43289	2.45446
H	-3.53598	-1.07954	2.36507
C	1.14148	-0.97486	-0.15445
H	0.90441	-0.94010	-1.21978
C	2.50419	0.79933	-0.31905
H	3.09314	0.01400	-0.79569
O	1.92090	1.65091	-1.09403
H	1.88889	1.29975	-2.04840
H	0.65608	-0.27093	1.76075
H	3.16403	0.44044	1.68600
H	1.14156	0.55408	-3.92565
O	1.91184	0.48383	-3.34527
H	2.68922	0.55344	-3.91680
C	2.02439	-2.09676	0.30998
H	2.99360	-2.09545	-0.20036
H	1.55135	-3.05770	0.08529
H	2.19629	-2.04744	1.38838

E(0 K) = -796.5039829
E(0 K) + ZPE = -796.205445
H (195 K) = -796.195332
G (195 K) = -796.230671

anti-T1-H

C	-0.08313	-0.15429	-0.76380
C	-2.68386	0.57734	-2.01638
H	-2.91132	-0.41264	-2.41904
H	-3.55006	1.22103	-2.20554
C	0.67061	0.93113	-0.14815
H	0.23203	1.26659	0.79890
H	0.82106	1.77867	-0.82543
Si	2.45291	0.28938	0.30429
C	2.23907	-1.22788	1.38931
H	1.76717	-2.04652	0.83622
H	1.62174	-1.00286	2.26503
H	3.21337	-1.57816	1.74422
C	3.28085	1.69412	1.22906
H	3.29549	2.60646	0.62554
H	4.31472	1.42744	1.47034
H	2.75537	1.90526	2.16521
C	3.34314	-0.13230	-1.29286
H	3.37923	0.73298	-1.96159
H	2.85018	-0.95643	-1.81790
H	4.37200	-0.43851	-1.07888
C	-1.00670	-0.93768	-0.12389
C	-2.50773	0.51639	-0.53825
H	-1.98529	1.32575	-0.02466
O	-3.49989	-0.03663	0.10515
H	-3.40694	0.13843	1.09167
H	0.10169	-0.35346	-1.82214
H	-1.81206	0.99883	-2.51535
H	-2.86511	-0.17309	3.21267
O	-2.83355	0.50475	2.52366
H	-3.12459	1.32581	2.94243
H	-1.11017	-0.79471	0.95369
C	-1.56235	-2.20763	-0.69834
H	-2.63873	-2.28075	-0.51095
H	-1.08829	-3.06978	-0.21956
H	-1.38075	-2.27423	-1.77415

E(0 K) = -796.501713
E(0 K) + ZPE = -796.201519
H (195 K) = -796.191867
G (195 K) = -796.226274

anti-T2-H

C	2.21611	2.00656	0.09013
H	3.03377	2.70013	-0.13989
H	1.44364	2.55032	0.63555
C	1.71823	1.50916	-1.22223
H	2.40696	0.89217	-1.80460
O	0.94324	2.31523	-1.89479
H	0.96209	2.13282	-2.88899
H	2.61950	1.19836	0.70038
H	0.40301	1.68951	-4.96646
O	1.16730	1.88121	-4.40700
H	1.69027	2.54068	-4.88271
C	-0.02601	0.23895	-0.07401
C	0.15625	0.06501	1.36396
H	0.04231	1.00098	1.92272
H	1.10432	-0.42065	1.61730

Si	-1.24815	-1.10355	2.02124
C	-2.90731	-0.29985	1.66185
H	-3.10324	-0.25268	0.58589
H	-2.95624	0.71572	2.06707
H	-3.71044	-0.88506	2.12120
C	-0.95661	-1.29177	3.86427
H	0.03176	-1.71558	4.06605
H	-1.70892	-1.95941	4.29643
H	-1.02813	-0.32443	4.37043
C	-1.10292	-2.74177	1.11538
H	-0.11840	-3.19681	1.26380
H	-1.26209	-2.60924	0.04010
H	-1.85827	-3.44385	1.48288
C	0.69695	-0.38188	-1.05702
H	1.51930	-1.03054	-0.74954
H	-0.84650	0.88643	-0.39479
C	0.21452	-0.52797	-2.47202
H	1.03411	-0.44339	-3.19180
H	-0.55518	0.21272	-2.70657
H	-0.22865	-1.52031	-2.60061

E(0 K) = -796.5017622
E(0 K) + ZPE = -796.202831
H (195 K) = -796.192843
G (195 K) = -796.227835

anti-T3-H

C	0.26005	0.56497	0.72401
C	-0.83618	0.96382	-0.15297
H	-0.70992	0.58332	-1.17284
H	-0.99800	2.04717	-0.15521
Si	-2.48644	0.16627	0.48825
C	-3.81956	0.71811	-0.71148
H	-3.59966	0.36538	-1.72398
H	-3.90728	1.80827	-0.73570
H	-4.78807	0.30559	-0.41221
C	-2.80892	0.77935	2.23266
H	-2.03630	0.43319	2.92666
H	-3.77133	0.39858	2.58920
H	-2.84408	1.87245	2.27150
C	-2.27306	-1.69859	0.44488
H	-1.51354	-2.03961	1.15535
H	-1.98760	-2.03822	-0.55592
H	-3.21803	-2.18476	0.70819
C	1.16634	-0.43451	0.47060
H	1.06634	-0.98445	-0.46580
C	2.16309	1.19597	-0.47761
O	1.74668	1.11798	-1.71966
H	1.09058	1.84153	-1.96223
H	0.33354	1.07643	1.68632
H	0.68522	3.78682	-2.82567
O	0.20035	3.07726	-2.38145
H	-0.56725	2.89614	-2.94023
C	1.98606	-1.07676	1.55178
H	2.93685	-1.45823	1.17557
H	1.42959	-1.93610	1.94184
H	2.17355	-0.39199	2.38305
C	3.55646	0.70552	-0.23796
H	4.20804	1.43902	-0.72717
H	3.72715	-0.26794	-0.70062
H	3.80565	0.68302	0.82166
H	1.87359	2.09040	0.07624

E(0 K) = -796.5007433
E(0 K) + ZPE = -796.200894
H (195 K) = -796.191156
G (195 K) = -796.225727

anti-T3-H (*Z*-CH_3CHOH^+)

C	0.24208	0.57109	0.74330
C	-0.87041	0.95928	-0.12015
H	-0.72685	0.61691	-1.15029
H	-1.04889	2.04003	-0.10135
Si	-2.50300	0.12834	0.50995
C	-3.83715	0.63501	-0.70903
H	-3.59507	0.27863	-1.71504
H	-3.94689	1.72281	-0.74597
H	-4.80069	0.20501	-0.41848
C	-2.85348	0.75674	2.24406
H	-2.07488	0.44010	2.94562
H	-3.80834	0.36080	2.60412
H	-2.91214	1.84953	2.26411
C	-2.25049	-1.73301	0.49860
H	-1.48669	-2.04353	1.21864
H	-1.95207	-2.08322	-0.49482
H	-3.18528	-2.23627	0.76630
C	1.13970	-0.43745	0.49818
H	1.01595	-1.01688	-0.41784
C	2.10018	1.19168	-0.53249
O	1.64276	1.06447	-1.75419
H	2.09783	0.32236	-2.26080
H	0.34605	1.10428	1.69146
H	2.26376	-1.45827	-3.52559
O	2.81589	-0.89719	-2.96377
H	3.59818	-0.68571	-3.49197
C	1.99412	-1.04944	1.56906
H	2.95096	-1.40400	1.18062
H	1.47099	-1.92364	1.97219
H	2.17360	-0.35490	2.39389
C	3.51188	0.79818	-0.22492
H	4.14232	1.53880	-0.73212
H	3.76143	-0.19314	-0.60835
H	3.71805	0.85671	0.84294
H	1.74141	2.10124	-0.05764

E(0 K) = -796.5007181
E(0 K) + ZPE = -796.200648
H (195 K) = -796.190879

G (195 K) = -796.225525

syn-T1-F

C	0.68424	0.08931	0.43550
C	-0.33136	0.98513	0.09252
H	-0.49568	1.21423	-0.95998
H	-0.61503	1.76292	0.79840
C	1.47248	-0.69977	-0.39473
H	1.23987	-0.68400	-1.46135
C	3.27992	0.70173	-0.65881
H	0.89275	-0.01291	1.50676
Si	-2.51166	-0.26411	0.36443
C	-1.94320	-1.24153	-1.14728
H	-0.96393	-1.69602	-0.96822
H	-1.84019	-0.57909	-2.01345
H	-2.67111	-2.02168	-1.38607
C	-3.23575	1.46432	0.09701
H	-2.79215	1.95628	-0.77286
H	-3.04281	2.09674	0.97000
H	-4.31813	1.39317	-0.04545
C	-1.87946	-0.73587	2.08413
H	-1.45180	0.12301	2.60898
H	-1.09083	-1.49056	1.99089
H	-2.69582	-1.15398	2.68000
F	-4.04267	-1.06654	0.53704
O	4.25051	-0.04442	-0.90640
C	2.18953	-1.91846	0.11276
H	3.19493	-1.99287	-0.32511
H	1.65422	-2.85082	-0.11487
H	2.30717	-1.86733	1.20279
H	3.14383	1.08059	0.36890
C	2.65664	1.55380	-1.73864
H	3.26283	2.46159	-1.85563
H	1.63888	1.85260	-1.47561
H	2.66155	1.01382	-2.68965

E(0 K) = -819.6120356
E(0 K) + ZPE = -819.349891
H (195 K) = -819.340850
G (195 K) = -819.373933

syn-T2-F

C	0.58677	0.35226	0.59175
C	-0.40645	1.16478	0.04129
H	-0.55496	1.16504	-1.03854
H	-0.68460	2.07806	0.56186
C	1.36778	-0.62120	-0.02135
H	1.11869	-0.89222	-1.04757
C	3.09591	0.76009	-0.57244
H	0.80233	0.51449	1.65369
Si	-2.63564	0.03850	0.46798
C	-2.11669	-1.10772	-0.93693
H	-1.09093	-1.45861	-0.79529
H	-2.15548	-0.56608	-1.88833
H	-2.79352	-1.96490	-0.99520
C	-3.31262	1.75261	0.03084
H	-2.73850	2.24554	-0.75673
H	-3.28785	2.39696	0.91726
H	-4.35423	1.65822	-0.29153
C	-2.01193	-0.30117	2.22043
H	-1.60735	0.60319	2.68344
H	-1.20584	-1.04203	2.18584
H	-2.82683	-0.69055	2.83741
F	-4.20329	-0.66895	0.71496
C	2.15597	-1.62066	0.77893
H	3.04434	-1.96054	0.23061
H	1.58013	-2.51547	1.05371
H	2.51447	-1.15417	1.70367
O	3.95884	0.69464	0.32656
H	2.38047	1.59978	-0.59308
C	3.35921	0.10399	-1.91490
H	3.66836	-0.93637	-1.77444
H	4.18732	0.63940	-2.39694
H	2.48537	0.14648	-2.56883

E(0 K) = -819.6100459
E(0 K) + ZPE = -819.347694
H (195 K) = -819.338619
G (195 K) = -819.371906

syn-T3-F

C	0.61813	0.10317	0.31185
C	3.46672	1.14629	0.41552
H	4.41263	1.69033	0.29639
H	2.73128	1.82576	0.85452
C	-0.34521	0.99474	-0.17103
H	-0.38029	1.16491	-1.24744
H	-0.60703	1.84910	0.45216
C	1.42179	-0.76690	-0.41090
H	1.21521	-0.86969	-1.47575
C	2.99153	0.70267	-0.95282
H	3.48835	-0.20540	-1.34337
O	2.52007	1.53552	-1.75351
H	0.77785	0.09732	1.39541
H	3.63713	0.29892	1.08557
Si	-2.52694	-0.10565	0.07027
C	-1.98983	-1.18368	-1.38458
H	-0.99891	-1.61199	-1.21016
H	-1.92706	-0.57116	-2.29095
H	-2.71340	-1.98588	-1.55378
C	-3.21697	1.61960	-0.30291
H	-2.63594	2.13950	-1.06837
H	-3.19477	2.23168	0.60628
H	-4.25663	1.53812	-0.63430
C	-1.99824	-0.52383	1.84307
H	-1.55472	0.34143	2.34438

H	-1.23810	-1.31269	1.82082
H	-2.85506	-0.87886	2.42235
F	-4.09961	-0.84780	0.24675
C	2.16247	-1.90040	0.24858
H	3.20079	-1.98326	-0.10975
H	1.69016	-2.87523	0.06981
H	2.20405	-1.75350	1.33425

E(0 K) = -819.6116318
E(0 K) + ZPE = -819.349190
H (195 K) = -819.340065
G (195 K) = -819.373428

anti-T1-F

C	0.68424	0.08931	0.43550
C	-0.33136	0.98513	0.09252
H	-0.49568	1.21423	-0.95998
H	-0.61503	1.76292	0.79840
C	1.47248	-0.69977	-0.39473
H	1.23987	-0.68400	-1.46135
C	3.27992	0.70173	-0.65881
H	0.89275	-0.01291	1.50676
Si	-2.51166	-0.26411	0.36443
C	-1.94320	-1.24153	-1.14728
H	-0.96393	-1.69602	-0.96822
H	-1.84019	-0.57909	-2.01345
H	-2.67111	-2.02168	-1.38607
C	-3.23575	1.46432	0.09701
H	-2.79215	1.95628	-0.77286
H	-3.04281	2.09674	0.97000
H	-4.31813	1.39317	-0.04545
C	-1.87946	-0.73587	2.08413
H	-1.45180	0.12301	2.60898
H	-1.09083	-1.49056	1.99089
H	-2.69582	-1.15398	2.68000
F	-4.04267	-1.06654	0.53704
O	4.25051	-0.04442	-0.90640
C	2.18953	-1.91846	0.11276
H	3.19493	-1.99287	-0.32511
H	1.65422	-2.85082	-0.11487
H	2.30717	-1.86733	1.20279
H	3.14383	1.08059	0.36890
C	2.65664	1.55380	-1.73864
H	3.26283	2.46159	-1.85563
H	1.63888	1.85260	-1.47561
H	2.66155	1.01382	-2.68965

E(0 K) = -819.6134605
E(0 K) + ZPE = -819.351442
H (195 K) = -819.342288
G (195 K) = -819.375729

anti-T2-F

C	0.68357	0.12422	0.41983
C	-0.34745	0.95148	-0.03785
H	-0.48397	1.04840	-1.11591
H	-0.59879	1.83756	0.54334
C	1.46430	-0.77558	-0.29678
H	1.21694	-0.91590	-1.35137
C	3.28826	0.43987	-0.66310
H	3.51281	-0.37828	-1.37507
H	0.90391	0.17567	1.49148
Si	-2.47215	-0.17427	0.39870
C	-1.97379	-1.36151	-0.98361
H	-0.96724	-1.75465	-0.81463
H	-1.96198	-0.82945	-1.94146
H	-2.68593	-2.18842	-1.05259
C	-3.21774	1.50898	-0.06168
H	-2.66979	2.01406	-0.86054
H	-3.20901	2.16489	0.81692
H	-4.25821	1.37296	-0.37139
C	-1.86452	-0.47839	2.16654
H	-1.40986	0.41907	2.59626
H	-1.09831	-1.26213	2.15723
H	-2.69206	-0.80327	2.80327
F	-4.04015	-0.90572	0.67207
C	2.15631	-1.91913	0.39991
H	3.00296	-2.29824	-0.18686
H	1.48966	-2.76981	0.59755
H	2.55820	-1.57605	1.36057
O	3.96737	0.52569	0.38410
C	2.67789	1.66493	-1.29968
H	3.48418	2.24707	-1.76352
H	2.18241	2.28350	-0.54682
H	1.94862	1.39677	-2.06907

E(0 K) = -819.6094134
E(0 K) + ZPE = -819.347678
H (195 K) = -819.338664
G (195 K) = -819.371722

anti-T3-F

C	0.59417	0.33992	0.52508
C	3.41199	-0.13330	-2.01442
H	3.46648	-1.19602	-1.76930
C	-0.38803	1.16564	-0.01624
H	-0.54858	1.16716	-1.09404
H	-0.67692	2.06921	0.51449
C	1.36027	-0.63160	-0.10711
H	1.10440	-0.88167	-1.13691
C	3.07085	0.73427	-0.81725
O	2.71408	1.91285	-0.99700
H	0.80510	0.47888	1.59120
H	2.67287	0.02771	-2.80378
Si	-2.60481	0.04958	0.49576

C	-2.12747	-1.18234	-0.85006
H	-1.05107	-1.36090	-0.88402
H	-2.44151	-0.78487	-1.82257
H	-2.65151	-2.12949	-0.68904
C	-3.29625	1.74061	-0.00590
H	-2.73681	2.20936	-0.81821
H	-3.26690	2.41750	0.85593
H	-4.34096	1.62506	-0.31064
C	-1.96944	-0.19185	2.25945
H	-1.51126	0.72270	2.64679
H	-1.20352	-0.97504	2.27166
H	-2.79131	-0.48968	2.91700
F	-4.17439	-0.64659	0.78902
C	2.12681	-1.66326	0.68016
H	3.13064	-1.84876	0.26902
H	1.62325	-2.63889	0.72498
H	2.26343	-1.32293	1.71376
H	4.39208	0.18237	-2.39510
H	3.55302	0.44526	0.13439

E(0 K) = -819.6083625
E(0 K) + ZPE = -819.345360
H (195 K) = -819.336376
G (195 K) = -819.369424

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(1) To avoid confusion, those figures and tables in the Supporting Information are designated with the prefix "SI-" and those referred to in the main text are designated with the prefix "T-".

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