

## Supporting Information

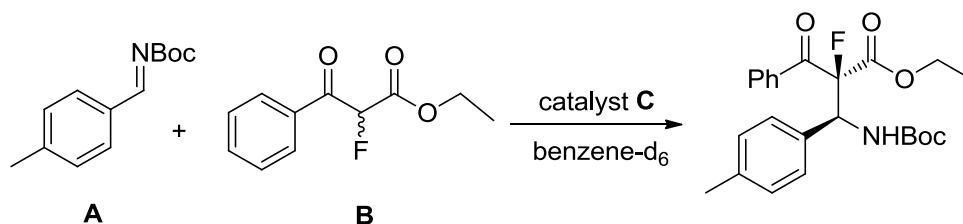
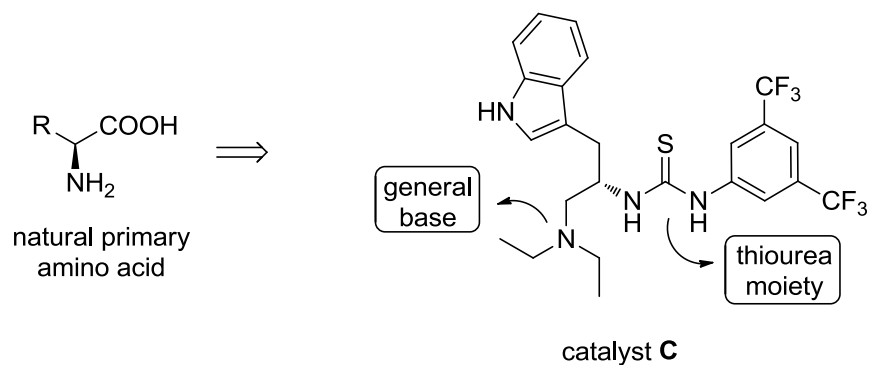
### Kinetic Evidence of an Apparent Negative Activation Enthalpy in an Organocatalytic Process

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### 1. Representative Procedure of Asymmetric Mannich Reaction of Fluorinated Ketoester with Imine Catalyzed by a Tryptophan Derived Catalyst

Ketoester **B** and 1,4-dimethoxybenzene stock solution (0.5 M **B** and 0.25 M 1,4-dimethoxybenzene; 100  $\mu\text{L}$ ), imine **A** stock solution (0.25 M, 200  $\mu\text{L}$ ), deuterated benzene (150  $\mu\text{L}$ ) and catalyst **C** (0.1 M, 50  $\mu\text{L}$ ) were added into a dried NMR tube, mixed well, and submitted to kinetic experiment immediately. The total volume is assumed to be 500  $\mu\text{L}$ .

### 2. Mannich Reaction of Imine and Fluorinated Ketoester (1:10) Catalyzed by Trp-1

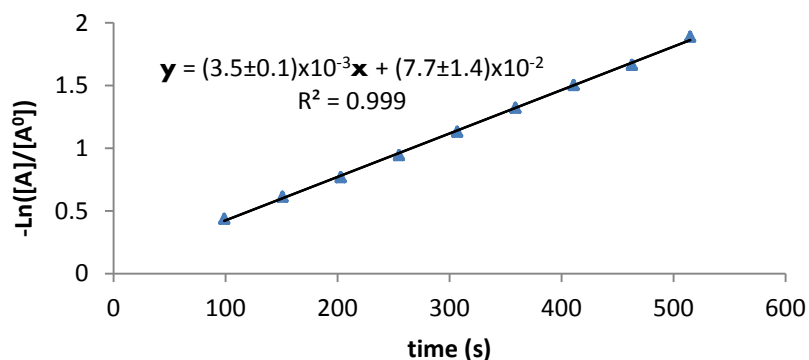
In our reaction, the rate is given by  $\text{rate} = k [\text{A}]^a [\text{B}]^b [\text{C}]^c$  where  $k$  is the rate constant,  $[\text{A}]$ ,  $[\text{B}]$  and  $[\text{C}]$  represent the concentrations of the species A, B and the Catalyst (M, mole/liter), and  $a$ ,  $b$  and  $c$  are reaction orders on A, B, and C, respectively, to be determined experimentally.

The kinetic measurement was first carried out with imine **A** (0.05 mmol), ketoester **B** (0.5 mmol), catalyst **C** (0.005 mmol) in benzene- $d_6$  at 285K and monitored by  $^1\text{H}$  NMR spectroscopy. Since B is in 10 fold excess to A, [B] can be treated as a constant. The rate law can be simplified to:  $\text{rate} = k_{\text{obs}} [\text{A}]^a$

**Table 1** | Mannich reaction of imine and a large excess of fluorinated ketoester carried out in the presence of 10 mol% catalyst<sup>†</sup>.

Entry	Time (s)	$I_A^{\ddagger}$	$[A]^{\S}$ (M)	$-\ln([A]/[A]^0)$
1	99	0.6456	0.06456	0.4376
2	151	0.5426	0.05426	0.6114
3	203	0.4639	0.04639	0.7681
4	255	0.3891	0.03891	0.9439
5	307	0.3229	0.03229	1.1304
6	359	0.2665	0.02665	1.3224
7	411	0.2225	0.02225	1.5028
8	463	0.1894	0.01894	1.6639
9	515	0.1515	0.01515	1.8885

<sup>†</sup>Reaction was carried out with imine (0.05 mmol) and ketoester (0.5 mmol) in benzene- $d_6$  at 285K. <sup>‡</sup>Integration value of imine. <sup>§</sup>Concentration of imine.



**Figure 1** |  $-\ln([A]/[A]_0)$  vs. time for the Mannich reaction monitored by  $^1\text{H}$  NMR spectroscopy in the presence of 10 mol% catalyst.

From the above data, plotting  $-\ln([A]/[A]^0)$  versus time gave a straight line ( $R^2 = 0.999$ ), indicating the reaction was first-order to imine **A**.

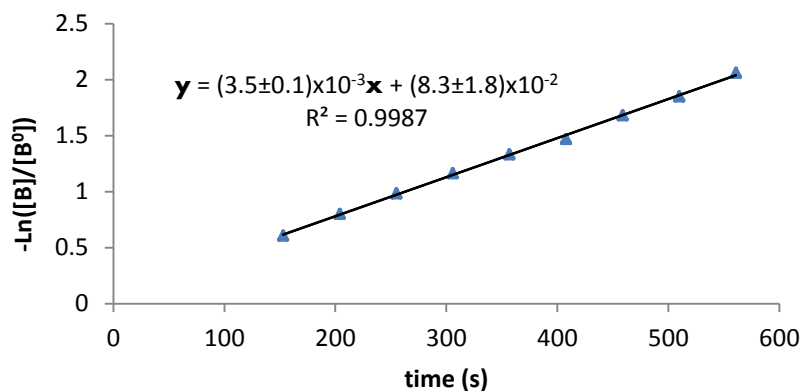
### 3. Mannich Reaction of Imine and Fluorinated Ketoester (10:1) Catalyzed by Trp-1

By the same procedure with A in 10 fold excess, it was determined that the reaction is first order to ketoester **B**.

**Table 2** | Mannich reaction of ketoester and a large excess of imine carried out in the presence of 10 mol% catalyst<sup>†</sup>.

Entry	Time (s)	$I_B^{\ddagger}$	$[B]^{\S}$ (M)	$-\ln([B]/[B]^0)$
1	153	1.6336	0.05445	0.6078
2	204	1.3487	0.04496	0.7995
3	255	1.1229	0.03743	0.9827
4	306	0.9377	0.03126	1.1629
5	357	0.791	0.02637	1.3331
6	408	0.691	0.02303	1.4682
7	459	0.5594	0.01865	1.6795
8	510	0.4716	0.01572	1.8502
9	561	0.3818	0.01273	2.0615

<sup>†</sup>Reaction was carried out with imine (0.5 mmol) and ketoester (0.05 mmol) in benzene- $d_6$  at 285K. <sup>‡</sup>Integration value of ketoester. <sup>§</sup>Concentration of ketoester.



**Figure 2** |  $-\ln([B]/[B]_0)$  vs. time for the Mannich reaction monitored by  $^1\text{H}$  NMR spectroscopy in the presence of 10 mol% catalyst.

#### 4. Mannich Reaction of Imine and Fluorinated Ketoester (1:1) Catalyzed by Trp-1 with Different Catalyst Loading

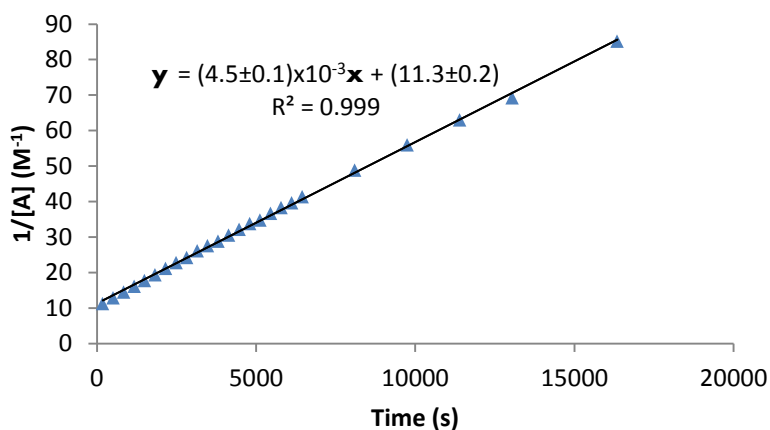
As the rate law for the Mannich reaction is  $\text{rate} = k [\text{A}][\text{B}][\text{C}]^c$ , when  $[\text{A}]_0 = [\text{B}]_0$  (and therefore  $[\text{A}]_t = [\text{B}]_t$ ), the integrated second order rate law,  $1/[\text{A}] = kt + 1/[\text{A}]_0$ , can be utilized. The kinetics was carried out with imine **A** (0.05 mmol), ketoester **B** (0.05 mmol), and catalyst **C** (10 mol%, 15 mol%, 20 mol%, 25 mol%) in benzene- $d_6$  at 298K. The volume of the mixture was fixed to 500  $\mu\text{L}$ .

**Table 3** | Mannich reaction of ketoester and imine carried out in the presence of 10 mol% catalyst†.

Entry	Time (s)	$I_A^\ddagger$	$[\text{A}]^{\S}$ (M)	$1/[\text{A}]$ ( $\text{M}^{-1}$ )
1	179	0.8940	0.0894	11.1857
2	509	0.7785	0.0779	12.8452
3	839	0.6936	0.0694	14.4175
4	1169	0.6217	0.0622	16.0849
5	1499	0.5656	0.0566	17.6803
6	1829	0.5183	0.0518	19.2938
7	2159	0.4733	0.0473	21.1282
8	2489	0.4404	0.0440	22.7066
9	2819	0.4130	0.0413	24.2131
10	3149	0.3837	0.0384	26.0620
11	3479	0.3640	0.0364	27.4725

12	3809	0.3473	0.0347	28.7936
13	4139	0.3276	0.0328	30.5250
14	4469	0.3114	0.0311	32.1130
15	4799	0.2962	0.0296	33.7610
16	5129	0.2880	0.0288	34.7222
17	5459	0.2734	0.0273	36.5764
18	5789	0.2614	0.0261	38.2555
19	6119	0.2524	0.0252	39.6197
20	6449	0.2422	0.0242	41.2882
21	8099	0.2048	0.0205	48.8281
22	9749	0.1789	0.0179	55.8971
23	11399	0.1588	0.0159	62.9723
24	13049	0.1445	0.0145	69.2042
25	16349	0.1175	0.0118	85.1064

†Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in benzene-d<sub>6</sub>. ‡Integration value of imine. §Concentration of imine.



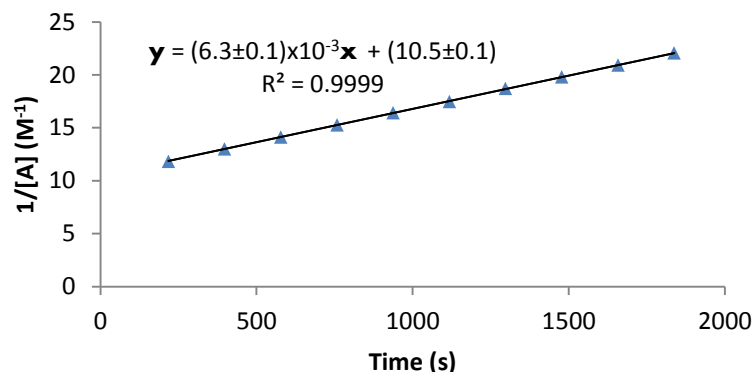
**Figure 3** |  $1/[A]$  vs. time for the Mannich reaction monitored by  $^1\text{H}$  NMR spectroscopy in the presence of 10 mol% catalyst.

**Table 4** | Mannich reaction of ketoester and imine carried out in the presence of 15 mol% catalyst†.

Entry	time (s)	$I_A$ ‡	$[A]$ § (M)	$1/[A]$ (M <sup>-1</sup> )
1	218	0.8457	0.0846	11.8245
2	398	0.7686	0.0769	13.0107
3	578	0.7073	0.0707	14.1383
4	758	0.6548	0.0655	15.2718
5	938	0.6086	0.0609	16.4312
6	1118	0.5721	0.0572	17.4795
7	1298	0.5342	0.0534	18.7196

8	1478	0.5052	0.0505	19.7941
9	1658	0.4783	0.0478	20.9074
10	1838	0.4534	0.0453	22.0556

†Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in benzene-d<sub>6</sub>. ‡Integration value of imine. §Concentration of imine.

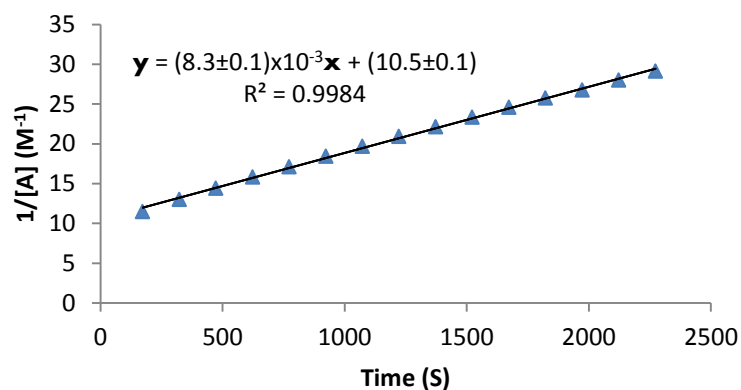


**Figure 4** |  $1/[A]$  vs. time for the Mannich reaction monitored by  $^1\text{H}$  NMR spectroscopy in the presence of 15 mol% catalyst.

**Table 5** | Mannich reaction of ketoester and imine carried out in the presence of 20 mol% catalyst†.

Entry	Time (s)	$I_A^\ddagger$	$[A]^\S$ (M)	$1/[A]$ ( $M^{-1}$ )
1	173	0.8704	0.0870	11.4890
2	323	0.7674	0.0767	13.0310
3	473	0.6929	0.0693	14.4321
4	623	0.6325	0.0633	15.8103
5	773	0.5847	0.0585	17.1028
6	923	0.5427	0.0543	18.4264
7	1073	0.5075	0.0508	19.7044
8	1223	0.4780	0.0478	20.9205
9	1373	0.4519	0.0452	22.1288
10	1523	0.4281	0.0428	23.3590
11	1673	0.4067	0.0407	24.5881
12	1823	0.3885	0.0389	25.7400
13	1973	0.3737	0.0374	26.7594
14	2123	0.3572	0.0357	27.9955
15	2273	0.3431	0.0343	29.1460

†Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in benzene-d<sub>6</sub>. ‡Integration value of imine. §Concentration of imine.



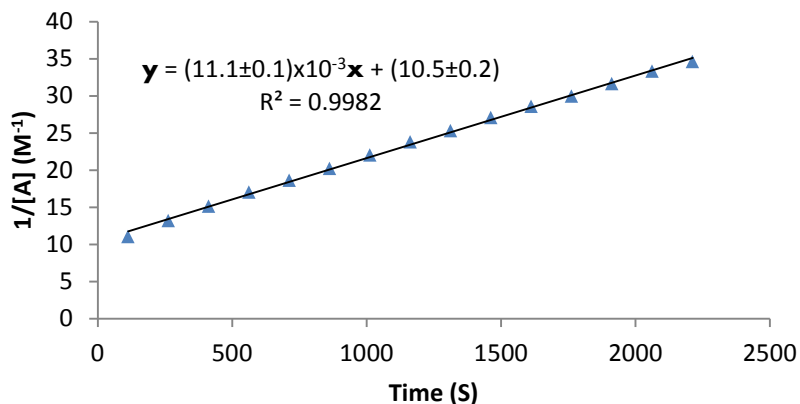
**Figure 5** |  $1/[A]$  vs. time for the Mannich reaction monitored by  $^1\text{H}$  NMR spectroscopy in the presence of 20 mol% catalyst.

**Table 6** | Mannich reaction of ketoester and imine carried out in the presence of 25 mol% catalyst†.

Entry	Time (s)	$I_A^\ddagger$	$[A]^\S$ (M)	$1/[A]$ ( $\text{M}^{-1}$ )
1	113	0.9072	0.0907	11.0229
2	263	0.7581	0.0758	13.1909
3	413	0.6612	0.0661	15.1240
4	563	0.5867	0.0587	17.0445
5	713	0.5374	0.0537	18.6081
6	863	0.4943	0.0494	20.2306
7	1013	0.4536	0.0454	22.0459
8	1163	0.4202	0.0420	23.7982
9	1313	0.3949	0.0395	25.3229
10	1463	0.3691	0.0369	27.0929
11	1613	0.3497	0.0350	28.5959
12	1763	0.3337	0.0334	29.9670
13	1913	0.3159	0.0316	31.6556
14	2063	0.3000	0.0300	33.3333
15	2213	0.2890	0.0289	34.6021

†Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in benzene- $d_6$ .  $^\ddagger$ Integration value of imine.  $^\S$ Concentration of imine.

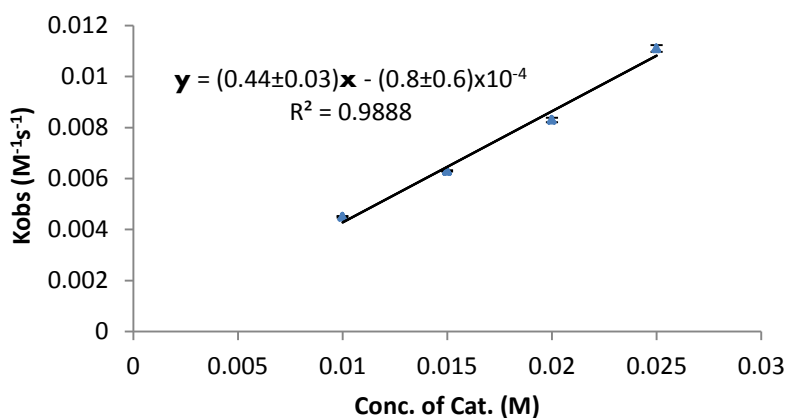




**Figure 6** |  $1/[A]$  vs. time for the mannich reaction monitored by <sup>1</sup>H NMR spectroscopy in the presence of 25 mol% catalyst.

**Table 7** | Observed reaction rate based on imine.

Cat. Loading (mol%)	[A] <sub>0</sub> (M)	[B] <sub>0</sub> (M)	[Cat.] (M)	K <sub>obs</sub> (M <sup>-1</sup> s <sup>-1</sup> )
10	0.1000	0.1000	0.0100	$(4.5 \pm 0.1) \times 10^{-3}$
15	0.1000	0.1000	0.0150	$(6.3 \pm 0.1) \times 10^{-3}$
20	0.1020	0.1000	0.0200	$(8.3 \pm 0.1) \times 10^{-3}$
25	0.1000	0.1000	0.0250	$(11.1 \pm 0.1) \times 10^{-3}$



**Figure 7** |  $K_{obs}$  based on imine vs. concentration of catalyst for the Mannich reaction.

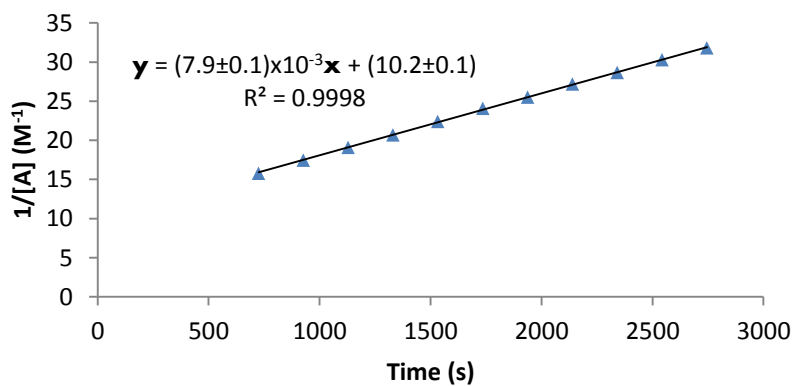
The plot of the concentration of catalyst C with  $k_{obs}$  gives a straight line with zero intercept, suggesting the reaction is also first order to C.

5. Mannich Reaction of Imine and Fluorinated Ketoester (1:1) Catalyzed by Trp-1 at Different Temperatures

**Table 8** | Mannich reaction of imine and fluorinated ketoester carried out in the presence of 12 mol% catalyst at 283K<sup>†</sup>

Entry	Time (s)	$I_A^{\ddagger}$	$[A]^{\S}$ (M)	$1/[A]$ ( $M^{-1}$ )
1	119	0.9387	0.0939	10.6530
2	321	0.8083	0.0808	12.3716
3	523	0.7089	0.0709	14.1064
4	725	0.6334	0.0633	15.7878
5	927	0.5726	0.0573	17.4642
6	1129	0.5237	0.0524	19.0949
7	1331	0.4831	0.0483	20.6996
8	1533	0.4465	0.0447	22.3964
9	1735	0.4157	0.0416	24.0558
10	1937	0.3919	0.0392	25.5167
11	2139	0.3678	0.0368	27.1887
12	2341	0.3492	0.0349	28.6369
13	2543	0.3302	0.0330	30.2847
14	2745	0.3144	0.0314	31.8066

<sup>†</sup>Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in benzene-d<sub>6</sub>. <sup>‡</sup>Integration value of imine. <sup>§</sup>Concentration of imine.

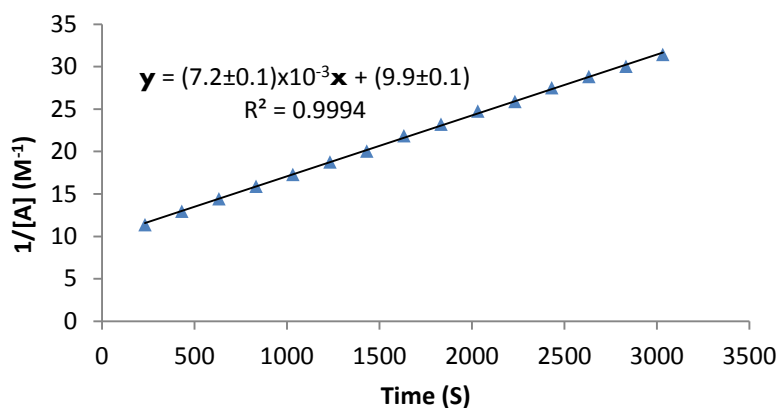


**Figure 8** |  $1/[A]$  vs. time monitored by <sup>1</sup>H NMR spectroscopy in the presence of 12 mol% catalyst at 283K.

**Table 9** | Mannich reaction of imine and fluorinated ketoester carried out in the presence of 12 mol% catalyst at 293K<sup>†</sup>

Entry	Time (s)	I <sub>A</sub> <sup>‡</sup>	[A] <sup>§</sup> (M)	1/[A] (M <sup>-1</sup> )
1	233	0.8803	0.0880	11.3598
2	433	0.7720	0.0772	12.9534
3	633	0.6931	0.0693	14.4279
4	833	0.6297	0.0630	15.8806
5	1033	0.5781	0.0578	17.2980
6	1233	0.5334	0.0533	18.7477
7	1433	0.4990	0.0499	20.0401
8	1633	0.4579	0.0458	21.8388
9	1833	0.4311	0.0431	23.1965
10	2033	0.4039	0.0404	24.7586
11	2233	0.3864	0.0386	25.8799
12	2433	0.3638	0.0364	27.4876
13	2633	0.3469	0.0347	28.8268
14	2833	0.3329	0.0333	30.0391
15	3033	0.3184	0.0318	31.4070

<sup>†</sup>Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in benzene-d<sub>6</sub>. <sup>‡</sup>Integration value of imine. <sup>§</sup>Concentration of imine.

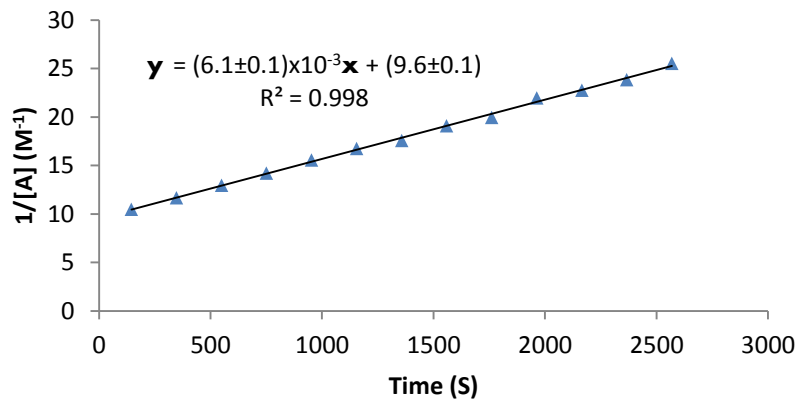


**Figure 9** | 1/[A] vs. time monitored by <sup>1</sup>H NMR spectroscopy in the presence of 12 mol% catalyst at 293K.

**Table 10** | Mannich reaction of imine and fluorinated ketoester carried out in the presence of 12 mol% catalyst at 303K<sup>†</sup>

Entry	Time (s)	$I_A^{\ddagger}$	$[A]^{\S}$ (M)	$1/[A]$ ( $M^{-1}$ )
1	145	0.9568	0.0957	10.4515
2	347	0.8581	0.0858	11.6537
3	549	0.7728	0.0773	12.9400
4	751	0.7046	0.0705	14.1924
5	953	0.6435	0.0644	15.5400
6	1155	0.5977	0.0598	16.7308
7	1357	0.5698	0.0570	17.5500
8	1559	0.5241	0.0524	19.0803
9	1761	0.5017	0.0502	19.9322
10	1963	0.4554	0.0455	21.9587
11	2165	0.4397	0.0440	22.7428
12	2367	0.4197	0.0420	23.8265
13	2569	0.3921	0.0392	25.5037

<sup>†</sup>Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in benzene-d<sub>6</sub>. <sup>‡</sup>Integration value of imine. <sup>§</sup>Concentration of imine.

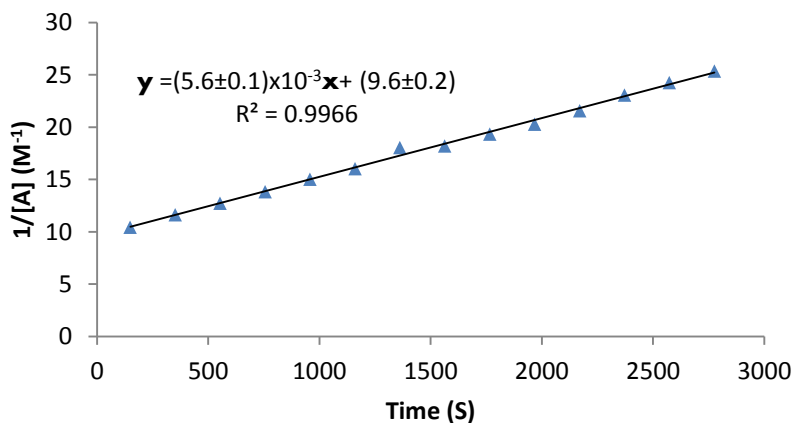


**Figure 10** |  $1/[A]$  vs. time monitored by <sup>1</sup>H NMR spectroscopy in the presence of 12 mol% catalyst at 303K.

**Table 11** | Mannich reaction of imine and fluorinated ketoester carried out in the presence of 12 mol% catalyst at 323K<sup>†</sup>

Entry	Time (s)	$I_A^{\ddagger}$	$[A]^{\S}$ (M)	$1/[A]$ ( $M^{-1}$ )
1	150	0.9574	0.0957	10.4450
2	352	0.8592	0.0859	11.6387
3	554	0.7865	0.0787	12.7146
4	756	0.7232	0.0723	13.8274
5	958	0.6652	0.0665	15.0331
6	1160	0.6241	0.0624	16.0231
7	1362	0.5542	0.0554	18.0440
8	1564	0.5491	0.0549	18.2116
9	1766	0.5173	0.0517	19.3311
10	1968	0.4935	0.0494	20.2634
11	2170	0.4641	0.0464	21.5471
12	2372	0.4339	0.0434	23.0468
13	2574	0.4123	0.0412	24.2542
14	2776	0.3945	0.0395	25.3485

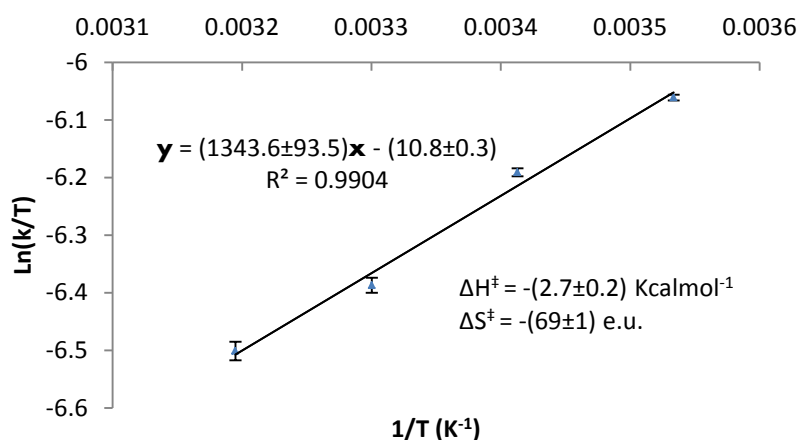
<sup>†</sup>Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in benzene-d<sub>6</sub>. <sup>‡</sup>Integration value of imine. <sup>§</sup>Concentration of imine.



**Figure 11** |  $1/[A]$  vs. time monitored by <sup>1</sup>H NMR spectroscopy in the presence of 12 mol% catalyst at 313K.

**Table 12** | Activation parameters for Mannich reaction of imine and fluorinated ketoester catalyzed by **Trp-1** at different temperature

Entry	T (K)	$K_{obs}$ ( $M^{-1}s^{-1}$ )	k ( $M^{-2}s^{-1}$ )	ee (%)
1	283	$(7.9 \pm 0.1) \times 10^{-3}$	$0.66 \pm 0.01$	93
2	293	$(7.2 \pm 0.1) \times 10^{-3}$	$0.60 \pm 0.01$	93
3	303	$(6.1 \pm 0.1) \times 10^{-3}$	$0.51 \pm 0.01$	93
4	313	$(5.6 \pm 0.1) \times 10^{-3}$	$0.47 \pm 0.01$	93



**Figure 12** | Eyring plots showing the temperature dependent behavior of the Mannich reaction measured by  $^1H$  NMR spectroscopy.

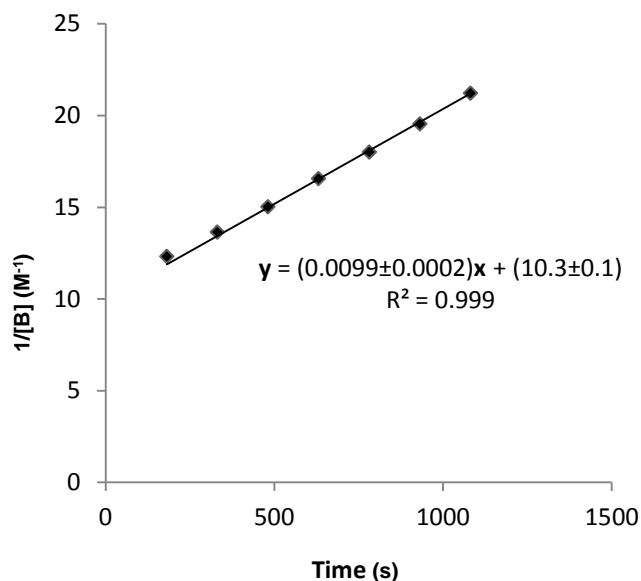
## 6. Mannich Reaction of Imine and Fluorinated Ketoester Catalyzed by DABCO at Different Temperatures

**Table 13.** Mannich reaction of imine and fluorinated ketoester carried out in the presence of 30 mol% DABCO at 293K<sup>a</sup>.

Entry	Time (S)	$I_B^b$	$[B]^c$ (M)	$1/[B]$ ( $M^{-1}$ )
1	182	2.4373	0.0812	12.3087
2	332	2.1989	0.0733	13.6432
3	482	1.9983	0.0666	15.0128
4	632	1.8129	0.0604	16.5481
5	782	1.6672	0.0556	17.9942
6	932	1.5357	0.0512	19.5351

7	1082	1.4144	0.0471	21.2104
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[a] Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in the 0.5 ml solvent. [b] Integration value of ketoester. [c] Concentration of ketoester.

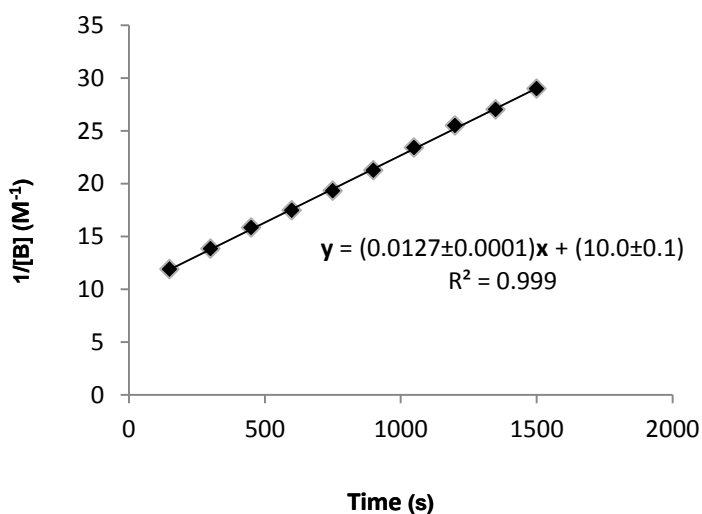


**Figure 13.**  $1/[B]$  vs. time monitored by  $^1\text{H}$  NMR spectroscopy in the presence of 30 mol% DABCO at 283K.

**Table 14.** Mannich reaction of imine and fluorinated ketoester carried out in the presence of 30 mol% DABCO at 293K<sup>a</sup>.

Entry	Time (S)	$I_B^b$	$[B]^c$ (M)	$1/[B]$ ( $\text{M}^{-1}$ )
1	150	2.5231	0.0841	11.8901
2	300	2.1692	0.0723	13.8300
3	450	1.8929	0.0631	15.8487
4	600	1.7155	0.0572	17.4876
5	750	1.5513	0.0517	19.3386
6	900	1.4101	0.0470	21.2751
7	1050	1.2808	0.0427	23.4229
8	1200	1.1761	0.0392	25.5080
9	1350	1.1100	0.0370	27.0270
10	1500	1.0347	0.0345	28.9939

[a] Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in the 0.5 ml solvent. [b] Integration value of ketoester. [c] Concentration of ketoester.



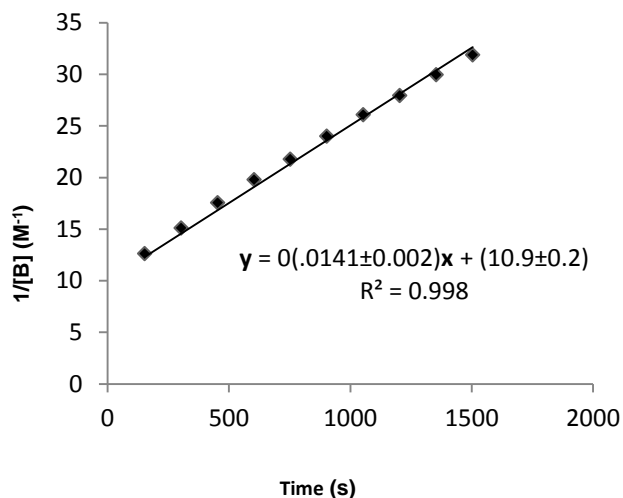
**Figure 14.**  $1/[B]$  vs. time monitored by  $^1H$  NMR spectroscopy in the presence of 30 mol% DABCO at 293K.

**Table 15.** Mannich reaction of imine and fluorinated ketoester carried out in the presence of 30 mol% DABCO at 303K<sup>a</sup>.

Entry	Time (S)	$I_B^b$	$[B]^c$ (M)	$1/[B]$ ( $M^{-1}$ )
1	154	2.3769	0.0792	12.6215
2	304	1.9857	0.0662	15.1080
3	454	1.7097	0.0570	17.5469
4	604	1.5168	0.0506	19.7785
5	754	1.3782	0.0459	21.7675
6	904	1.2495	0.0417	24.0096
7	1054	1.1508	0.0384	26.0688
8	1204	1.0734	0.0358	27.9486
9	1354	1.0021	0.0334	29.9371
10	1504	0.9411	0.0314	31.8776

[a] Reaction was carried out with imine (0.05 mmol) and ketoester (0.05 mmol) in the 0.5 ml solvent. [b] Integration value of ketoester. [c] Concentration of ketoester.

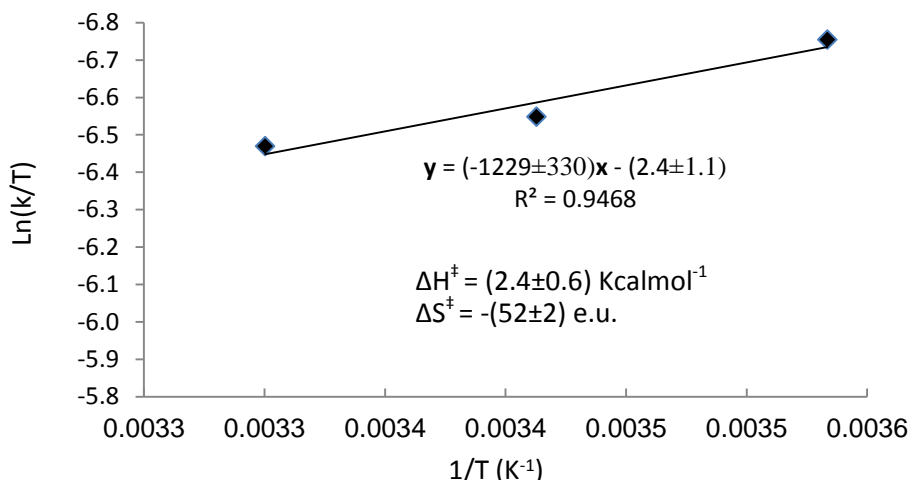




**Figure 15.**  $1/[B]$  vs. time monitored by  $^1\text{H}$  NMR spectroscopy in the presence of 30 mol% DABCO at 303K.

**Table 16.** Activation parameters for Mannich reaction of imine and fluorinated ketoester catalyzed by **DABCO** at different temperature

Entry	T (K)	$K_{\text{obs}}$ ( $10^{-2}\text{M}^{-1}\text{s}^{-1}$ )	k ( $\text{M}^{-2}\text{s}^{-1}$ )
1	283	$0.99\pm 0.02$	$0.33\pm 0.01$
2	293	$1.27\pm 0.01$	$0.42\pm 0.01$
3	303	$1.41\pm 0.02$	$0.47\pm 0.01$



**Figure 17.** Eyring plots showing the temperature dependent behavior of the Mannich reaction measured by  $^1\text{H}$  NMR spectroscopy

## 7. Thermodynamic Data and Cartesian

## Catalyst

### Coordinates of Optimized Stationary Points

Zero-point correction=  
0.481034  
Sum of electronic and thermal Enthalpies=  
-2145.698396  
Sum of electronic and thermal Free Energies=  
-2145.806283

### Imine

Zero-point correction=  
0.278425  
Sum of electronic and thermal Enthalpies=  
-710.419828  
Sum of electronic and thermal Free Energies=  
-710.483570

H	-1.18511	1.982047	0.321025
C	-0.31412	2.581517	0.561368
C	1.951983	4.088844	1.155788
C	0.953343	2.102041	0.193915
C	-0.43516	3.795129	1.215649
C	0.693949	4.571147	1.524977
C	2.082192	2.870144	0.498197
H	-1.42033	4.156749	1.495954
H	3.067269	2.507929	0.218352
H	2.837647	4.672993	1.385831
C	0.539834	5.886759	2.233511
H	-0.061	6.583327	1.640566
H	1.507073	6.355249	2.424661
H	0.030747	5.75848	3.193539
C	1.119993	0.828556	-0.49196
H	2.143909	0.525352	-0.74243
N	0.126297	0.077042	-0.79743
C	0.476459	-1.12937	-1.44294
O	1.602379	-1.56631	-1.58582
O	-0.64186	-1.71831	-1.86096
C	-0.60771	-2.99687	-2.5702
C	-0.0233	-4.08033	-1.66991
H	-0.56798	-4.12126	-0.72289
H	1.032048	-3.90149	-1.46569
H	-0.12515	-5.05133	-2.16228
C	-2.08283	-3.26286	-2.8436
H	-2.6429	-3.32257	-1.90753
H	-2.19809	-4.20765	-3.38051
H	-2.51166	-2.46208	-3.45061
C	0.162832	-2.8524	-3.8786
H	0.064136	-3.77465	-4.45761
H	1.221211	-2.6646	-3.69933
H	-0.24988	-2.03306	-4.47327

C	-2.71904	5.479489	2.383684
S	-4.13396	4.613973	2.549666
N	-2.42569	6.641211	3.071978
H	-1.70458	7.207639	2.648779
N	-1.71634	5.150393	1.533281
H	-0.76846	5.413648	1.809641
C	-3.13301	7.282936	4.093425
C	-4.40318	8.694478	6.163963
C	-3.84766	6.591683	5.078974
C	-3.05323	8.675392	4.158618
C	-3.67884	9.369048	5.190163
C	-4.47622	7.30443	6.091691
H	-3.90994	5.514117	5.046092
H	-2.51045	9.223444	3.395421
H	-4.896	9.23544	6.961629
C	-5.28382	6.572563	7.129288
C	-3.51964	10.86155	5.26374
C	-1.69122	3.937189	0.731277
H	-2.09774	3.115395	1.33305
C	-0.21994	3.670084	0.373343
H	0.049233	4.324492	-0.46152
H	-0.12721	2.636165	0.008593
N	0.694789	3.953617	1.47628
C	2.061571	4.174185	0.998603
H	2.734737	4.063579	1.851636
H	2.34998	3.391976	0.274224
C	2.276272	5.554653	0.394797
H	3.314424	5.666142	0.070181
H	2.06468	6.333349	1.132543
H	1.642504	5.733135	-0.47767
C	0.633733	2.913136	2.50783
H	1.189212	2.015691	2.182902
H	-0.41008	2.605801	2.611045
C	1.132479	3.379611	3.867594
H	2.184684	3.675005	3.851925
H	1.032651	2.572135	4.597753
H	0.547012	4.231993	4.221573

C	-2.54922	4.071524	-0.53903
H	-2.1531	4.898565	-1.13902
H	-3.56013	4.352757	-0.22919
C	-2.59653	2.818766	-1.35509
C	-3.25709	1.587849	-1.00466
C	-3.03291	0.672817	-2.06325
H	-1.44717	3.285037	-3.19588
F	-6.60639	6.668121	6.882935
F	-5.08423	7.081687	8.361776
F	-4.98542	5.264626	7.184445
F	-4.49895	11.44438	5.973911
F	-3.51604	11.42773	4.040857
F	-2.35132	11.20579	5.849074
H	-1.98745	0.936846	-3.88986
N	-2.27351	1.321254	-3.00713
C	-2.0207	2.606489	-2.58067
C	-3.54639	-0.62597	-2.04838
H	-3.36743	-1.31647	-2.86635
C	-4.02999	1.181883	0.095257
C	-4.54208	-0.10594	0.113404
H	-5.14345	-0.43176	0.955358
C	-4.30041	-1.00089	-0.94631
H	-4.71574	-2.00217	-0.90277
H	-4.23035	1.870258	0.910793

### Ketoenol

Zero-point correction=  
0.204304  
Sum of electronic and thermal Enthalpies=  
-750.952148  
Sum of electronic and thermal Free Energies=  
-751.009074

C	-0.04282	2.006306	0.258996
C	0.076334	4.475755	1.58168
C	-0.1877	2.074126	1.653509
C	0.154624	3.195247	-0.4607
C	0.21876	4.417122	0.19686
C	-0.13075	3.302142	2.303081
H	-0.35378	1.175157	2.2297
H	0.257567	3.147141	-1.53742
H	0.378087	5.325636	-0.37399
H	-0.2503	3.339977	3.380523
H	0.123662	5.430185	2.0954
C	-0.1062	0.747367	-0.50043
C	-0.0129	-0.5193	0.011089

C	-0.07288	-1.6943	-0.82916
O	-0.25035	0.910693	-1.81707
H	-0.26346	0.006228	-2.22951
O	-0.21188	-1.6254	-2.05693
O	0.035139	-2.84337	-0.17388
C	-0.01534	-4.04086	-0.97449
H	0.799546	-4.0074	-1.70201
H	-0.9581	-4.05075	-1.52711
C	0.107323	-5.21533	-0.03464
H	1.052233	-5.18284	0.511936
H	0.072059	-6.14608	-0.60643
H	-0.7107	-5.2247	0.688798
F	0.166451	-0.73283	1.333504

### pTS1-I

Zero-point correction=  
0.968485  
Sum of electronic and thermal Enthalpies=  
-3607.081855  
Sum of electronic and thermal Free Energies=  
-3607.267971

C	-3.27606	0.226236	-4.88636
S	-4.64924	1.213225	-4.93272
N	-2.66567	-0.29854	-5.98291
N	-2.67033	-0.13468	-3.72563
C	-2.98503	-0.14073	-7.33459
C	-3.48999	0.043598	-10.097
C	-2.71876	-1.22421	-8.18302
C	-3.48988	1.0416	-7.88311
C	-3.73825	1.117738	-9.25087
C	-2.97361	-1.12618	-9.54527
H	-2.32457	-2.14499	-7.76837
H	-3.69933	1.884527	-7.24017
H	-3.70131	0.111312	-11.1563
C	-2.66409	-2.28276	-10.4531
C	-4.22499	2.421535	-9.81762
C	-3.28041	0.076527	-2.4321
H	-4.07771	0.805473	-2.5878
C	-2.26038	0.613874	-1.43959
H	-1.44759	-0.10529	-1.31741
H	-2.75148	0.77601	-0.4793
C	-3.93478	-1.21277	-1.89157
H	-3.16036	-1.97315	-1.76159
H	-4.61211	-1.56499	-2.67749
C	-4.68979	-1.00893	-0.61623

C	-5.86394	-0.19552	-0.42051	C	0.28691	-5.46422	-7.66417
C	-6.22341	-0.297	0.947152	C	1.059259	-3.31121	-8.42012
F	-1.46188	-2.13543	-11.0561	H	0.888587	-1.70994	-6.98683
F	-3.57246	-2.39906	-11.4426	H	-0.43599	-5.55454	-5.64408
F	-2.63236	-3.45515	-9.80043	H	0.093937	-6.51513	-7.85371
F	-4.75857	2.279889	-11.0448	H	1.476873	-2.68015	-9.19798
F	-3.21411	3.316216	-9.93625	H	1.071373	-5.08979	-9.63481
F	-5.15627	3.000995	-9.04048	H	-1.1418	1.770006	-2.76554
N	-1.6372	1.912364	-1.85758	N	1.790605	0.988328	-3.2481
C	-2.6583	2.987843	-2.09604	C	1.090092	1.597803	-4.27162
H	-3.28521	2.634476	-2.91827	C	2.106185	-0.25221	-3.30056
H	-3.28107	3.047053	-1.20019	H	1.748073	-0.8944	-4.1102
C	-0.53896	2.30586	-0.91371	C	2.943404	-0.88111	-2.28491
H	-0.00893	3.131375	-1.3887	C	4.603611	-2.13545	-0.38681
H	0.149033	1.459336	-0.89304	C	3.222431	-2.24839	-2.37776
C	-2.05428	4.331185	-2.45859	C	3.504247	-0.14205	-1.23192
H	-1.36913	4.240578	-3.30395	C	4.318635	-0.76272	-0.30027
H	-1.52969	4.80605	-1.6264	C	4.040853	-2.86443	-1.43659
H	-2.86618	4.997239	-2.7583	H	2.785047	-2.83418	-3.18024
C	-1.00428	2.677465	0.480795	H	3.296982	0.920867	-1.16862
H	-1.48139	1.84442	1.000093	H	4.750713	-0.18035	0.508588
H	-1.69266	3.525496	0.479796	H	4.239608	-3.92818	-1.51988
H	-0.12949	2.968452	1.066804	C	5.511633	-2.78949	0.61557
H	-1.88561	-0.95114	-5.77985	H	5.442567	-3.8779	0.567425
O	-0.599	-1.70557	-4.92689	H	5.271179	-2.47612	1.635176
C	-0.14706	-2.89935	-4.86581	H	6.5555	-2.51472	0.430338
C	0.077923	-3.56971	-3.66615	O	-0.00774	2.12011	-4.10128
C	-0.21299	-3.08569	-2.35293	O	1.793601	1.64535	-5.39187
O	-0.75152	-2.01094	-2.0718	C	1.373508	2.430697	-6.56973
H	-1.88686	-0.80153	-3.77983	C	1.292339	3.904135	-6.19183
F	0.683959	-4.80183	-3.70712	H	1.1136	4.495328	-7.09361
O	0.175612	-3.95466	-1.38695	H	2.232807	4.239215	-5.74643
C	-0.06446	-3.5487	-0.04234	H	0.477307	4.091788	-5.49286
H	0.448837	-2.60098	0.148993	C	2.515379	2.183896	-7.54584
H	-1.13676	-3.37763	0.098833	H	2.326594	2.721108	-8.47818
C	0.443208	-4.64904	0.861957	H	2.605349	1.119277	-7.7729
H	1.513644	-4.80887	0.714623	H	3.463882	2.530753	-7.12931
H	-0.07395	-5.58966	0.659319	C	0.060954	1.894397	-7.11846
H	0.275538	-4.38029	1.908771	H	-0.16845	2.400194	-8.05988
C	0.205615	-3.56519	-6.16218	H	-0.76124	2.061374	-6.42458
C	0.833251	-4.66435	-8.6655	H	0.137548	0.823641	-7.31885
C	0.734927	-2.76564	-7.18258	H	-5.33975	-1.43308	2.504853
C	-0.01669	-4.92333	-6.41776	C	-6.65325	0.593086	-1.27444

H	-6.4132	0.679517	-2.33022
C	-7.33049	0.366591	1.480617
H	-7.59483	0.276612	2.529442
C	-8.08701	1.14243	0.614809
H	-8.95614	1.668984	0.994768
C	-4.3989	-1.55659	0.60664
H	-3.60481	-2.23673	0.878943
N	-5.30906	-1.12849	1.548138
C	-7.75317	1.25295	-0.74834
H	-8.37294	1.861205	-1.39842

### TS1-I

Zero-point correction=  
0.968022  
Sum of electronic and thermal Enthalpies=  
-3607.072109  
Sum of electronic and thermal Free Energies=  
-3607.252602  
Imaginary frequency = 225.64i cm<sup>-1</sup>

C	-0.0528	0.216481	0.058654
S	-0.1214	0.272822	1.74549
N	1.110806	0.268686	-0.64901
N	-1.14859	0.13133	-0.72748
C	2.419293	0.346072	-0.1541
C	5.103719	0.493612	0.659592
C	3.311614	1.199731	-0.80344
C	2.876756	-0.4415	0.90786
C	4.205263	-0.35406	1.30537
C	4.644121	1.26238	-0.40186
H	2.954498	1.830516	-1.6099
H	2.19567	-1.11411	1.408923
H	6.137338	0.548879	0.975563
C	5.589876	2.148171	-1.16034
C	4.678987	-1.16781	2.47727
C	-2.50036	0.18263	-0.21548
H	-2.42162	0.033452	0.862481
C	-3.34898	-0.91353	-0.84497
H	-3.33721	-0.81072	-1.93294
H	-4.37051	-0.81455	-0.47488
C	-3.14158	1.569999	-0.43635
H	-3.20427	1.768639	-1.50886
H	-2.44241	2.299003	-0.01171
C	-4.48503	1.71517	0.205188
C	-4.78642	1.675816	1.61435
C	-6.18665	1.850815	1.750822

F	5.986708	1.572717	-2.32043
F	6.705727	2.423301	-0.46439
F	5.023673	3.323497	-1.49457
F	4.565353	-0.48826	3.637211
F	5.977045	-1.5115	2.35772
F	3.97811	-2.3072	2.623084
N	-2.87887	-2.30514	-0.55779
C	-2.64288	-2.5593	0.898007
H	-1.86683	-1.86024	1.215657
H	-3.56039	-2.30298	1.434717
C	-3.77526	-3.31275	-1.21122
H	-3.25833	-4.27045	-1.14042
H	-3.78456	-3.04446	-2.26895
C	-2.18965	-3.97652	1.197538
H	-1.32447	-4.25004	0.589345
H	-2.97528	-4.72079	1.049201
H	-1.88711	-4.0229	2.24589
C	-5.17337	-3.40947	-0.63024
H	-5.74078	-2.48286	-0.73648
H	-5.17075	-3.69158	0.425276
H	-5.71645	-4.18624	-1.1738
H	1.02137	0.267276	-1.66722
O	0.384526	0.010212	-3.35224
C	0.332433	-0.04108	-4.5964
C	-0.93906	0.047912	-5.26722
C	-2.04144	0.799428	-4.66807
O	-2.29691	0.846609	-3.47373
H	-1.03814	0.182051	-1.74436
F	-0.8878	0.173392	-6.63052
O	-2.78591	1.418921	-5.59732
C	-3.91685	2.152109	-5.11482
H	-4.58963	1.462121	-4.59681
H	-3.57599	2.897996	-4.39085
C	-4.58399	2.791256	-6.31023
H	-4.91399	2.03154	-7.02199
H	-3.89776	3.468987	-6.82279
H	-5.45596	3.36546	-5.98533
C	1.601902	-0.23373	-5.36932
C	4.090153	-0.56644	-6.62881
C	2.787288	0.172641	-4.74252
C	1.685489	-0.81721	-6.64089
C	2.921758	-0.98874	-7.25785
C	4.019298	0.019223	-5.36578

H	2.726325	0.615414	-3.75625
H	0.79198	-1.14803	-7.15116
H	2.969172	-1.45234	-8.23772
H	4.921257	0.354666	-4.86536
H	5.050047	-0.69227	-7.1188
H	-1.9462	-2.45573	-1.06351
C	-1.66736	-2.01086	-4.97736
N	-1.73213	-2.26776	-3.67244
C	-0.67289	-2.84231	-3.05283
H	-0.81586	-2.36327	-5.56112
C	-2.92271	-1.89272	-5.7447
C	-5.31156	-1.75935	-7.25568
C	-2.9016	-2.02213	-7.13751
C	-4.15825	-1.6926	-5.11794
C	-5.32882	-1.62602	-5.86182
C	-4.07571	-1.95605	-7.87815
H	-1.9549	-2.17534	-7.64488
H	-4.18329	-1.58642	-4.04018
H	-6.27758	-1.4709	-5.35484
H	-4.03163	-2.05896	-8.95848
C	-6.58486	-1.72634	-8.0543
H	-6.42107	-1.3066	-9.04977
H	-7.35416	-1.13089	-7.55666
H	-6.98877	-2.73584	-8.18859
O	-0.66678	-3.03808	-1.82219
O	0.331469	-3.25844	-3.83588
C	1.491511	-3.99318	-3.32347
C	1.040805	-5.31717	-2.71543
H	1.919851	-5.91918	-2.46955
H	0.434843	-5.87848	-3.43217
H	0.461739	-5.15842	-1.80635
C	2.311361	-4.24029	-4.5839
H	3.219941	-4.79337	-4.33278
H	2.597886	-3.2956	-5.05073
H	1.738928	-4.8269	-5.30724
C	2.273965	-3.13673	-2.33628
H	3.195386	-3.65718	-2.06023
H	1.695848	-2.94444	-1.43363
H	2.544493	-2.18352	-2.7952
H	-7.66818	2.17386	0.267952
C	-4.00367	1.525407	2.771453
H	-2.92648	1.404315	2.701263
C	-6.81978	1.870631	2.995604

H	-7.89273	2.008041	3.084584
C	-6.02207	1.713309	4.119343
H	-6.48067	1.726296	5.10246
C	-5.6823	1.910912	-0.4339
H	-5.88383	2.012545	-1.4907
N	-6.70563	1.986519	0.48559
C	-4.62884	1.54441	4.008626
H	-4.03499	1.432922	4.909513

### pTS-II

Zero-point correction=  
0.968099  
Sum of electronic and thermal Enthalpies=  
-3607.081195  
Sum of electronic and thermal Free Energies=  
-3607.268581

C	-0.95014	1.191242	-0.58368
S	-1.85106	2.591705	-0.8451
N	-0.31844	0.476023	-1.55837
N	-0.77392	0.650847	0.646066
C	-0.05297	0.797706	-2.89551
C	0.610755	1.260295	-5.58919
C	1.11096	0.244662	-3.44976
C	-0.88898	1.572113	-3.70263
C	-0.54155	1.799436	-5.03355
C	1.427983	0.471522	-4.78096
H	1.761784	-0.36184	-2.83117
H	-1.79677	1.988221	-3.29
H	0.861186	1.437544	-6.62753
C	2.677051	-0.11194	-5.37729
C	-1.43435	2.675087	-5.86882
C	-1.42169	1.146653	1.840434
C	-0.40554	1.290686	2.966984
H	0.003025	0.315117	3.234985
H	-0.89722	1.73356	3.833923
C	-2.58256	0.22755	2.271764
H	-2.19325	-0.7708	2.496371
H	-3.23422	0.122542	1.397502
C	-3.35908	0.750058	3.438362
C	-4.13076	1.966067	3.493845
C	-4.67979	2.055775	4.797882
H	-3.05612	-0.76309	5.030142
F	3.30062	-0.96277	-4.54767
F	3.569076	0.84833	-5.70523
F	2.413747	-0.78849	-6.51667

F	-1.24376	2.482052	-7.1882	H	3.729084	-6.09956	2.654084
F	-1.21064	3.985261	-5.63203	H	-1.84517	2.120455	1.585304
F	-2.73792	2.454305	-5.61865	H	0.0637	-0.42529	-1.2767
N	0.765995	2.144407	2.603806	H	0.009688	0.006874	0.805786
C	0.345456	3.547051	2.272676	O	0.224505	-2.42717	-1.58584
H	-0.27342	3.471086	1.376088	N	-1.27559	-3.70861	-0.37409
H	-0.28886	3.896543	3.091868	C	-0.81827	-3.63635	0.81718
C	1.842205	2.044994	3.640409	H	0.240306	-3.43392	1.016198
H	2.71308	2.552686	3.224501	C	-1.67245	-3.83442	1.986322
H	2.084226	0.98185	3.689491	C	-3.26659	-4.23624	4.273602
C	1.499424	4.496044	2.013374	C	-1.10475	-3.79673	3.263111
H	2.162277	4.095927	1.244502	C	-3.04905	-4.0736	1.859663
H	2.079487	4.718885	2.911991	C	-3.82892	-4.2666	2.9873
H	1.085516	5.438552	1.647812	C	-1.89541	-3.99669	4.391509
C	1.474063	2.608494	4.999583	H	-0.03897	-3.61654	3.366211
H	0.644698	2.072435	5.465513	H	-3.48416	-4.10721	0.866842
H	1.21894	3.670138	4.958583	H	-4.89377	-4.45009	2.87675
H	2.338294	2.506697	5.660135	H	-1.43888	-3.97545	5.376904
H	1.224397	1.745442	1.739596	C	-0.41158	-3.45915	-1.43726
O	2.275754	1.824132	0.393812	O	-0.44829	-4.48125	-2.28195
O	1.523563	-0.55808	1.803546	C	0.273411	-4.4743	-3.56181
C	2.531597	-1.04735	1.195213	C	1.772501	-4.34439	-3.32393
C	3.117612	1.040187	-0.07948	H	2.11735	-5.12495	-2.64059
C	3.292407	-0.33015	0.272358	H	2.030403	-3.37034	-2.91087
F	4.362573	-0.94568	-0.32216	H	2.299109	-4.46666	-4.27395
O	3.990611	1.456614	-1.01501	C	-0.27912	-3.36793	-4.45081
C	3.894588	2.826583	-1.41995	H	0.183491	-3.43287	-5.4391
H	4.062173	3.469624	-0.55012	H	-0.06967	-2.38133	-4.03893
H	2.884275	3.023173	-1.78947	H	-1.35956	-3.48051	-4.57187
C	4.939389	3.056132	-2.48718	C	-0.06396	-5.84522	-4.13286
H	5.941203	2.851224	-2.10283	H	0.292727	-6.63727	-3.47023
H	4.902665	4.096463	-2.82135	H	0.410817	-5.96793	-5.10932
H	4.76409	2.411829	-3.351	H	-1.14382	-5.95664	-4.25419
C	2.914774	-2.45715	1.544398	H	-4.51842	0.719654	6.437271
C	3.499413	-5.0848	2.345836	N	-4.25887	0.948019	5.494178
C	3.396505	-3.39222	0.620978	C	-3.47271	0.168491	4.674526
C	2.722976	-2.86237	2.871646	C	-5.49204	3.120184	5.195318
C	3.026049	-4.15876	3.274636	H	-5.90667	3.174247	6.19688
C	3.674985	-4.69794	1.019294	C	-5.75441	4.10721	4.256959
H	3.545923	-3.10208	-0.41083	H	-6.38348	4.947408	4.531269
H	2.332848	-2.13873	3.579387	C	-5.22547	4.036175	2.954324
H	2.892693	-4.44931	4.312245	H	-5.45812	4.822106	2.243856
H	4.037047	-5.41425	0.288759	C	-4.41966	2.978237	2.563201

H	-4.02587	2.933019	1.552016
C	-4.12536	-4.47423	5.483583
H	-4.52147	-5.49467	5.486466
H	-3.56305	-4.33353	6.409031
H	-4.98464	-3.79696	5.498808

## TS-II

Zero-point correction=

0.968290

Sum of electronic and thermal Enthalpies=

-3607.050207

Sum of electronic and thermal Free Energies=

-3607.230296

Imaginary frequency = 349.56i cm<sup>-1</sup>

C	-0.27811	0.360171	-0.18541
S	0.014344	0.058683	1.451469
N	0.72345	0.639799	-1.05166
N	-1.52332	0.309939	-0.72944
C	2.076702	0.720053	-0.63664
C	4.761585	0.890207	0.111735
C	2.963758	-0.29262	-0.99158
C	2.529406	1.822047	0.08237
C	3.86847	1.900253	0.45379
C	4.300066	-0.20308	-0.61604
H	2.601092	-1.14427	-1.55214
H	1.833914	2.608226	0.348066
H	5.80322	0.959026	0.401496
C	5.27612	-1.28385	-0.98398
C	4.344033	3.066601	1.274081
C	-2.71182	0.058175	0.058609
C	-3.61876	-0.98339	-0.60546
H	-4.23161	-0.51833	-1.37735
H	-4.26322	-1.43698	0.148095
C	-3.49926	1.352206	0.332945
H	-3.78637	1.799313	-0.62454
H	-2.80538	2.045425	0.821148
C	-4.71156	1.143913	1.184204
C	-4.74071	0.711924	2.558615
C	-6.10193	0.645366	2.948153
H	-6.42185	1.650592	-0.13617
F	4.692654	-2.30383	-1.63872
F	5.877881	-1.80421	0.105261
F	6.263894	-0.81815	-1.77775
F	5.652132	3.320141	1.078016
F	4.185636	2.844612	2.595389

F	3.669933	4.195119	0.986355
N	-2.85122	-2.07058	-1.28698
C	-2.00559	-2.84874	-0.32315
H	-1.36547	-2.12214	0.180585
H	-2.67824	-3.27123	0.426996
C	-3.74671	-2.91753	-2.14274
H	-3.08906	-3.52306	-2.76733
H	-4.26588	-2.21815	-2.79978
C	-1.15798	-3.91375	-0.9921
H	-0.56394	-3.48735	-1.80338
H	-1.74901	-4.74501	-1.38391
H	-0.46971	-4.32124	-0.24872
C	-4.72531	-3.78484	-1.37595
H	-5.41248	-3.19935	-0.76218
H	-4.22374	-4.51561	-0.73821
H	-5.3277	-4.34105	-2.09756
H	-2.20732	-1.61134	-1.97098
O	-1.08146	-1.40061	-3.34187
O	-3.27519	0.335312	-3.16587
C	-3.25898	0.205945	-4.40399
C	-1.08083	-0.9956	-4.50763
C	-1.97199	0.039543	-5.06598
F	-2.01452	-0.01999	-6.43433
O	-0.26602	-1.48303	-5.43253
C	0.707382	-2.44904	-5.00591
H	0.20026	-3.24473	-4.45334
H	1.401604	-1.94574	-4.32851
C	1.39346	-2.97333	-6.24439
H	0.683664	-3.48217	-6.90071
H	2.172722	-3.68481	-5.95915
H	1.856487	-2.15913	-6.80461
C	-4.54775	0.279189	-5.15246
C	-7.08162	0.354619	-6.34349
C	-4.77626	-0.36825	-6.37427
C	-5.60687	0.960138	-4.53665
C	-6.86108	1.006892	-5.13039
C	-6.03998	-0.33648	-6.95738
H	-3.97248	-0.89829	-6.86704
H	-5.41893	1.460679	-3.59415
H	-7.66672	1.555208	-4.65309
H	-6.20731	-0.84738	-7.89966
H	-8.0611	0.388075	-6.80943
H	-2.34574	-0.32559	1.013941



H	0.585884	0.649938	-2.07141
H	-1.66142	0.532068	-1.713
C	-1.06568	1.795351	-4.78089
O	1.245173	0.752494	-3.80524
N	0.062417	1.818369	-5.50724
H	-1.00282	1.683593	-3.69064
C	-2.10985	2.763229	-5.22049
C	-4.01907	4.678256	-6.03774
C	-2.91414	3.414812	-4.28385
C	-2.25759	3.090033	-6.573
C	-3.20344	4.024557	-6.97075
C	-3.85067	4.363838	-4.68828
H	-2.79492	3.192063	-3.22785
H	-1.60339	2.613407	-7.2934
H	-3.30411	4.264746	-8.02577
H	-4.45253	4.874152	-3.94112
C	1.163723	1.323751	-4.91091
O	2.243875	1.534349	-5.69125
C	3.604597	1.370188	-5.21961
C	3.912412	-0.0941	-4.92305
H	3.700822	-0.70962	-5.80146
H	3.317195	-0.45163	-4.08399
H	4.971827	-0.20716	-4.67687
C	3.859951	2.26486	-4.0099
H	4.921472	2.23666	-3.74829
H	3.280559	1.937885	-3.14678
H	3.593066	3.298754	-4.24459
C	4.430011	1.847808	-6.41046
H	4.209006	1.244666	-7.2945
H	5.497081	1.765289	-6.18775
H	4.198624	2.890088	-6.64163
H	-7.85632	1.108966	1.849222
N	-6.85608	1.016223	1.860377
C	-6.01893	1.318772	0.810068
C	-6.49358	0.263008	4.232952
H	-7.53987	0.219799	4.517955
C	-5.4906	-0.05498	5.136545
H	-5.75865	-0.35337	6.144487
C	-4.13197	0.008691	4.77334
H	-3.37445	-0.23957	5.50889
C	-3.74655	0.389182	3.497391
H	-2.69428	0.443541	3.233752
C	-5.04638	5.682073	-6.48367

H	-5.91271	5.184626	-6.93335
H	-5.40769	6.282861	-5.64578
H	-4.63814	6.363016	-7.23567

### pTS-III

Zero-point correction=  
0.968862  
Sum of electronic and thermal Enthalpies=  
-3607.073525  
Sum of electronic and thermal Free Energies=  
-3607.260952

C	-3.34232	0.348059	-5.52479
S	-4.63821	1.432399	-5.59515
N	-2.69525	-0.14301	-6.6173
N	-2.84556	-0.13966	-4.35886
C	-2.85291	0.217851	-7.95791
C	-3.03191	0.829665	-10.6979
C	-2.69978	-0.7842	-8.92223
C	-3.08369	1.533209	-8.37502
C	-3.17519	1.821587	-9.73188
C	-2.78934	-0.47307	-10.2757
H	-2.52265	-1.8068	-8.60811
H	-3.20192	2.31586	-7.63942
H	-3.11644	1.063939	-11.751
C	-2.58053	-1.55397	-11.2982
C	-3.35604	3.250178	-10.1605
C	-3.57231	-0.05952	-3.11125
H	-4.36797	0.671369	-3.2687
C	-2.65738	0.391447	-1.97973
H	-1.89994	-0.37181	-1.79252
H	-3.25066	0.553833	-1.07924
C	-4.22407	-1.41252	-2.75946
H	-3.43821	-2.16805	-2.66676
H	-4.84197	-1.6927	-3.61993
C	-5.0559	-1.37643	-1.517
C	-6.25196	-0.60441	-1.29117
C	-6.69285	-0.88858	0.02611
F	-1.26916	-1.70553	-11.5995
F	-3.20919	-1.28306	-12.4575
F	-3.01958	-2.75092	-10.8743
F	-3.93259	3.350273	-11.3721
F	-2.16525	3.893963	-10.2474
F	-4.10755	3.954539	-9.29801
N	-1.9204	1.660847	-2.27937
C	-2.85103	2.810682	-2.54064

H	-3.44503	2.528649	-3.4141	C	2.807374	1.420018	-2.75756
H	-3.52421	2.877048	-1.68258	H	3.329651	1.740237	-1.8518
C	-0.88188	1.933303	-1.2303	C	3.222973	0.11265	-3.26319
H	-0.24198	2.724477	-1.62112	C	4.164241	-2.40193	-4.12722
H	-0.27455	1.02775	-1.18284	C	4.434579	-0.40458	-2.78372
C	-2.13951	4.122848	-2.80562	C	2.471589	-0.65699	-4.16616
H	-1.41155	4.02249	-3.61298	C	2.941627	-1.8909	-4.58582
H	-1.63453	4.524168	-1.92418	C	4.903349	-1.63684	-3.22002
H	-2.88638	4.854975	-3.12006	H	5.017284	0.172124	-2.07075
C	-1.4394	2.289576	0.134034	H	1.495855	-0.32935	-4.50656
H	-2.0395	1.486615	0.566098	H	2.334918	-2.48572	-5.26009
H	-2.03991	3.201569	0.116466	H	5.848333	-2.01616	-2.8437
H	-0.59911	2.467733	0.808987	C	4.639753	-3.74888	-4.58791
H	-2.04187	-0.92482	-6.42475	H	5.578943	-4.02963	-4.10758
O	-0.96599	-1.87737	-5.48323	H	4.795622	-3.7582	-5.671
C	-0.54764	-3.07628	-5.35639	H	3.894524	-4.51782	-4.36476
C	-0.1884	-3.63817	-4.13395	O	0.002055	1.906139	-4.37317
C	-0.25083	-3.00445	-2.85548	O	1.941297	2.468762	-5.41047
O	-0.74533	-1.90035	-2.60792	C	1.37919	2.610248	-6.7694
H	-2.08697	-0.83798	-4.42682	C	0.300462	3.685246	-6.77789
F	0.380146	-4.88912	-4.13355	H	0.01198	3.893351	-7.81124
O	0.309623	-3.76129	-1.87751	H	0.680678	4.612296	-6.34017
C	0.310989	-3.19834	-0.56957	H	-0.58711	3.366943	-6.23209
H	0.856818	-2.24897	-0.58264	C	2.592383	3.054625	-7.57424
H	-0.71775	-2.98088	-0.26279	H	2.312903	3.177906	-8.62315
C	0.964735	-4.20003	0.35569	H	3.388965	2.309788	-7.51232
H	1.990428	-4.40646	0.041716	H	2.977715	4.007093	-7.20275
H	0.413614	-5.14324	0.360192	C	0.86873	1.260493	-7.25085
H	0.988229	-3.80775	1.376328	H	0.53291	1.353597	-8.28688
C	-0.38471	-3.88036	-6.61182	H	0.03169	0.909006	-6.64817
C	-0.1345	-5.24793	-9.0483	H	1.669086	0.516963	-7.21857
C	0.053211	-3.21563	-7.76374	H	-5.88684	-2.21176	1.47459
C	-0.70316	-5.24037	-6.69905	C	-7.00021	0.284922	-2.08072
C	-0.58785	-5.91438	-7.91173	H	-6.70008	0.512816	-3.09919
C	0.190285	-3.89472	-8.97026	C	-7.8411	-0.31039	0.571568
H	0.285425	-2.15783	-7.69793	H	-8.16763	-0.5408	1.580652
H	-1.05112	-5.76766	-5.81929	C	-8.55581	0.567482	-0.2299
H	-0.85433	-6.96489	-7.96853	H	-9.45489	1.032126	0.16082
H	0.538292	-3.36693	-9.85199	C	-4.83119	-2.07836	-0.36105
H	-0.04181	-5.77703	-9.9911	H	-4.0452	-2.78376	-0.13261
H	-1.37051	1.517766	-3.14853	N	-5.80413	-1.78529	0.568847
N	1.935676	2.246739	-3.19123	C	-8.14077	0.860729	-1.54263
C	1.204847	2.14107	-4.361	H	-8.7291	1.544875	-2.14467

### TS-III

Zero-point correction=

0.968333

Sum of electronic and thermal Enthalpies=

-3607.049714

Sum of electronic and thermal Free Energies=

-3607.228635

Imaginary frequency = 125.52i cm<sup>-1</sup>

C	0.044883	0.104719	-0.24298
S	0.069841	0.354834	1.429295
N	1.13767	0.162757	-1.04833
N	-1.10073	-0.16527	-0.91505
C	2.478723	0.322043	-0.67632
C	5.215921	0.634946	-0.11972
C	3.300746	1.049031	-1.54275
C	3.037155	-0.26499	0.462469
C	4.392244	-0.09773	0.729367
C	4.65419	1.198031	-1.26119
H	2.86871	1.482593	-2.43669
H	2.416522	-0.84469	1.130221
H	6.268483	0.758251	0.098949
C	5.526198	1.935857	-2.23604
C	4.962877	-0.69821	1.982999
C	-2.40913	-0.14872	-0.30323
H	-2.25037	-0.23837	0.774305
C	-3.25029	-1.31487	-0.80682
H	-3.47704	-1.1897	-1.869
H	-4.18496	-1.34027	-0.24586
C	-3.14243	1.185227	-0.55489
H	-3.23605	1.34839	-1.63411
H	-2.48465	1.971766	-0.17057
C	-4.48747	1.272842	0.092827
C	-4.77258	1.256237	1.505177
C	-6.17939	1.35338	1.64961
H	-5.91458	1.446394	-1.59812
F	5.943308	1.130894	-3.24057
F	6.634703	2.430593	-1.65471
F	4.883531	2.967642	-2.81411
F	4.780244	0.102095	3.05429
F	6.288894	-0.91475	1.884081
F	4.389974	-1.88074	2.283643
N	-2.58285	-2.64718	-0.69085
C	-2.01304	-2.90724	0.669019
H	-1.31331	-2.09548	0.875315
H	-2.82891	-2.83228	1.392702

C	-3.48478	-3.7358	-1.18972
H	-2.85443	-4.61256	-1.34122
H	-3.8198	-3.41203	-2.17742
C	-1.28985	-4.23798	0.763211
H	-0.53522	-4.33337	-0.02094
H	-1.96213	-5.09747	0.711812
H	-0.77586	-4.28071	1.725608
C	-4.66418	-4.06018	-0.29219
H	-5.32284	-3.2043	-0.13278
H	-4.3521	-4.4421	0.681983
H	-5.25703	-4.84123	-0.77353
H	0.988107	0.194987	-2.06847
O	1.392511	-0.04764	-3.82853
C	1.066898	0.268776	-4.9931
C	-0.08194	1.081529	-5.2423
C	-0.59351	2.137608	-4.36931
O	-1.46048	2.920108	-4.72574
H	-1.07029	-0.36375	-1.92677
F	-0.35258	1.393194	-6.54454
O	-0.04706	2.162272	-3.13652
C	-0.43196	3.267078	-2.29768
H	-1.5004	3.454269	-2.42089
H	-0.23634	2.915753	-1.28326
C	0.376352	4.508766	-2.61287
H	0.168861	4.860408	-3.62511
H	1.446861	4.313164	-2.51575
H	0.111145	5.305711	-1.91213
C	1.927979	-0.21549	-6.12259
C	3.723654	-1.11942	-8.08206
C	3.275318	-0.44646	-5.81087
C	1.489986	-0.4543	-7.4318
C	2.383181	-0.91104	-8.39807
C	4.168491	-0.88334	-6.78191
H	3.609483	-0.27255	-4.79473
H	0.452803	-0.30355	-7.69686
H	2.026595	-1.1021	-9.40514
H	5.211031	-1.03782	-6.5237
H	4.417169	-1.46279	-8.84295
H	-1.77294	-2.66404	-1.39076
C	-1.8154	-0.48693	-4.64886
N	-1.39761	-1.21164	-3.61983
C	-0.7221	-2.38601	-3.58674
O	-0.74219	-3.07812	-2.54747

O	-0.02148	-2.74578	-4.65624
C	0.865989	-3.92537	-4.65395
C	1.970771	-3.7328	-3.62357
H	2.717118	-4.52259	-3.74673
H	1.581227	-3.7769	-2.60684
H	2.45871	-2.76775	-3.77377
C	0.059753	-5.1994	-4.42073
H	0.715818	-6.0628	-4.56171
H	-0.7553	-5.2797	-5.1462
H	-0.35301	-5.23579	-3.41378
C	1.439024	-3.92036	-6.06432
H	2.101399	-4.78042	-6.19059
H	2.009971	-3.01065	-6.25125
H	0.641887	-3.98666	-6.80877
N	-6.71558	1.422048	0.385875
C	-5.69855	1.380799	-0.5412
H	-7.68836	1.553826	0.172052
C	-6.80231	1.372981	2.899486
H	-7.88053	1.451066	2.995037
C	-5.98739	1.296232	4.019111
H	-6.43769	1.312727	5.005907
C	-4.58751	1.206106	3.900002
H	-3.98097	1.15856	4.798
C	-3.97229	1.186654	2.657998
H	-2.89024	1.131512	2.580664
C	-2.28438	-0.8751	-5.98841
C	-2.28076	-2.17616	-6.51449
C	-2.88577	0.139804	-6.75286
C	-2.84388	-2.43881	-7.75582
H	-1.84031	-2.98626	-5.95176
C	-3.43376	-0.12928	-7.99926
H	-2.90845	1.152767	-6.36342
C	-3.42127	-1.42335	-8.5276
H	-2.83704	-3.45673	-8.13562
H	-3.88285	0.678993	-8.56862
C	-3.99175	-1.7142	-9.88666
H	-4.42506	-2.71638	-9.93316
H	-4.76651	-0.99335	-10.1573
H	-3.21224	-1.66014	-10.6546
H	-2.28237	0.442957	-4.33254

pTS-IV

Zero-point correction=  
0.968761  
Sum of electronic and thermal Enthalpies=  
-3607.081735  
Sum of electronic and thermal Free Energies=  
-3607.268409

C	-3.06756	0.192117	-5.23788
S	-4.32612	1.296557	-5.46354
N	-2.31036	-0.36224	-6.22742
N	-2.68085	-0.21961	-4.00746
C	-2.2889	-0.15534	-7.60842
C	-2.03848	0.122216	-10.4036
C	-1.15108	-0.62842	-8.27917
C	-3.31118	0.444601	-8.35437
C	-3.16866	0.576963	-9.73218
C	-1.03512	-0.48625	-9.65617
H	-0.36502	-1.10838	-7.70565
H	-4.19878	0.803569	-7.85427
H	-1.94359	0.234084	-11.4759
C	0.178786	-1.0411	-10.3447
C	-4.24582	1.276541	-10.5146
C	-3.47085	-0.03748	-2.80885
H	-4.25781	0.677186	-3.0552
C	-2.59255	0.490008	-1.68242
H	-1.77714	-0.21862	-1.51124
H	-3.18883	0.600968	-0.7764
C	-4.13482	-1.36642	-2.38839
H	-3.35442	-2.1181	-2.24084
H	-4.73969	-1.69469	-3.24099
C	-4.97731	-1.26664	-1.15753
C	-6.18804	-0.50571	-0.98373
C	-6.62585	-0.71417	0.349104
F	1.29813	-0.87623	-9.61137
F	0.397316	-0.46171	-11.5388
F	0.064141	-2.36916	-10.5731
F	-4.38479	0.759112	-11.7517
F	-3.96651	2.589835	-10.6784
F	-5.44519	1.206041	-9.91555
N	-1.96488	1.816863	-1.98368
C	-2.99444	2.893943	-2.18255
H	-3.56612	2.597234	-3.06503
H	-3.66036	2.865176	-1.31693
C	-0.90638	2.149907	-0.97284
H	-0.38069	3.024436	-1.35564
H	-0.20224	1.316792	-1.00087

C	-2.40619	4.27445	-2.39984	H	2.004579	4.199624	-8.17793
H	-1.68169	4.26744	-3.21592	H	2.412903	2.502322	-7.87081
H	-1.932	4.68499	-1.50559	H	3.166426	3.7829	-6.90273
H	-3.219	4.948022	-2.67982	C	-0.17518	2.899179	-7.07631
C	-1.42749	2.385311	0.431247	H	-0.45167	3.599708	-7.86895
H	-1.8961	1.496596	0.857466	H	-1.00637	2.824553	-6.37626
H	-2.13998	3.211895	0.479587	H	-0.01029	1.922953	-7.53678
H	-0.58141	2.646343	1.07095	H	-5.7911	-1.92087	1.881376
H	-1.59032	-1.02349	-5.90912	C	-6.9516	0.317791	-1.82778
O	-0.27072	-2.21108	-5.57868	H	-6.65411	0.485375	-2.85857
C	-0.17342	-3.36816	-5.13172	C	-7.78552	-0.12387	0.855732
C	-0.35589	-3.7638	-3.77437	H	-8.10968	-0.2962	1.8771
C	-0.60538	-2.92124	-2.68896	C	-8.51524	0.688444	0.000142
O	-0.68045	-1.6558	-2.77851	H	-9.42346	1.159947	0.360244
H	-1.8728	-0.8522	-3.88809	C	-4.7393	-1.88954	0.040919
F	-0.20527	-5.10655	-3.5346	H	-3.93576	-2.55919	0.314465
H	-1.43548	1.746732	-2.87821	N	-5.72073	-1.55745	0.94746
N	1.699819	1.296889	-3.49659	C	-8.10369	0.90565	-1.32833
C	0.911438	2.015499	-4.36709	H	-8.70393	1.539136	-1.97264
C	1.855256	0.028993	-3.56443	O	0.146698	-4.40294	-5.93315
H	1.3307	-0.5804	-4.30643	C	0.326238	-4.1142	-7.32267
C	2.741291	-0.68309	-2.64659	H	-0.60489	-3.70764	-7.72839
C	4.457721	-2.10977	-0.9286	H	1.103107	-3.35242	-7.43682
C	2.826496	-2.0769	-2.72299	C	0.708523	-5.405	-8.00864
C	3.524882	-0.00491	-1.70263	H	1.63807	-5.80498	-7.59712
C	4.366904	-0.71142	-0.85817	H	-0.07329	-6.15782	-7.88546
C	3.671537	-2.77843	-1.87116	H	0.851306	-5.22513	-9.07714
H	2.210133	-2.61299	-3.43746	C	-0.78244	-3.51208	-1.31742
H	3.465688	1.077109	-1.65045	C	-0.28328	-2.78917	-0.22697
H	4.971442	-0.17562	-0.13192	C	-1.49094	-4.69421	-1.07296
H	3.714823	-3.86123	-1.93606	C	-0.46785	-3.24401	1.07466
C	5.398406	-2.86519	-0.03323	H	0.261836	-1.87171	-0.42031
H	5.035219	-3.87621	0.163925	C	-1.6967	-5.13745	0.231846
H	5.535113	-2.35683	0.924184	H	-1.88675	-5.26496	-1.90401
H	6.385851	-2.95657	-0.49881	C	-1.18118	-4.4195	1.309347
O	-0.24078	2.355551	-4.10882	H	-0.05314	-2.68406	1.907266
O	1.593741	2.386942	-5.43879	H	-2.25623	-6.05121	0.405042
C	1.096549	3.389414	-6.40086	H	-1.32908	-4.776	2.323878
C	0.903985	4.719384	-5.68399				
H	0.657968	5.490643	-6.41839				
H	1.82258	5.017305	-5.17173				
H	0.090776	4.666123	-4.96006				
C	2.243727	3.472397	-7.39838				

## TS-IV

Zero-point correction=  
 0.968070  
 Sum of electronic and thermal Enthalpies=  
 -3607.069904  
 Sum of electronic and thermal Free Energies=  
 -3607.250473  
 Imaginary frequency = 235.20i cm<sup>-1</sup>

C	-0.00011	0.146003	0.2451
S	-0.08747	-0.0403	1.919891
N	1.156456	0.285706	-0.46755
N	-1.09292	0.132195	-0.55059
C	2.487129	0.355179	-0.05303
C	5.237247	0.515768	0.546799
C	3.452612	0.050737	-1.02019
C	2.911107	0.760599	1.21874
C	4.27168	0.829151	1.499015
C	4.806573	0.13246	-0.71835
H	3.126366	-0.24732	-2.01015
H	2.180654	1.012023	1.973652
H	6.291499	0.575577	0.781587
C	5.800958	-0.17016	-1.80117
C	4.706128	1.212235	2.887053
C	-2.44862	0.168184	-0.04772
H	-2.39351	-0.10388	1.00716
C	-3.32557	-0.81822	-0.80599
H	-3.29535	-0.5955	-1.8758
H	-4.34861	-0.7222	-0.43916
C	-3.03268	1.595806	-0.12844
H	-3.05112	1.914525	-1.17434
H	-2.31882	2.245482	0.390359
C	-4.3877	1.72727	0.490325
C	-4.73372	1.530402	1.875863
C	-6.12729	1.760259	1.998479
F	5.500795	-1.31231	-2.4579
F	7.052391	-0.30087	-1.33236
F	5.832985	0.803937	-2.73984
F	5.930871	1.774748	2.894666
F	4.77034	0.137694	3.702926
F	3.862821	2.086711	3.462259
N	-2.91337	-2.24999	-0.67333
C	-2.69273	-2.67197	0.746293
H	-1.88391	-2.04854	1.132664
H	-3.59761	-2.43258	1.311643
C	-3.84742	-3.14074	-1.43475

H	-3.36834	-4.11954	-1.47502
H	-3.84527	-2.75383	-2.45512
C	-2.30788	-4.13316	0.888257
H	-1.45603	-4.37815	0.250341
H	-3.12832	-4.81825	0.662965
H	-2.00948	-4.30719	1.92426
C	-5.24999	-3.24683	-0.86639
H	-5.77936	-2.29209	-0.8631
H	-5.2615	-3.64961	0.149074
H	-5.82269	-3.93242	-1.49545
H	1.044555	0.238159	-1.48084
C	-1.49632	-1.61256	-5.05787
C	-0.69299	-2.73433	-3.19108
N	-1.65332	-1.99958	-3.7929
H	-1.98515	-2.38826	-1.18919
C	-0.65873	0.42121	-5.10336
F	-0.60697	0.6472	-6.45493
H	-0.99568	0.320608	-1.55389
O	-1.81796	0.988682	-3.15455
C	-1.66592	1.159979	-4.37381
C	0.65435	0.168165	-4.52778
O	0.896063	0.030738	-3.33205
H	-0.61562	-1.92528	-5.62102
C	-2.69442	-1.38455	-5.88707
C	-4.97845	-1.06117	-7.5232
C	-2.58335	-1.37439	-7.28173
C	-3.96695	-1.23912	-5.32253
C	-5.08601	-1.07989	-6.12743
C	-3.70787	-1.21725	-8.08385
H	-1.60723	-1.49432	-7.7399
H	-4.06229	-1.25686	-4.24332
H	-6.06458	-0.96752	-5.66851
H	-3.59673	-1.21707	-9.16425
C	-6.18932	-0.85273	-8.38893
H	-6.05705	-1.30085	-9.37645
H	-6.38144	0.215744	-8.53655
H	-7.08476	-1.28583	-7.93607
O	-0.73916	-3.00937	-1.97637
O	0.274868	-3.23005	-3.98126
C	1.244729	-4.22314	-3.51927
C	0.520033	-5.49095	-3.07892
H	1.253933	-6.2742	-2.87029
H	-0.14109	-5.84748	-3.87357

H	-0.06667	-5.31641	-2.17749
C	2.064463	-4.4954	-4.77522
H	2.841212	-5.23379	-4.56186
H	2.546753	-3.58097	-5.12808
H	1.428442	-4.88089	-5.57589
C	2.127666	-3.65273	-2.4162
H	2.918658	-4.36954	-2.17908
H	1.554062	-3.44722	-1.51366
H	2.601095	-2.72682	-2.74848
H	-7.54348	2.34575	0.532272
C	-3.99556	1.200514	3.025007
H	-2.92337	1.03614	2.968538
C	-6.7969	1.661254	3.220082
H	-7.86403	1.843054	3.298541
C	-6.04308	1.327571	4.335478
H	-6.53057	1.245351	5.301145
C	-5.55333	2.064045	-0.14833
H	-5.71614	2.31277	-1.18715
N	-6.59945	2.078509	0.747769
C	-4.65685	1.101878	4.239426
H	-4.09691	0.852844	5.134486
O	1.59929	0.06384	-5.47377
C	2.944271	-0.14651	-5.0238
H	3.232014	0.681824	-4.37063
H	2.983883	-1.06973	-4.43973
C	3.828371	-0.22096	-6.24587
H	3.532884	-1.04937	-6.89381
H	3.773432	0.704442	-6.82325
H	4.865374	-0.37472	-5.9376
C	-2.59675	2.100701	-5.0813
C	-3.86606	2.285429	-4.51972
C	-2.23224	2.873907	-6.19
C	-4.76048	3.198684	-5.06216
H	-4.1339	1.697281	-3.64965
C	-3.12132	3.80564	-6.72005
H	-1.25201	2.761261	-6.63339
C	-4.38855	3.965268	-6.16611
H	-5.74606	3.319843	-4.62389
H	-2.82026	4.407865	-7.57085
H	-5.08106	4.68645	-6.58798

PC-I

Zero-point correction=  
0.968834  
Sum of electronic and thermal Enthalpies=  
-3607.086763  
Sum of electronic and thermal Free Energies=  
-3607.268682

C	-0.32546	0.310026	-0.13817
S	-0.49272	0.572509	1.517888
N	0.874406	0.2953	-0.79567
N	-1.37578	0.117571	-0.96404
C	2.17479	0.367647	-0.29151
C	4.864236	0.493282	0.527128
C	3.147198	0.94085	-1.11887
C	2.559701	-0.15395	0.948201
C	3.890893	-0.07615	1.342816
C	4.475339	0.994882	-0.71036
H	2.857206	1.358363	-2.07676
H	1.819111	-0.60028	1.595886
H	5.895044	0.552636	0.851253
C	5.507338	1.564384	-1.64069
C	4.295667	-0.69124	2.654202
C	-2.75804	0.211797	-0.54501
H	-2.75363	0.148026	0.544343
C	-3.5682	-0.92606	-1.14845
H	-3.47848	-0.89909	-2.23756
H	-4.61203	-0.79279	-0.85789
C	-3.36439	1.580918	-0.92434
H	-3.35197	1.68893	-2.01192
H	-2.68575	2.338605	-0.51698
C	-4.74581	1.796234	-0.39324
C	-5.13633	1.910333	0.989325
C	-6.54012	2.104949	1.015996
H	-6.03034	1.911791	-2.19817
F	5.995603	0.618613	-2.47921
F	6.563149	2.073072	-0.98181
F	5.009649	2.543159	-2.41871
F	5.398609	-0.1121	3.166055
F	4.579974	-2.00652	2.515358
F	3.328123	-0.60129	3.581094
N	-3.12694	-2.29232	-0.74587
C	-3.00337	-2.4594	0.731234
H	-2.2517	-1.74132	1.063928
H	-3.95549	-2.17863	1.191819
C	-3.97675	-3.32833	-1.40822
H	-3.46488	-4.28123	-1.26604

H	-3.92299	-3.10509	-2.47582	C	-2.74192	-2.9252	-7.03574
C	-2.56944	-3.8548	1.144788	C	-4.04419	-1.93771	-5.28755
H	-1.66108	-4.1535	0.617018	C	-5.20924	-2.24451	-5.98518
H	-3.34025	-4.61032	0.976226	C	-3.90756	-3.23626	-7.72971
H	-2.34837	-3.84413	2.214352	H	-1.77907	-3.19324	-7.45973
C	-5.41227	-3.40908	-0.92062	H	-4.10109	-1.43677	-4.32822
H	-5.97008	-2.48653	-1.09476	H	-6.17279	-1.97217	-5.56177
H	-5.48078	-3.65481	0.141983	H	-3.83805	-3.74835	-8.68553
H	-5.91998	-4.20368	-1.47278	C	-6.4241	-3.26915	-7.95383
H	0.81836	0.282121	-1.81059	H	-6.29999	-3.16395	-9.03476
O	0.291885	0.056154	-3.62138	H	-7.26327	-2.64014	-7.64712
C	0.296844	-0.12817	-4.82925	H	-6.70544	-4.30975	-7.75887
C	-1.02702	-0.48883	-5.50395	O	-0.89446	-3.03652	-1.73456
C	-2.07395	0.582579	-5.21026	O	0.26051	-3.33785	-3.66412
O	-2.46736	0.843567	-4.09631	C	1.154025	-4.33877	-3.10244
H	-1.20974	-0.04489	-1.95751	C	0.37014	-5.5713	-2.65953
F	-0.84384	-0.57912	-6.87388	H	1.066354	-6.3683	-2.38327
O	-2.48757	1.190057	-6.31793	H	-0.25618	-5.9358	-3.47878
C	-3.51077	2.188707	-6.14495	H	-0.26287	-5.3449	-1.80215
H	-4.3865	1.708188	-5.70056	C	2.052296	-4.68911	-4.28484
H	-3.14676	2.944572	-5.44413	H	2.795025	-5.43314	-3.98563
C	-3.81242	2.767603	-7.50585	H	2.576972	-3.8017	-4.64706
H	-4.16219	1.992215	-8.1906	H	1.462508	-5.1001	-5.10826
H	-2.92552	3.236655	-7.93745	C	1.982301	-3.75124	-1.96389
H	-4.59274	3.527759	-7.41633	H	2.711256	-4.49029	-1.61875
C	1.573567	-0.05599	-5.59237	H	1.34595	-3.4618	-1.12897
C	4.081884	0.182903	-6.80474	H	2.533649	-2.87221	-2.3083
C	2.734399	-0.4543	-4.91372	N	-6.97601	2.106052	-0.28739
C	1.684201	0.470747	-6.88638	C	-5.89746	1.926022	-1.12583
C	2.936732	0.598741	-7.47921	H	-7.92222	2.264023	-0.58506
C	3.978723	-0.34887	-5.51967	C	-7.25038	2.262296	2.208187
H	2.643192	-0.85828	-3.9123	H	-8.32522	2.412945	2.212909
H	0.802976	0.796344	-7.42177	C	-6.52676	2.22417	3.390848
H	3.015627	1.023295	-8.47419	H	-7.04606	2.345379	4.335643
H	4.867349	-0.66981	-4.98764	C	-5.13127	2.037437	3.388372
H	5.054407	0.276092	-7.2765	H	-4.59716	2.019956	4.332358
H	-2.11992	-2.49761	-1.18682	C	-4.42958	1.881402	2.203091
C	-1.50713	-1.94346	-5.05231	H	-3.35203	1.745378	2.213899
N	-1.66283	-2.08323	-3.64313				
C	-0.79588	-2.80979	-2.98188				
H	-0.71455	-2.57943	-5.46402				
C	-2.78997	-2.27102	-5.80327				
C	-5.16439	-2.90247	-7.21781				

**PC-II**

Zero-point correction=  
0.969779



Sum of electronic and thermal Enthalpies=  
-3607.062329  
Sum of electronic and thermal Free Energies=  
-3607.245188

C	0.524063	0.003836	-0.17391
S	0.622647	-0.44831	1.45029
N	1.599575	0.049983	-1.00218
N	-0.64086	0.306619	-0.80475
C	2.92344	-0.27462	-0.64845
C	5.591491	-0.90233	-0.0637
C	3.613421	-1.20542	-1.42017
C	3.572583	0.351033	0.418845
C	4.894009	0.029706	0.703553
C	4.94185	-1.511	-1.12951
H	3.106842	-1.69986	-2.24024
H	3.044249	1.084646	1.012027
H	6.621877	-1.1436	0.164754
C	5.678835	-2.47844	-2.01039
C	5.578024	0.66828	1.880525
C	-1.88594	0.511743	-0.09789
C	-3.04362	-0.25351	-0.73956
H	-3.33942	0.187275	-1.69484
H	-3.89887	-0.2272	-0.06424
C	-2.22612	2.012769	0.002371
H	-2.28747	2.438026	-1.00553
H	-1.37038	2.489994	0.493019
C	-3.48708	2.303412	0.752093
C	-3.77413	1.996993	2.130745
C	-5.08943	2.456596	2.395134
H	-4.78063	3.326896	-0.73115
F	4.87973	-3.47806	-2.43788
F	6.725401	-3.0435	-1.3847
F	6.163256	-1.87657	-3.1183
F	6.895258	0.845877	1.657777
F	5.473211	-0.09154	2.990637
F	5.057406	1.870985	2.178796
N	-2.73351	-1.68833	-1.05369
C	-2.11094	-2.43795	0.084591
H	-1.23962	-1.87058	0.415214
H	-2.8321	-2.43436	0.904639
C	-3.93595	-2.38631	-1.63546
H	-3.56055	-3.29321	-2.11137
H	-4.30094	-1.73337	-2.42679
C	-1.69142	-3.84413	-0.29773

H	-1.04002	-3.83955	-1.176
H	-2.53428	-4.51128	-0.49035
H	-1.11797	-4.26539	0.530369
C	-5.02514	-2.71173	-0.63201
H	-5.39999	-1.82646	-0.11434
H	-4.71335	-3.44495	0.114691
H	-5.86591	-3.14249	-1.1804
H	-2.05596	-1.64176	-1.83378
O	-1.47281	-1.43321	-3.58474
O	-4.15955	-0.34606	-3.97257
C	-3.6799	-0.34058	-5.09701
C	-1.29148	-0.8869	-4.66184
C	-2.241	0.155467	-5.25859
F	-1.94842	0.321372	-6.5938
O	-0.28556	-1.15481	-5.46615
C	0.72242	-2.05548	-4.96666
H	0.242888	-2.99999	-4.69588
H	1.141262	-1.60714	-4.06287
C	1.754874	-2.22812	-6.05317
H	1.31186	-2.66657	-6.95007
H	2.548355	-2.89248	-5.70137
H	2.200202	-1.26815	-6.31986
C	-4.4936	-0.78166	-6.26091
C	-6.17819	-1.70243	-8.29083
C	-3.9544	-1.38864	-7.40281
C	-5.88419	-0.64366	-6.14711
C	-6.7205	-1.08881	-7.16151
C	-4.79874	-1.85838	-8.40414
H	-2.88343	-1.49894	-7.50964
H	-6.28826	-0.1706	-5.25948
H	-7.79393	-0.9588	-7.07462
H	-4.37565	-2.33759	-9.28036
H	-6.83065	-2.05534	-9.08277
H	-1.71887	0.135129	0.913864
H	1.413199	0.359149	-1.96859
H	-0.54686	0.658447	-1.77153
C	-2.04236	1.570708	-4.54155
O	0.404428	1.06666	-3.28213
N	-0.81597	2.163958	-4.93234
H	-2.12478	1.337342	-3.46801
C	-3.18314	2.501773	-4.92998
C	-5.26649	4.268169	-5.67933
C	-4.2908	2.696143	-4.10624

C	-3.12138	3.214152	-6.13189
C	-4.1492	4.073073	-6.50049
C	-5.31618	3.567524	-4.47393
H	-4.36203	2.154038	-3.16833
H	-2.23928	3.099554	-6.75068
H	-4.07863	4.614311	-7.44035
H	-6.16741	3.70427	-3.81158
C	0.265174	1.869407	-4.26897
O	1.342527	2.537541	-4.77993
C	2.611558	2.671942	-4.11898
C	3.371167	1.347112	-4.13741
H	3.52611	1.022809	-5.17001
H	2.813837	0.569539	-3.6175
H	4.349746	1.45651	-3.66144
C	2.452021	3.242849	-2.7105
H	3.435161	3.465318	-2.28551
H	1.934292	2.552987	-2.04528
H	1.880296	4.173857	-2.75313
C	3.344517	3.687118	-4.9944
H	3.409926	3.322535	-6.02229
H	4.356495	3.857869	-4.61652
H	2.806906	4.638057	-5.00439
H	-6.45988	3.464304	1.127407
N	-5.56888	3.01235	1.233415
C	-4.60472	2.923663	0.255903
C	-5.69047	2.323734	3.648549
H	-6.69709	2.683678	3.835459
C	-4.94788	1.719256	4.65188
H	-5.38302	1.602949	5.638734
C	-3.63764	1.262525	4.415888
H	-3.08117	0.805347	5.227005
C	-3.04395	1.396019	3.170189
H	-2.02603	1.053015	3.010598
C	-6.36245	5.216928	-6.08218
H	-6.75268	4.974706	-7.07538
H	-7.1967	5.185539	-5.37743
H	-5.99841	6.248734	-6.12142

### PC-III

Zero-point correction=  
0.969162  
Sum of electronic and thermal Enthalpies=  
-3607.077621

Sum of electronic and thermal Free Energies=  
-3607.258676

C	-0.88406	0.320331	-0.20695
S	-1.26743	0.931766	1.320348
N	0.377718	0.328404	-0.74051
N	-1.80049	-0.2077	-1.03742
C	1.583969	0.730357	-0.15681
C	4.096824	1.503459	0.851413
C	2.553505	1.281284	-1.00026
C	1.886569	0.553369	1.19832
C	3.127987	0.948731	1.683862
C	3.794398	1.657092	-0.49642
H	2.330466	1.410381	-2.05231
H	1.149554	0.125073	1.861815
H	5.056465	1.812085	1.24499
C	4.82302	2.200482	-1.44453
C	3.460192	0.701996	3.129089
C	-3.20549	-0.3045	-0.71754
H	-3.29736	-0.19707	0.365899
C	-3.73548	-1.6633	-1.16205
H	-3.69818	-1.73843	-2.25166
H	-4.7693	-1.76375	-0.82697
C	-4.01288	0.836605	-1.36964
H	-3.87978	0.796989	-2.45467
H	-3.54869	1.769358	-1.03145
C	-5.46601	0.825407	-1.01646
C	-6.04227	1.022534	0.289723
C	-7.44918	0.920505	0.149478
H	-6.51186	0.45713	-2.93823
F	5.441786	1.210983	-2.13194
F	5.787326	2.894132	-0.81589
F	4.280094	3.01908	-2.3689
F	4.336799	1.606789	3.607248
F	4.028865	-0.51342	3.30608
F	2.375399	0.738569	3.919716
N	-2.94416	-2.82005	-0.64932
C	-2.78746	-2.79811	0.835997
H	-2.28071	-1.86251	1.078994
H	-3.78454	-2.7597	1.284689
C	-3.47908	-4.10746	-1.18794
H	-2.72839	-4.86762	-0.96915
H	-3.49501	-3.98713	-2.27354
C	-1.97453	-3.96345	1.370851

H	-1.0157	-4.04249	0.853913
H	-2.49706	-4.91988	1.294266
H	-1.77161	-3.78473	2.428947
C	-4.84109	-4.52309	-0.66188
H	-5.62541	-3.80398	-0.90643
H	-4.84013	-4.67689	0.419633
H	-5.11518	-5.47351	-1.12587
H	0.460935	0.055278	-1.71832
O	1.322179	-0.30415	-3.50211
C	1.150116	-0.45749	-4.70586
C	-0.29665	-0.28044	-5.16156
C	-0.786	1.082236	-4.60276
O	-1.87295	1.274621	-4.11497
H	-1.52354	-0.63609	-1.94949
F	-0.41864	-0.10658	-6.54353
O	0.122236	2.026374	-4.8221
C	-0.24359	3.372023	-4.44468
H	-1.16506	3.635948	-4.96963
H	-0.45069	3.382717	-3.37164
C	0.905802	4.276655	-4.81477
H	1.100674	4.243539	-5.88892
H	1.818283	3.992011	-4.28688
H	0.66033	5.305938	-4.5415
C	2.306875	-0.73338	-5.59831
C	4.627781	-1.208	-7.09416
C	3.569125	-0.74297	-4.98185
C	2.226222	-0.95858	-6.98085
C	3.382831	-1.19781	-7.71738
C	4.718937	-0.97697	-5.72118
H	3.627282	-0.55909	-3.91585
H	1.271011	-0.95015	-7.48438
H	3.307247	-1.37294	-8.7852
H	5.685442	-0.97548	-5.22907
H	5.525572	-1.39074	-7.6756
H	-1.9256	-2.78527	-1.08031
C	-1.30606	-1.40634	-4.73909
N	-1.25092	-1.77837	-3.34484
C	-0.46091	-2.70657	-2.84673
O	-0.58377	-3.09612	-1.64361
O	0.504819	-3.24549	-3.62488
C	1.411523	-4.28471	-3.14124
C	2.273036	-3.75121	-2.0007
H	3.029227	-4.49609	-1.73608

H	1.668791	-3.53153	-1.12159
H	2.786825	-2.83838	-2.31177
C	0.635872	-5.53798	-2.7451
H	1.339016	-6.35367	-2.55252
H	-0.02604	-5.84434	-3.55996
H	0.042616	-5.36614	-1.84809
C	2.282141	-4.58284	-4.35777
H	3.039409	-5.32616	-4.09555
H	2.791921	-3.67954	-4.70088
H	1.680226	-4.98026	-5.17811
N	-7.70917	0.671796	-1.17686
C	-6.51933	0.622964	-1.87034
H	-8.62279	0.600626	-1.58818
C	-8.32036	1.070019	1.230889
H	-9.39593	0.991954	1.108161
C	-7.75772	1.329634	2.47188
H	-8.4055	1.454123	3.333223
C	-6.36372	1.442242	2.633489
H	-5.95939	1.655126	3.617313
C	-5.50188	1.292904	1.557969
H	-4.42872	1.393761	1.692565
C	-1.45273	-2.53607	-5.75338
C	-0.40552	-3.21588	-6.37737
C	-2.75487	-2.92318	-6.08284
C	-0.65331	-4.23638	-7.2899
H	0.619108	-2.95662	-6.14928
C	-3.0053	-3.95509	-6.98344
H	-3.59329	-2.39841	-5.63189
C	-1.95597	-4.63276	-7.60691
H	0.186565	-4.73596	-7.766
H	-4.0319	-4.22416	-7.21673
C	-2.21324	-5.75824	-8.57108
H	-1.48923	-5.75554	-9.39003
H	-2.13588	-6.73054	-8.07222
H	-3.21382	-5.6911	-9.00475
H	-2.24763	-0.85342	-4.82398

#### PC-IV

Zero-point correction=  
 0.969022  
 Sum of electronic and thermal Enthalpies=  
 -3607.088463  
 Sum of electronic and thermal Free Energies=  
 -3607.272797

C	-0.84261	0.351304	-0.4598	H	-1.37978	-3.66101	2.451192
S	-0.97874	0.849427	1.149731	C	-4.88336	-4.45308	-0.08973
N	0.312639	0.431508	-1.18309	H	-5.67359	-3.71426	-0.23686
N	-1.86232	-0.2008	-1.14649	H	-4.70909	-4.56175	0.983027
C	1.577812	0.870662	-0.77109	H	-5.26066	-5.41008	-0.45795
C	4.184559	1.705482	-0.12385	H	0.299918	0.030218	-2.11936
C	2.689263	0.19286	-1.27822	O	1.050523	-0.30534	-3.92798
C	1.776802	1.983398	0.052668	C	0.689079	-0.60219	-5.04858
C	3.071597	2.378685	0.37285	C	-0.77186	-0.52902	-5.48126
C	3.975736	0.614972	-0.96053	C	-1.34348	0.839321	-5.03392
H	2.538196	-0.66097	-1.92606	O	-2.11136	0.893597	-4.09527
H	0.926773	2.529558	0.434846	H	-1.71009	-0.58241	-2.09642
H	5.186078	2.027974	0.129336	F	-0.84071	-0.57911	-6.87032
C	5.144318	-0.09273	-1.58035	H	-2.01958	-2.83226	-1.04838
C	3.270504	3.540073	1.306188	C	-1.51871	-1.80768	-4.96316
C	-3.2042	-0.30262	-0.62087	N	-1.50294	-1.94456	-3.52724
H	-3.12635	-0.16811	0.460117	C	-0.76823	-2.89469	-2.99984
C	-3.79714	-1.66889	-0.93541	H	-0.94674	-2.60913	-5.44483
H	-3.9046	-1.79823	-2.01515	C	-2.92189	-1.89676	-5.54718
H	-4.78292	-1.73232	-0.47093	C	-5.51381	-2.16411	-6.67011
C	-4.10748	0.827884	-1.15819	C	-3.12973	-2.61901	-6.72359
H	-4.16017	0.766892	-2.24903	C	-4.03344	-1.30899	-4.93911
H	-3.59139	1.765581	-0.92518	C	-5.3028	-1.4395	-5.49215
C	-5.48103	0.834119	-0.56641	C	-4.4015	-2.74988	-7.27669
C	-5.82816	1.069893	0.812502	H	-2.28322	-3.08483	-7.21948
C	-7.23839	0.969038	0.914803	H	-3.88725	-0.73068	-4.03653
H	-6.83701	0.41233	-2.27156	H	-6.14866	-0.96145	-5.00428
F	4.929593	-1.41831	-1.70709	H	-4.52822	-3.31692	-8.19473
F	6.275936	0.061783	-0.87123	C	-6.89416	-2.32324	-7.24657
F	5.404138	0.367968	-2.828	H	-6.85568	-2.57426	-8.30908
F	4.442452	4.169426	1.085579	H	-7.47958	-1.40631	-7.13762
F	3.281749	3.14752	2.597855	H	-7.44466	-3.1237	-6.74006
F	2.29704	4.46093	1.188866	O	-0.79163	-3.18742	-1.76318
N	-2.96776	-2.8177	-0.47085	O	0.071782	-3.59038	-3.8209
C	-2.59557	-2.72399	0.97295	C	0.807603	-4.77029	-3.39711
H	-2.03414	-1.79506	1.090338	C	-0.14282	-5.85301	-2.89246
H	-3.51477	-2.63096	1.55916	H	0.411962	-6.78208	-2.73356
C	-3.61375	-4.11174	-0.84874	H	-0.92414	-6.04611	-3.63311
H	-2.85837	-4.88626	-0.71105	H	-0.60722	-5.5562	-1.95298
H	-3.80453	-4.04462	-1.92232	C	1.476998	-5.23224	-4.68802
C	-1.73979	-3.88594	1.445011	H	2.085708	-6.12042	-4.50043
H	-0.86873	-4.01551	0.799106	H	2.12535	-4.44879	-5.08777
H	-2.28725	-4.83022	1.495162	H	0.727904	-5.47794	-5.44504

C	1.860265	-4.40389	-2.35541
H	2.468107	-5.28209	-2.11855
H	1.391196	-4.03849	-1.44281
H	2.526902	-3.62861	-2.74256
N	-7.71855	0.684458	-0.34102
C	-6.66332	0.611164	-1.22372
H	-8.68837	0.601735	-0.58918
C	-7.91473	1.150621	2.12322
H	-8.99546	1.072651	2.186011
C	-7.15087	1.441522	3.243821
H	-7.64392	1.591157	4.198557
C	-5.74969	1.552774	3.164669
H	-5.18516	1.7892	4.060258
C	-5.08149	1.37138	1.963759
H	-4.00071	1.468368	1.914431
O	1.495861	-1.02718	-6.00636
C	2.895463	-1.13371	-5.65937
H	2.992812	-1.87363	-4.86161
H	3.229127	-0.16971	-5.26877
C	3.643984	-1.53717	-6.90538
H	3.532153	-0.78739	-7.69166
H	4.707372	-1.63372	-6.67293
H	3.286218	-2.49557	-7.28775
C	-0.91423	2.079908	-5.74367
C	0.060732	2.112546	-6.7495
C	-1.50556	3.280786	-5.32624
C	0.436597	3.325708	-7.31833
H	0.520622	1.198592	-7.10221
C	-1.13474	4.48747	-5.90185
H	-2.25157	3.24245	-4.54083
C	-0.15966	4.512314	-6.89945
H	1.193656	3.342078	-8.09493
H	-1.59947	5.410056	-5.57116
H	0.13437	5.455404	-7.34831

## Product

Zero-point correction=  
0.486028  
Sum of electronic and thermal Enthalpies=  
-1461.396588  
Sum of electronic and thermal Free Energies=  
-1461.496200

C	-0.59506	0.3036	-0.32813
C	-0.92905	-0.91017	0.569336

C	-1.59407	1.453142	-0.12343
F	-0.72853	-0.12762	-1.64177
O	-0.12751	-1.26978	1.413404
O	-1.92715	2.205924	-1.00382
C	-2.21985	-1.6251	0.378138
C	-4.62453	-3.03445	0.179426
C	-3.16578	-1.27343	-0.59429
C	-2.49118	-2.6927	1.245184
C	-3.68533	-3.39278	1.147102
C	-4.36224	-1.977	-0.68844
H	-2.97097	-0.46924	-1.29283
H	-1.74977	-2.95247	1.992023
H	-3.88679	-4.21692	1.822912
H	-5.08771	-1.70113	-1.44589
H	-5.55844	-3.58125	0.100686
O	-2.00084	1.505255	1.14028
C	-2.8609	2.609546	1.494295
H	-3.76456	2.549751	0.882478
H	-2.34088	3.537563	1.245276
C	-3.15762	2.498366	2.969351
H	-3.66476	1.558476	3.198307
H	-3.80834	3.32233	3.273002
H	-2.23783	2.550665	3.555291
C	0.850374	0.856595	-0.19383
H	0.9769	1.43843	-1.11166
C	1.07642	1.807084	0.972514
C	1.526658	3.660918	3.06447
C	1.30437	1.368533	2.27973
C	1.080696	3.181364	0.7267
C	1.296673	4.093637	1.757442
C	1.525763	2.282005	3.303868
H	1.29363	0.307771	2.501296
H	0.922445	3.546208	-0.28411
H	1.299383	5.157077	1.535569
H	1.700043	1.915754	4.311957
C	1.802429	4.638499	4.173675
H	2.878585	4.729327	4.356089
H	1.340418	4.319694	5.111743
H	1.425826	5.634802	3.931042
N	1.812416	-0.20947	-0.28876
H	1.819306	-0.93321	0.41181
C	2.831343	-0.15823	-1.19147
O	2.971477	0.717169	-2.0261

O	3.637688	-1.22169	-1.01251
C	4.81197	-1.423	-1.85833
C	5.792072	-0.26825	-1.67962
H	6.038769	-0.14038	-0.62207
H	5.37723	0.663922	-2.06223
H	6.716717	-0.4904	-2.21967
C	5.400693	-2.71602	-1.30735
H	5.666304	-2.60018	-0.25372
H	6.301541	-2.98319	-1.8653
H	4.682032	-3.53445	-1.39502
C	4.388846	-1.60242	-3.31242
H	5.26212	-1.8708	-3.91358
H	3.955045	-0.68634	-3.71237
H	3.656192	-2.40946	-3.3978