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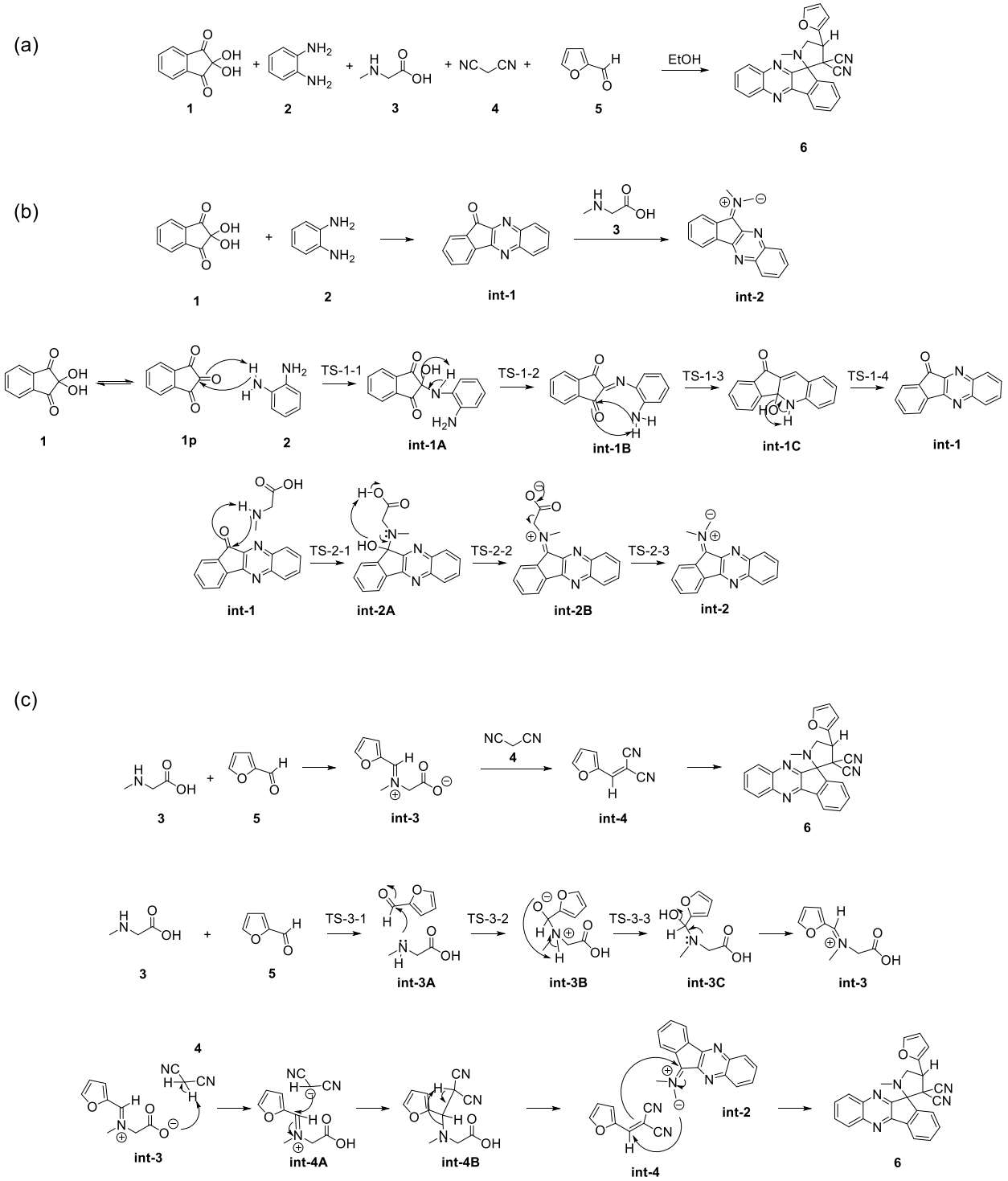
1. General reaction information



Scheme S1. Stepwise reaction pathway of the five-component reaction to construct spiro-pyrroidine **6**, including a) the formation of **int-1** and **int-2**, and b) the formation of **int-3**, **int-4**, and the product **6**.

2. Experimental details

2.1 Chemicals and materials

Ethanol (HPLC grade) was purchased from Acros Organics; Ninhydrin (99%) and o-Phenylenediamine (98%) were obtained from Alfa Aesar; Sarcosine (98.0%) was purchased from Tokyo Chemical Industry (TCI); Malononitrile (99%) and 2-furaldehyde (99%) were purchased from Acros Organics.

Fused silica capillary of 50 μm ID and 150 μm OD was obtained from BGB Analytik. Stainless steel tubing and T-junction purchased from Swagelok were used for building the nebulizer. PEEK unions purchased from IDEX Health & Scientific were employed to connect capillaries and syringe needle.

Borosilicate glass capillaries (1.5 mm OD and 0.86 mm ID) obtained from the World Precision Instruments (Sarasoto, FL) were used for manufacturing nanoESI tips using P-1000 micropipette puller (Shutter Instrument, Novato, CA). A platinum wire was inserted into the tip to provide efficient electrical contact with the solution and to initiate the electrospray.

2.2 Device for droplet reaction

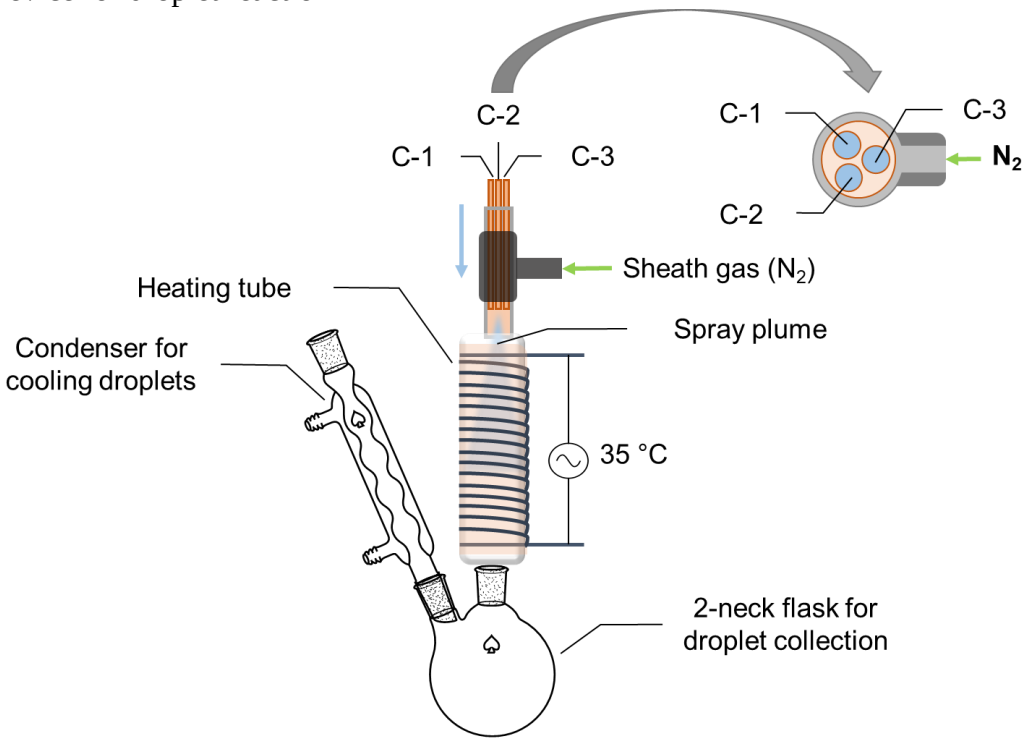


Figure S1. The heatable mix-at-spray setup for MCRs, with the front view and the top view of the device, where the blue arrow indicates the liquid flow, and the green arrows show the gas flow. C-1, C-2, and C-3 stand for the three fused silica capillaries. Reagent solutions were pumped into the capillaries at a flow rate of 10 μL/min. A heating power of 18 W was applied to the glass heating tube and the spray plume going through the heating tube was measured as 35 ºC by an IR thermometer.

2.3 Instrument

Low-resolution mass spectra were obtained with an LTQ XL mass spectrometer (Thermo Fisher Scientific, San Jose, CA). Instrumental conditions used for the positive-mode mass spectrometry is specified as: electrospray voltage: 1.0-2.0 kV; heated-capillary temperature: 275 °C; heated-capillary voltage: 44 V; tube lens voltage: 85 V.

High-resolution nanoESI mass spectrometric analysis was conducted on an Orbitrap Velos Pro (Thermo Fisher Scientific, San Jose, CA). The following MS parameters were used for data acquisitions. Samples were ionized with the applied spray voltage from 1.0-2.0 kV. S-lens RF level was set to be 67.9%, and capillary temperature was set at 200 °C. Full MS scans were acquired at m/z 50-750 with resolving power of 60,000. Maximum injection time of 500 ms and 1 micro-scan were used for full MS scans. MS/MS acquisitions were performed upon CID. The CID energy used for fragmentation was around 30 manufactural units.

The LC-MS analysis was conducted on a Q Exactive Focus (Thermo Fisher Scientific, San Jose, CA). The following MS parameters were used for data acquisitions. Injection volume: 10 μL. Acclaim LC parameters are following: C-18, 3 μm, 120 Å, 2.1 x 150 mm; Column Temperature: 25°C. Gradient elution procedure: 0-3 min: 20% acetonitrile; 3-5 min: 80% acetonitrile, 5-8 min maintain; 8-10 min: 80% acetonitrile + 2% THF, 10-20 min maintain. Samples were ionized with the applied spray voltage from 3.5 kV. S-lens RF level was set to be 70 %, and capillary temperature was set at 275 °C. Full MS scans were acquired at m/z 100-500 with resolving power of 70,000.

A syringe pump (model: Fusion 400, Chemyx Inc.) was used for supplying liquid flow in the droplet reactions. The temperature of heating tube was monitored via Surpeer IR5D infrared thermometer.

2.4 Heating power impact on the microdroplet/thin film reaction

2.4.1 Reagent mixing experiment

Reagents **1**, **2**, and **3** were introduced into the capillaries C-1, C-2, C-3 as shown in Figure S1, respectively. Different power was applied on the glass heating tube to justify the necessity of external heating. The deposition was rinsed off with EtOH-THF solvent and analyzed via nanoESI-MS. As the Figure S2 indicates, a considerable amount of organic salt was generated in each droplet reaction batch, which overwhelmingly suppressed the signals from the reactant and intermediate species. LC-MS was employed to separate the reaction intermediates and product from the reaction matrix (Figure S3). The plume temperature at 0 W, 18 W, and 36 W were measured to be 21 °C, 35 °C, and 55 °C, respectively. Both the nanoESI-MS and LC-MS analysis results indicate that **int-2** formation requires external heating, and the higher temperature can enhance the reaction efficiency. As Figure S3 suggests, with the assistance of 18 W heating, **2** can be depleted within 20 min of reaction time, and the transition from **int-1** to **int-2** was achieved in higher

temperature. When the heating power raises to 36 W, the conversion ratio for **int-2** is further enhanced.

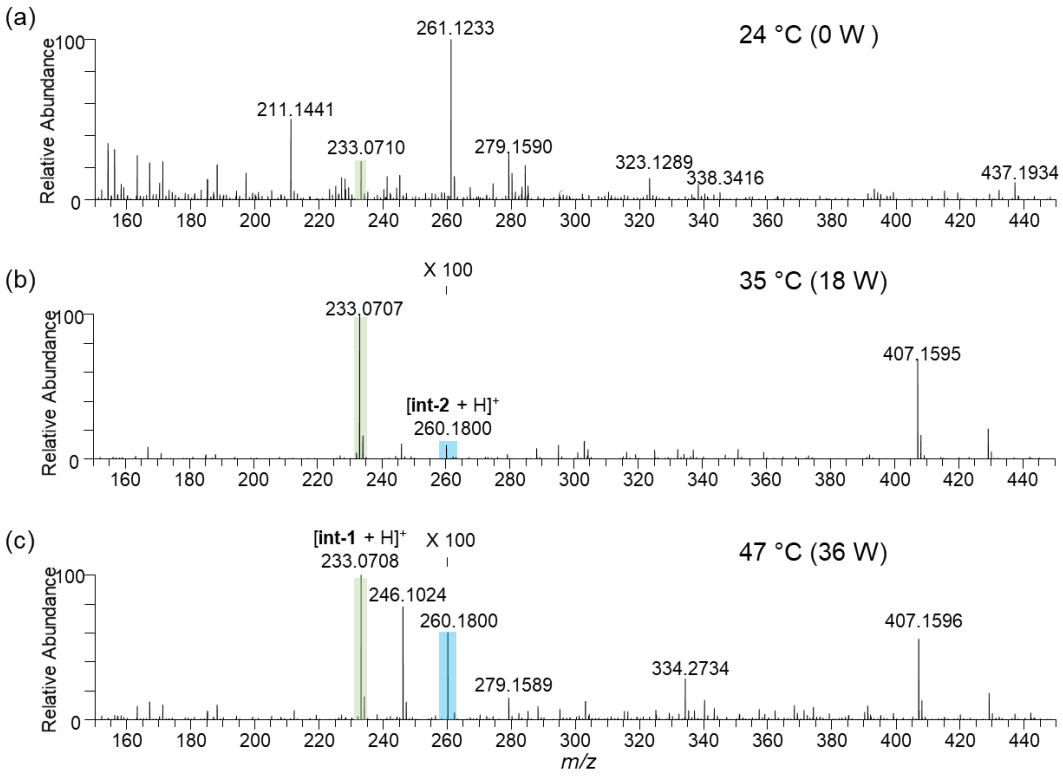


Figure S2. Mass spectra of 20-min droplet reactions among **1**, **2**, and **3** at different heating power including 0 W (a), 18 W (b), 36 W (c), respectively.

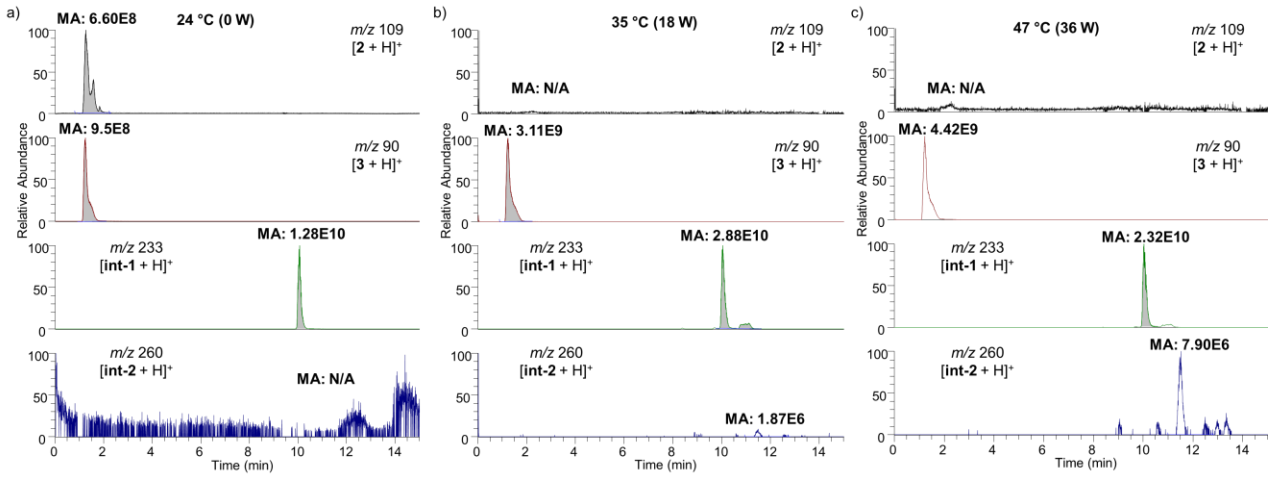


Figure S3. LC-MS of 20-min droplet reactions among **1**, **2**, and **3** at different heating power including 0 W (a), 18 W (b), 36 W (c), respectively. The peak area values were labeled as MA.

2.4.2 Five-component microdroplet/thin film reaction with different heating powers

In seeking optimal heating power for the five-component droplet reaction, we compared the reaction at different heating power to achieve different plume temperature. As Figure S4 demonstrate, the product **6** can still be generated even without external heating provided, while the reaction efficiency could be enhanced in higher plume temperature and longer deposition time. It is also noted that the relative abundance of **int-2** in reaction mixture reached the maximum level with 18 W heating power applied. By comparing Figure S4c and Figure S4d, it can be concluded that the product **6** has can be afforded with a higher efficiency when moderate heating power is applied. With the higher plume temperature, the intrinsic reaction rate and desolvation effect are both enhanced, while the latter can result in shorter microdroplet/thin film lifetime. The optimal reaction efficiency can be achieved by balancing these two factors with the mild heating power applied.

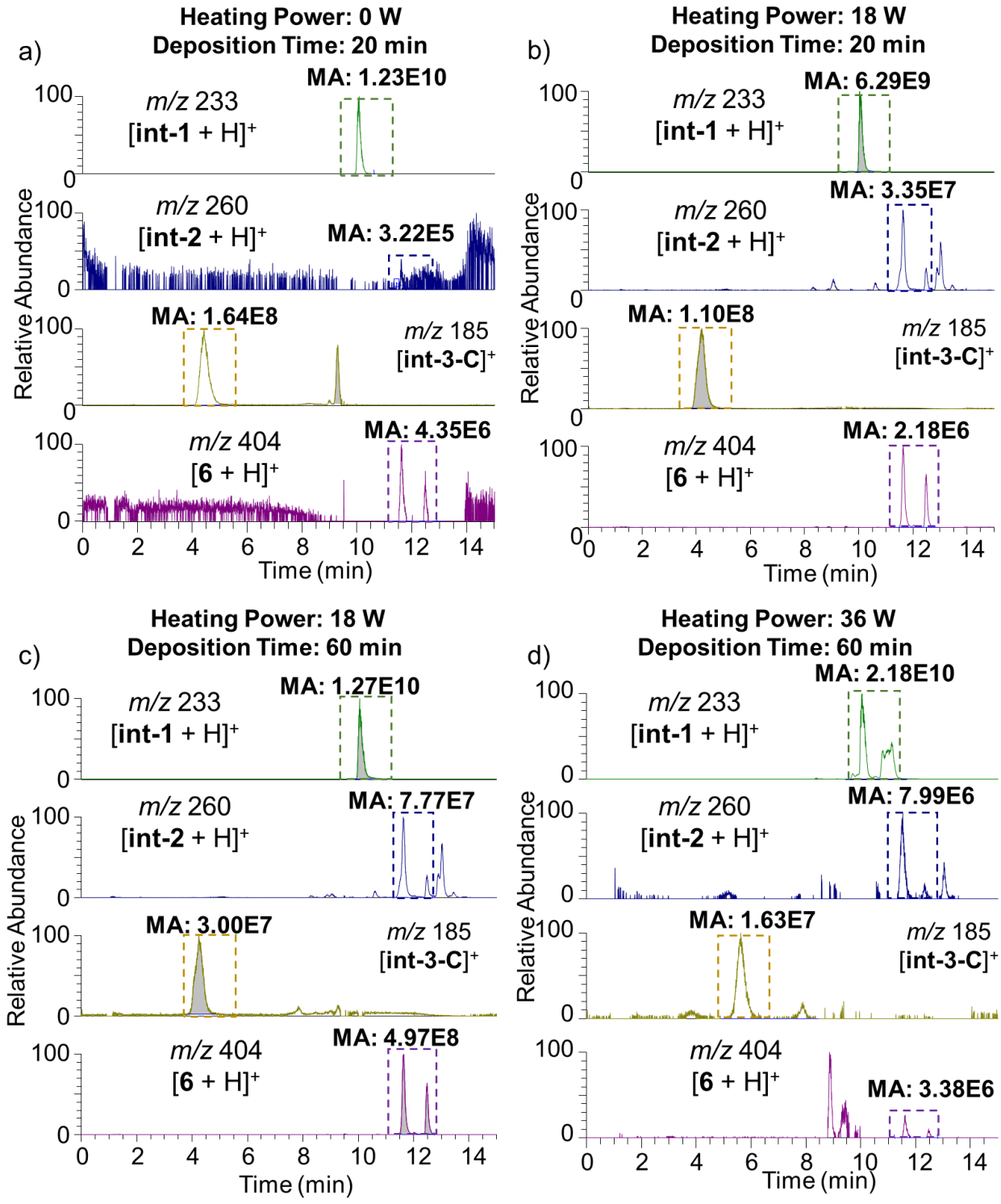


Figure S4. The LC-MS of reaction samples collected with different heating power at 20 min (a and b) and 60 min (c and d) deposition time. High-resolution MS was used to each species from the background signals, and the corresponding integration region was marked with dashed squares. The peak area values were labeled as MA.

2.5 Intermediate identification via collision-induced dissociation (CID) MS

The structures of **int-1**, **int-2**, and **int-3C** were confirmed via tandem MS in the high-resolution MS analysis of the droplet reaction sample.

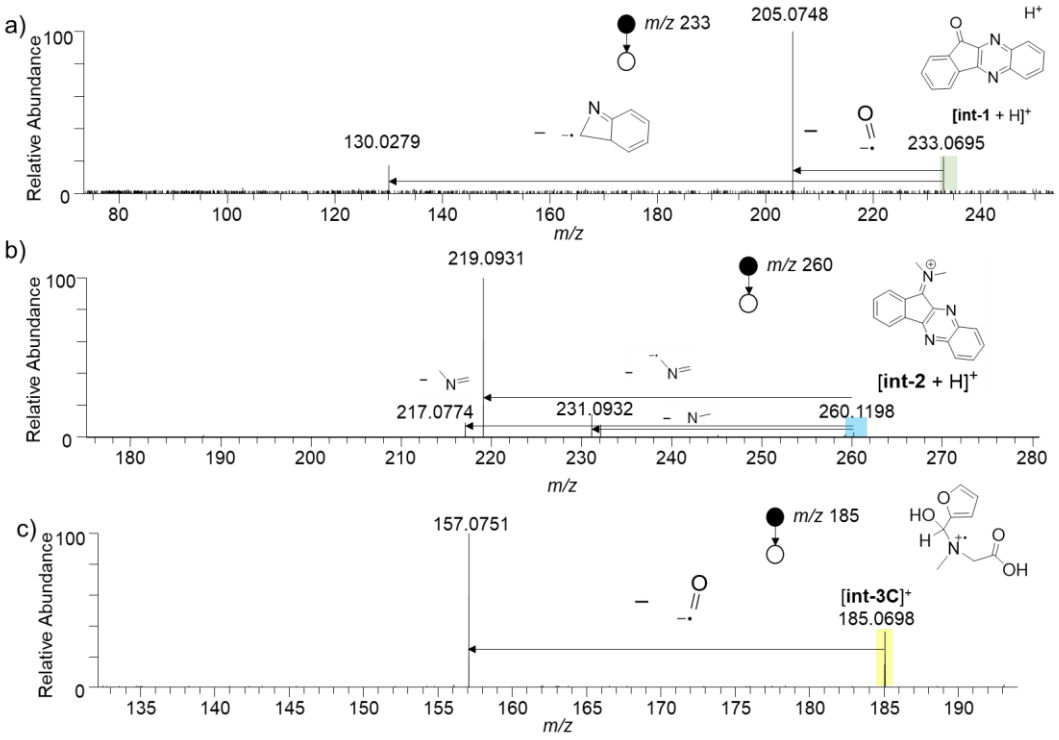


Figure S5. MS/MS of intermediates including **int-1** (a), **int-2** (b) and **int-3C** (c), which were captured in the droplet reaction monitoring.

2.6 Bulk-phase reaction monitoring

Reagent **1**, **2**, **4** and **5** were prepared in 100 μL ethanol to achieve the concentrations of 0.1 M . Reagent **3** was dissolved in ethanol to obtain the concentration of 0.12 M. They were readily mixed and heated to 35.0 °C. All the reaction mixture was dissolved in 2.00 mL chloroform at the designated time. 50 μL of the resulting clear solution was diluted in 400 μL ethanol, followed by adding 50 μL of internal standards (Girard's Reagent T and 2-phenylpyridine) . The obtained sample was then analyzed via liquid chromatography–mass spectrometry (LC-MS). The relative yield ratio in Figure 3a was plotted based on the integrated signal intensity of each intermediate which is calibrated with the corresponding internal standard.

2.7 Microdroplet/thin film reaction monitoring

We prepared the same concentrations of the reagents for both microdroplet reaction and bulk-phase reaction. Reagents **1** and **2** were prepared in ethanol to achieve 33.3 mM. Reagents **3**, **4**, and **5** were prepared in ethanol to obtain the concentrations of 0.12 M, 0.1 M, 0.1 M, respectively. They were mixed readily in identical volumes. The reagents were introduced into the capillaries at 10 μL/min via a syringe pump. The glass chamber was wrapped with Ni-Cr wires where 18 W heating power was applied. Microdroplets were

generated by supplying the nitrogen gas at 120 psi. After the designated spraying time, the liquid flow as well as heating were ceased, and the system was dried and cooled to room temperature by continuously providing the nitrogen flow. The heated mixing-at-spray device was rinsed with EtOH-$CHCl_3$-THF solvent (2:1:1, V:V:V) to collect the droplet reaction product and all the rinse-off solution was then combined and diluted to volume V_0. An aliquot of 50 μL of the resulting solution was combined with internal standards for LC-MS quantitative analysis.

2.8 Confirmation of the product structure in microdroplets

We performed the nuclear magnetic resonance (NMR) analysis of the synthesized product **6** and compared the tandem mass spectra of the standard compound with the product from the microdroplet reaction. The ^{1}H-NMR spectrum was recorded at 400 MHz by using a Bruker Avance 400M Spectrometer.

^{1}H NMR (DMSO-d^6, 400 MHz): δ = 7.80–8.19 (m, 9 H, ArH, furan-H4), 6.88 (d, J = 3.31 Hz, 1 H, furan-H2), 6.60 (dd, J = 3.3, 1.9 Hz, 1 H, furan-H3), 5.64–5.67 (dd, J = 10.4, 7.0 Hz, 1 H, CH), 4.01–4.04 (dd, J = 7.0, 9.6 Hz, 1 H, NCH_2), 3.91–3.95 (dd, J = 10.4, 9.6 Hz, 1 H, NCH_2), 2.06 (s, 3 H, NCH_3) ppm.

Chemical shifts were reported in parts per million (δ) relative to tetramethylsilane (TMS) in Figure S6a. All chemical shifts are in full agreement with the literature (M. Li, F.-M. Gong, L.-R. Wen and Z.-R. Li, *Eur. J. Org. Chem.*, 2011, **2011**, 3482-3490). The product **6** from the microdroplet reaction and standard bulk synthesis show the same fragment pattern as demonstrated in Figure S6b and d. The results confirm that the product structures in microdroplet reaction are the same with compound **6** in bulk-phase synthesis.

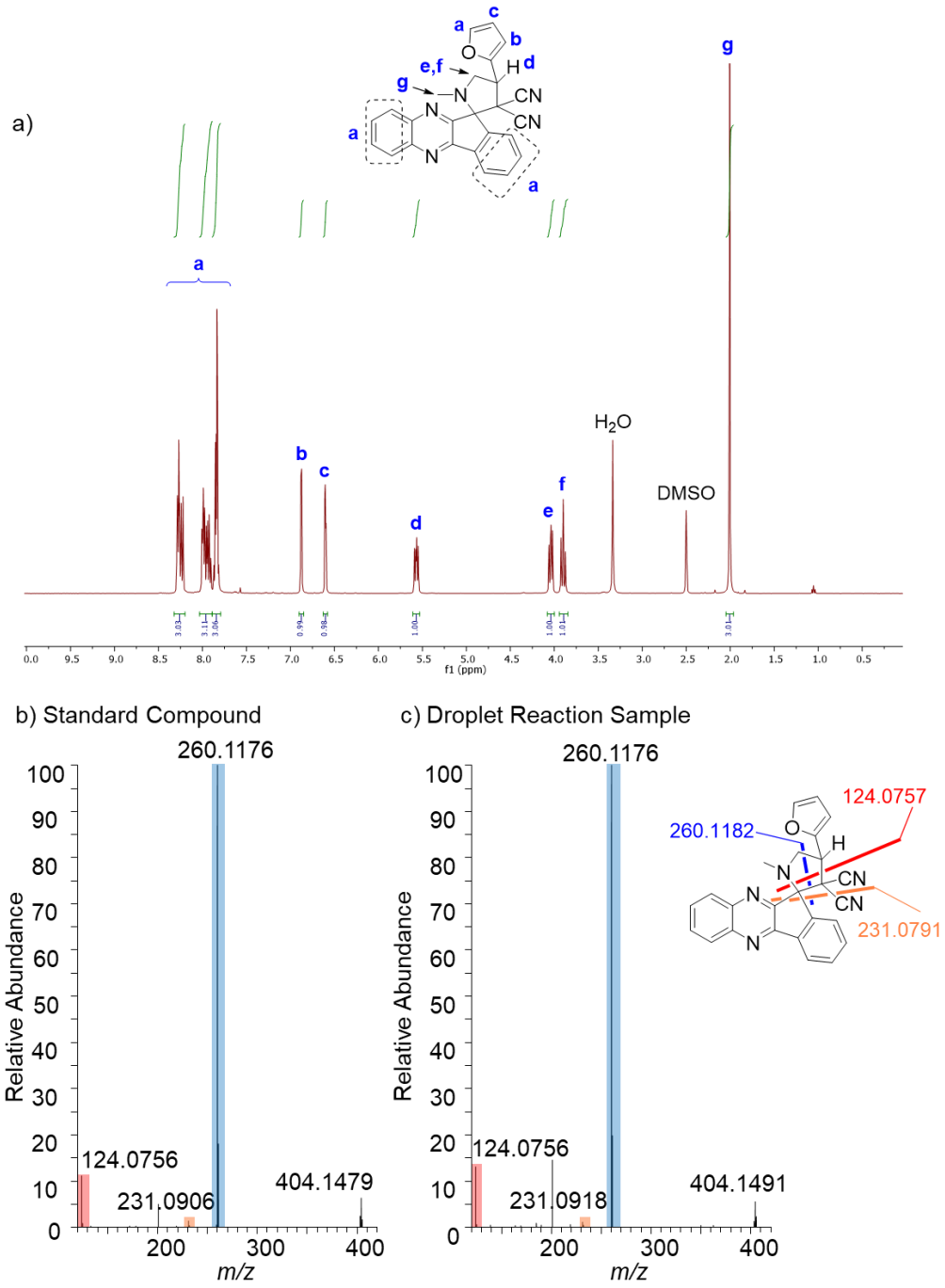


Figure S6. Characterization and structural confirmation of product **6** collected via ^{1}H-NMR (a) and high-resolution MS/MS of the standard compound synthesized in bulk-phase (b) and the droplet reaction sample (c).

3. DFT calculation details

3.1 General information

Benchmark was carried out among Hartree-Fock (HF), M06-2X, and B3LYP. The simulation efficacy was evaluated based on the geometry optimization output structures, with reference to the reported crystal structures (CCDC-793842 (**6g**) and -92227 (**7j**), geometries available on The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif).

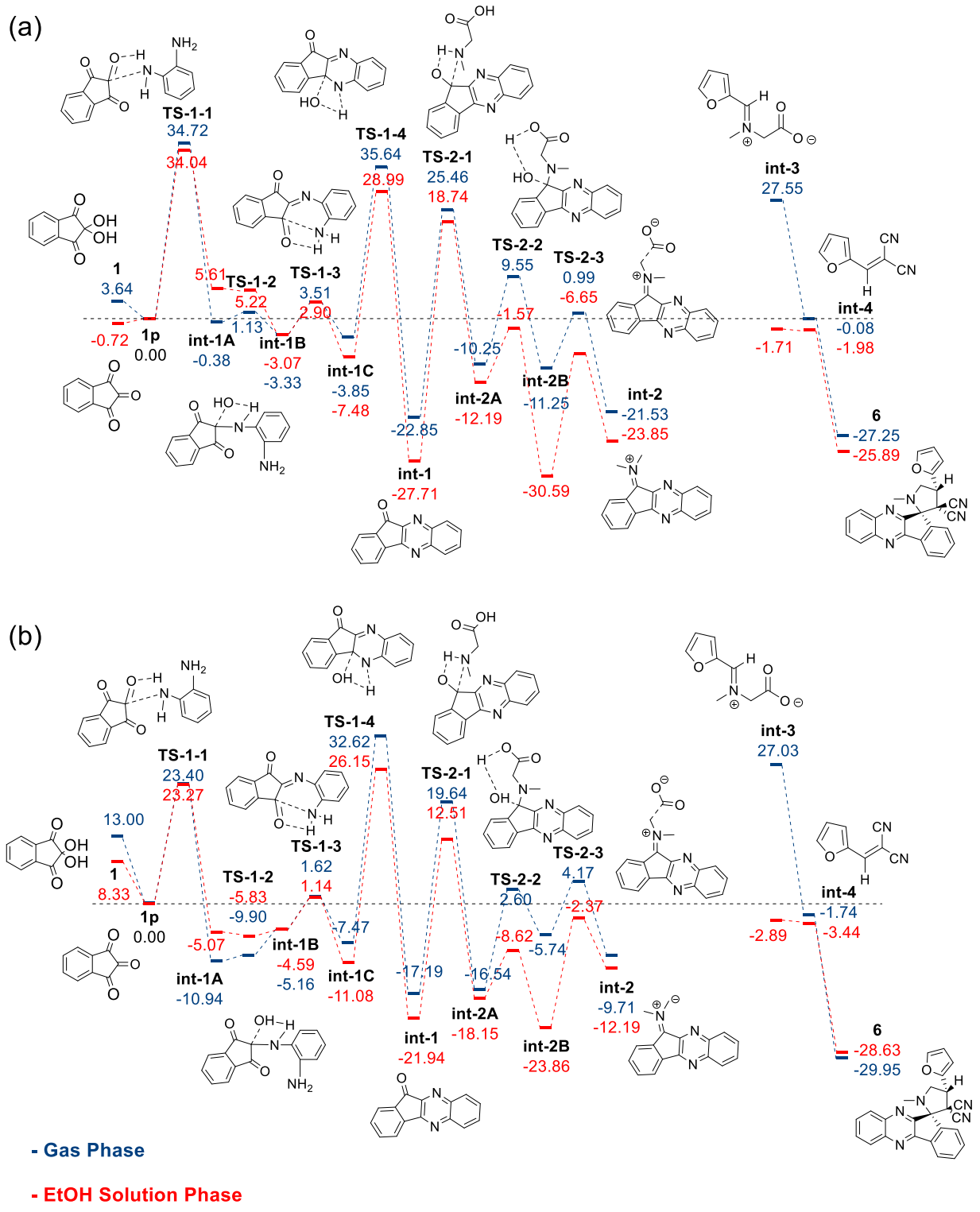
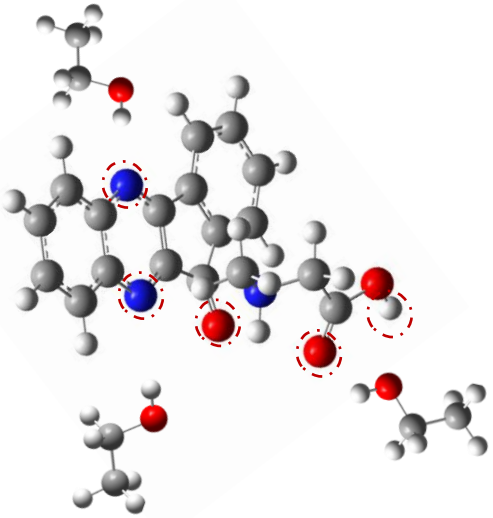


Figure S7. The free energy (a) and enthalpy (b) profiles of the five-component reaction, in both gas phase and solution phase (calculated using Solvation Model based on Density (SMD) model). Structures of **int-1A**, **int-1B**, **int-1C**, **int-2A,** and **int-2B** were omitted for spacing consideration, see Scheme S1 in SI for detailed reaction pathway.

3.2 Hydrogen bonding details

a) 

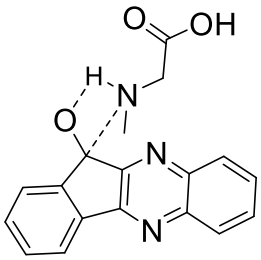
b) 

Figure S8. The atoms selected for hydrogen-bonding analysis. a) the representation of hydrogen-bonding between ethanol and probable sites on the **TS-2-1**; b) structure of **TS-2-1**.

Table S1. TS-2-1 energy state table in different hydrogen bonding conditions (with respect to the starting molecules, in unit of kcal/mol).

EtOH #	Gas		Solution		Gas		Solution	
	ΔG_{min}	ΔG_{max}	ΔG_{min}	ΔG_{max}	ΔH_{min}	ΔH_{max}	ΔH_{min}	ΔH_{max}
0	25.46		18.74		19.64		12.51	
1	23.96 (CO)	26.95 (COO)	19.90 (CO)	21.32 (N)	11.58 (CO)	14.40 (COO)	6.66 (CO)	7.96 (N)
2	19.62 (2O)	23.95 (CO,N)	22.31 (COO, N)		-8.31 (2O)	4.12 (CO,N)	0.63	
3	23.44		23.54		4.65		-5.11	

3.3 Energies and coordinates

Table S2. Gas-phase energies (Hartree), entropy values (in $cal \cdot mol^{-1} \cdot K^{-1}$) and the imaginary frequencies for transition states. Decimal places were minimized for table space consideration, see content below for the detailed information for each species.

Structure	Potential Energy	E+ZPE	Enthalpy	Entropy	G, 1 atm	G, 1 M	Imaginary Frequency (If applicable)
H_2O	-76.45	-76.43	-76.42	45.09	-76.44	-76.44	
CO_2	-188.64	-188.63	-188.63	51.06	-188.65	-188.65	
EtOH	-155.09	-155.01	-155.00	64.41	-155.03	-155.03	
1	-647.62	-647.49	-647.48	100.50	-647.52	-647.52	
1p	-571.15	-571.04	-571.03	93.15	-571.08	-571.08	
2	-343.04	-342.91	-342.90	79.82	-342.94	-342.94	
TS-1-1	-914.16	-913.92	-913.90	128.63	-913.96	-913.96	-1656.81
int-1A	-914.22	-913.97	-913.96	131.20	-914.02	-914.02	
TS-1-2	-914.22	-913.97	-913.95	129.64	-914.02	-914.01	-427.98

int-1B	-837.76	-837.54	-837.52	121.76	-837.58	-837.58	
TS-1-3	-837.75	-837.53	-837.51	121.51	-837.57	-837.57	-265.77
int-1C	-837.76	-837.54	-837.53	115.74	-837.58	-837.58	
TS-1-4	-837.69	-837.48	-837.46	117.76	-837.52	-837.52	-784.77
int-1	-761.33	-761.13	-761.12	108.11	-761.17	-761.17	
TS-2-1	-1085.10	-1084.80	-1084.78	144.68	-1084.85	-1084.84	-1727.79
int-2A	-1085.16	-1084.86	-1084.84	143.13	-1084.90	-1084.90	
TS-2-2	-1085.12	-1084.83	-1084.81	140.91	-1084.87	-1084.87	-727.98
int-2B	-1008.67	-1008.42	-1008.40	143.98	-1008.47	-1008.46	
TS-2-3	-1008.67	-1008.40	-1008.38	136.15	-1008.45	-1008.44	-204.84
int-2	-820.05	-819.79	-819.78	120.41	-819.83	-819.83	
3	-323.83	-323.72	-323.72	81.44	-323.76	-323.75	
4	-225.04	-224.99	-224.99	70.45	-225.02	-225.02	
5	-343.44	-343.36	-343.35	75.64	-343.39	-343.39	
int-3	-590.76	-590.62	-590.61	110.25	-590.66	-590.65	
int4	-492.03	-491.93	-491.92	95.41	-491.97	-491.97	
6	-1312.12	-1311.76	-1311.73	166.63	-1311.81	-1311.81	

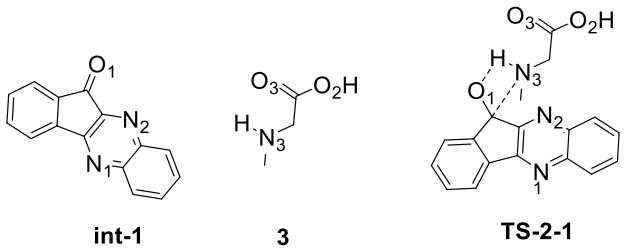
In the "G 1 M" column, the "1 M" refers to free energies adjusted for a standard state of 1 M instead of the default standard state of 1 atm by adding 0.001987*298.15*ln(24.5)/627.509.

Table S3. Solution-phase energies (Hartree) , entropy values (in cal·mol^{-1}·K^{-1}) and the imaginary frequencies for transition states, calculated using the SMD model. Decimal places were minimized for table space consideration, see content below for the detailed information for each species.

Structure	Potential Energy	E+ZPE	Enthalpy	Entropy	G, 1 atm	G, 1 M	Imaginary Vibration Frequency (If applicable)
H_2O	-76.46	-76.44	-76.43	45.12	-76.46	-76.45	
CO_2	-188.64	-188.63	-188.62	51.09	-188.65	-188.64	
EtOH	-155.10	-155.02	-155.01	64.61	-155.04	-155.04	

1	-647.65	-647.51	-647.50	101.54	-647.55	-647.54	
1p	-571.17	-571.06	-571.05	93.14	-571.10	-571.09	
2	-343.06	-342.93	-342.92	79.33	-342.96	-342.96	
TS-1-1	-914.20	-913.96	-913.94	129.98	-914.00	-914.00	-1748.28
int-1A	-914.25	-914.00	-913.98	130.29	-914.05	-914.04	
TS-1-2	-914.25	-914.00	-913.99	129.08	-914.05	-914.04	-167.19
int-1B	-837.78	-837.56	-837.55	122.26	-837.61	-837.60	
TS-1-3	-837.77	-837.55	-837.54	121.45	-837.60	-837.59	-309.16
int-1C	-837.79	-837.57	-837.56	115.30	-837.61	-837.61	
TS-1-4	-837.73	-837.51	-837.50	117.81	-837.56	-837.55	-247.58
int-1	-761.35	-761.15	-761.14	107.95	-761.19	-761.19	
TS-2-1	-1085.14	-1084.84	-1084.82	143.53	-1084.89	-1084.88	-1740.26
int-2A	-1085.19	-1084.89	-1084.87	144.43	-1084.94	-1084.93	
TS-2-2	-1085.17	-1084.87	-1084.85	140.73	-1084.92	-1084.92	-825.97
int-2B	-1008.72	-1008.46	-1008.44	148.21	-1008.51	-1008.51	
TS-2-3	-1008.70	-1008.43	-1008.41	140.00	-1008.47	-1008.47	-500.67
int-2	-820.08	-819.82	-819.80	120.01	-819.86	-819.85	
3	-323.85	-323.74	-323.73	82.16	-323.77	-323.77	
4	-225.05	-225.01	-225.00	70.20	-225.04	-225.03	
5b	-343.45	-343.37	-343.36	75.58	-343.40	-343.40	
int-3b	-590.82	-590.68	-590.66	108.68	-590.72	-590.71	
int4b	-492.05	-491.95	-491.94	95.77	-491.98	-491.98	
6p	-1312.15	-1311.78	-1311.76	166.03	-1311.84	-1311.83	

In the “G 1 M” column, the “1 M” refers to free energies adjusted for a standard state of 1 M instead of the default standard state of 1 atm by adding 0.001987*298.15*ln(24.5)/627.509.



int-1 **3** **TS-2-1**

Table S4. H-bonding investigation results in gas-phase (Energy values in Hartree, entropy values in cal·mol^{-1}·K^{-1})

Structure	Number of H-bonding	Potential Energy	E+ZPE	Enthalpy	Entropy	G, 1 atm	G, 1 M
3	0	-323.831821	-323.724265	-323.716506	81.442000	-323.755202	-323.752182
	1	-478.941640	-478.751699	-478.738587	112.306000	-478.791947	-478.788927
	1	-478.934578	-478.744917	-478.731533	113.476000	-478.785449	-478.782429
	2	-634.044011	-633.772103	-633.753275	144.575000	-633.821967	-633.818947
	3	-789.153070	-788.798887	-788.774602	173.989000	-788.857270	-788.854250
int-1	0	-761.326089	-761.134277	-761.121378	108.112000	-761.172745	-761.169725
	1	-916.428344	-916.154793	-916.135970	142.079000	-916.203476	-916.200456
	1	-916.428344	-916.154794	-916.135971	142.071000	-916.203473	-916.200453
	1	-916.428497	-916.154825	-916.136083	141.105000	-916.203126	-916.200106
	2	-1071.526025	-1071.171210	-1071.146270	177.898000	-1071.230795	-1071.227775
TS-2-1	0	-1085.096402	-1084.799321	-1084.779196	144.681000	-1084.847939	-1084.844919
	1	-1240.195282	-1239.816879	-1239.790684	180.193000	-1239.876300	-1239.873280
	1	-1240.200219	-1239.821144	-1239.795170	180.772000	-1239.881061	-1239.878041
	1	-1240.199193	-1239.820213	-1239.794247	177.537000	-1239.878601	-1239.875581
	2	-1395.310766	-1394.849513	-1394.818073	212.036000	-1394.918818	-1394.915798
	2	-1395.302998	-1394.842032	-1394.810214	213.801000	-1394.911797	-1394.908777
	2	-1395.309508	-1394.848272	-1394.816864	208.586000	-1394.915970	-1394.912950
	3	-1550.413573	-1549.870438	-1549.833154	244.725000	-1549.949431	-1549.946411

In the "G 1 M" column, the "1 M" refers to free energies adjusted for a standard state of 1 M instead of the default standard state of 1 atm by adding 0.001987*298.15*ln(24.5)/627.509.

Table S5. H-bonding investigation results in solution phase, calculated using SMD model (Energy values in Hartree, entropy values in cal·mol^{-1}·K^{-1})

Structure	Number of H-bonding	Potential Energy	E+ZPE	Enthalpy	Entropy	G, 1 atm	G, 1 M
3	0	-323.846221	-323.739119	-323.731284	82.164000	-323.770323	-323.767303
	1	-478.956595	-478.768267	-478.754767	115.692000	-478.809736	-478.806716

	1	-478.952177	-478.763326	-478.749821	114.673000	-478.804306	-478.801286
	2	-634.065649	-633.796066	-633.776814	154.335000	-633.850144	-633.847124
	2	-634.062898	-633.793093	-633.773862	147.464000	-633.843927	-633.840907
	3	-789.172735	-788.821716	-788.796901	174.026000	-788.879586	-788.876566
int-1	0	-761.346193	-761.154304	-761.141435	107.953000	-761.192727	-761.189707
	1	-916.450431	-916.177678	-916.158744	143.144000	-916.226757	-916.223737
	1	-916.452781	-916.179751	-916.160908	142.614000	-916.228668	-916.225648
	1	-916.452549	-916.179431	-916.160665	141.292000	-916.227798	-916.224778
	2	-1071.556432	-1071.202833	-1071.178701	170.829000	-1071.259867	-1071.256847
	2	-1071.556614	-1071.202731	-1071.177832	177.235000	-1071.262042	-1071.259022
	3	-1226.662456	-1226.227645	-1226.196702	210.870000	-1226.296894	-1226.293874
TS-2-1	0	-1085.135238	-1084.837701	-1084.817815	143.526000	-1084.886008	-1084.882988
	1 (O2)	-1240.243846	-1239.865447	-1239.839641	178.238000	-1239.924327	-1239.921307
	1 (N1)	-1240.241928	-1239.863406	-1239.837563	177.506000	-1239.921902	-1239.918882
	2 (O2N1)	-1395.353030	-1394.893216	-1394.861738	208.187000	-1394.960654	-1394.957634
	3 (O2O3N1)	-1550.461774	-1549.920738	-1549.883371	243.053000	-1549.998853	-1549.995833

In the “G 1 M” column, the “1 M” refers to free energies adjusted for a standard state of 1 M instead of the default standard state of 1 atm by adding 0.001987*298.15*ln(24.5)/627.509.

All geometry information in the following content is provided in the format: element charge x-coordinate y-coordinate z-coordinate.

3.3.1 Functional benchmark

Compound 6g

HF/6-311G**

E(RHF) = -1764.93133970

Zero-point correction= 0.415204 (Hartree/Particle)

Thermal correction to Energy= 0.439496

Thermal correction to Enthalpy= 0.440440

Thermal correction to Gibbs Free Energy= 0.360750

Sum of electronic and ZPE= -1764.516136

Sum of electronic and thermal Energies= -1764.491844

Sum of electronic and thermal Enthalpies= -1764.490900

Sum of electronic and thermal Free Energies= -1764.570589

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	275.788	96.095	167.721

Cl 0 1.3878853677 15.0899539832 7.8915184195

N 0 5.1664351242 11.2867209243 8.3893427748

N 0 4.8570017319 13.3292444796 6.0417461916

N 0 5.3433996639 11.8542134477 3.6863449135

N 0 2.0877111257 9.3743696855 9.0890578901

N 0 1.2655815392 11.7901979547 5.7567599723

C 0 2.9684143395 11.3782282413 7.6788506399

C 0 3.2036601943 12.6458968172 8.5709533244

H 0 3.310042987 13.4478672418 7.8648532785

C 0 4.6030658555 12.386757257 9.1627778466

H 0 5.1933137746 13.295599596 9.0729761645

H 0 4.5763265059 12.1125636564 10.2097748495

C 0 4.4318529562 11.1088269548 7.1569924816

C 0 5.2793318211 15.3602190462 4.839719994

H 0 5.093442238 15.9006671761 5.7492264704

C 0 5.594421244 15.9977767057 3.6789757677

H 0 5.6652397395 17.0700541923 3.6550078955

C 0 5.8266427798 15.2580271422 2.498729603

H 0 6.0727521528 15.7766699805 1.5897916918

C 0 5.7397863196 13.899740662 2.5048337188

H 0 5.9117465635 13.3161219339 1.6198909911

C 0 5.414256605 13.2170021441 3.6961210427

C 0 5.0376106956 11.3091072554 4.801837009

C 0 4.9478164347 9.8845494671 5.1338453806

C 0 5.1771632654 8.7835249445 4.3268886975

H 0 5.4023507206 8.91447668 3.2848882459

C 0 5.1211804974 7.5287166521 4.9023616849

H 0 5.2936173449 6.6545063651 4.3008443733

C 0 4.8592090616 7.3879419136 6.2605913621

H 0 4.8362142654 6.405739816 6.6970641929

C 0 4.6287304283 8.4930109802 7.0636031885

H 0 4.4383551112 8.3680811975 8.1109763169

C 0 4.6524117069 9.7505773409 6.4853995276

C 0 4.777231112 12.0583584933 5.9951307946

C 0 5.18201155 13.9541780979 4.8679073654

C 0 2.4768097598 10.2339613669 8.4715231808

C 0 2.0006050814 11.6145434569 6.5936638612

C 0 6.6119040526 11.2579564211 8.3261053188

H 0 6.9452191305 10.3651770958 7.8129090457

H 0 7.0041634576 11.2253951015 9.336310579

H 0 7.0320652522 12.1305245116 7.8242351217

C 0 2.1094773262 13.0222131684 9.5530825781

C 0 1.9286131845 12.3170656356 10.7421328342

H 0 2.5619657745 11.4788155142 10.9580651016

C 0 0.9452887119 12.6531325497 11.6499229158

H 0 0.8337971491 12.0789134729 12.551257362

C 0 0.1082562978 13.7240238906 11.3922443911

H 0 -0.6621797589 13.9966199708 12.0903720392

C 0 0.2660114504 14.4491506301 10.229429106

H 0 -0.3700446247 15.2856273951 10.0128673983

C 0 1.2560349323 14.0991913924 9.3271951057

Compound 6g

B3LYP/6-311G**

E(RB3LYP) = -1773.95825888

Zero-point correction= 0.386526 (Hartree/Particle)

Thermal correction to Energy= 0.412685

Thermal correction to Enthalpy= 0.413629

Thermal correction to Gibbs Free Energy= 0.330006

Sum of electronic and ZPE= -1773.571733

Sum of electronic and thermal Energies= -1773.545574

Sum of electronic and thermal Enthalpies= -1773.544630

Sum of electronic and thermal Free Energies= -1773.628253

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	258.964	103.802	175.999

Cl	0	1.331189788	15.0962433683	7.8974084006
N	0	5.1536511888	11.2861392048	8.3983743924
N	0	4.8338476305	13.3517171671	6.0348469674
N	0	5.3850371223	11.8499178503	3.661719879
N	0	2.0684564001	9.3751399252	9.1126493328
N	0	1.2455590438	11.806909478	5.7235497856
C	0	2.9401984672	11.3832357521	7.672902467
C	0	3.1880938279	12.6715280013	8.5655685868
H	0	3.2736587661	13.4768383824	7.8408811792
C	0	4.6021533786	12.4268355681	9.1404771799
H	0	5.1981001446	13.3381902313	8.9986858552
H	0	4.5933250532	12.1951297949	10.20844366
C	0	4.420969965	11.1049542589	7.1504232841
C	0	5.2718453634	15.3811890419	4.8214253337
H	0	5.064142678	15.9291610848	5.7325851275
C	0	5.6076277811	16.0202889442	3.6497678856
H	0	5.6722171331	17.1018365363	3.6224674043
C	0	5.8660419787	15.2769213394	2.4758962962
H	0	6.1269474267	15.7975920164	1.5616803358
C	0	5.7878401372	13.9035208237	2.4845555597
H	0	5.9813069715	13.311130681	1.5985834396
C	0	5.4459128326	13.2171808394	3.6724658135
C	0	5.057722235	11.2991678995	4.8020559129
C	0	4.9658286906	9.8773704963	5.128945023
C	0	5.2041797602	8.7648126813	4.3264981226
H	0	5.4510768074	8.8943092561	3.2797286294
C	0	5.1286714567	7.5025434718	4.9080533101
H	0	5.3076842307	6.6192285411	4.3057295292
C	0	4.8374245955	7.3637945691	6.2682060376
H	0	4.7974053819	6.3741849728	6.7086643394
C	0	4.5976562986	8.4803509787	7.0718783652
H	0	4.381003656	8.3606389987	8.124592193
C	0	4.6417515167	9.741894671	6.4902127972
C	0	4.7684622654	12.0529373826	5.9840367732
C	0	5.1810961025	13.9727816351	4.8594955108
C	0	2.456624062	10.2510050441	8.4725888342
C	0	1.9874262527	11.6238280367	6.5855106674
C	0	6.6066148745	11.2397289615	8.3339947296
H	0	6.9266840603	10.3327313365	7.8189122333
H	0	7.0033147545	11.203899457	9.351484915
H	0	7.0454693886	12.1119375284	7.8247117112
C	0	2.106017583	13.0284305898	9.5614432579
C	0	1.9508149313	12.311255819	10.7568715064
H	0	2.6069624381	11.4740129025	10.9571342827
C	0	0.9675286037	12.6310962508	11.6847203344
H	0	0.8747202332	12.0470721583	12.5924530803
C	0	0.106548162	13.6971137068	11.4411851242

H 0 -0.6646967578 13.957921354 12.1564770067

C 0 0.2369159562 14.4354547501 10.2712986998

H 0 -0.4201037923 15.2701094834 10.0649681804

C 0 1.2252731746 14.1005867774 9.349690727

Compound6g

M06-2X/6-311G**

E(RM062X) = -1773.44057741

Zero-point correction= 0.391752 (Hartree/Particle)

Thermal correction to Energy= 0.417570

Thermal correction to Enthalpy= 0.418514

Thermal correction to Gibbs Free Energy= 0.335501

Sum of electronic and ZPE= -1773.048825

Sum of electronic and thermal Energies= -1773.023008

Sum of electronic and thermal Enthalpies= -1773.022064

Sum of electronic and thermal Free Energies= -1773.105076

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 262.029 102.516 174.715

Cl 0 1.1913208844 14.929695982 7.8082702674

N 0 5.1584232038 11.2927159662 8.4161269443

N 0 4.8845633588 13.3573016971 6.073571136

N 0 5.3551721029 11.8498694993 3.685291649

N 0 2.0837326965 9.4609081998 9.1402156456

N 0 1.3368488995 11.8781716984 5.6814561441

C 0 2.9719601161 11.4349862894 7.6710586262

C 0 3.2241598493 12.7151579801 8.5463196374

H 0 3.2912840381 13.5279527637 7.8276990177

C 0 4.643816794 12.4810141976 9.1048921652

H 0 5.2516660182 13.3680672629 8.8866864829

H 0 4.6577524033 12.3109903497 10.1830021849

C 0 4.4304418574 11.1258537846 7.1716013493

C 0 5.3306481156 15.3752739673 4.8541661607

H 0 5.1491551229 15.9197863068 5.7727298751

C 0 5.6515615051 16.0094324065 3.6815072005

H 0 5.7331071159 17.0890390754 3.6543814357

C 0 5.8736446431 15.2638772752 2.5016024207

H 0 6.124518821 15.7813509874 1.583721322

C 0 5.772023745 13.8968489416 2.5102585122

H 0 5.9353867622 13.2991921247 1.6222221961

C 0 5.4420360135 13.2163511273 3.7037531843

C 0 5.0405156483 11.3096878972 4.8244160014

C 0 4.9210492555 9.8874728056 5.1566843514

C 0 5.1257077385 8.7717712563 4.356249554

H 0 5.3596780397 8.8935637485 3.3057343493

C 0 5.0339802365 7.5176739249 4.947838205

H 0 5.1865723742 6.6274866278 4.3497656188

C 0 4.7627043976 7.3917316589 6.3113541857

H 0 4.712814275 6.40528444 6.7560743979

C 0 4.5566456984 8.5131922622 7.1122183544

H 0 4.35703026 8.4120812924 8.1712977659

C 0 4.6161814096 9.7646923735 6.5170441916

C 0 4.7936720529 12.066885958 6.0157321919

C 0 5.218008488 13.969093219 4.8893893987

C 0 2.4713937565 10.3195340839 8.4847287387

C 0 2.0402383349 11.6795797829 6.5661339476

C 0 6.6060007529 11.2492851293 8.3045141168

H 0 6.907398233 10.3245692449 7.8097641963

H 0 7.0358677345 11.2543855387 9.3074107572

H 0 7.0107385921 12.1063001528 7.7461048112

C 0 2.1362509779 13.0261817315 9.5427962799

C 0 2.043771743 12.3316173999 10.7526506015

H 0 2.764544699 11.5514953017 10.967248545

C 0 1.039071707 12.598173099 11.670439543

H 0 0.9914243264 12.0359582192 12.594300433

C 0 0.09595502 13.5814224823 11.3959311886

H 0 -0.6929779887 13.7995705848 12.1050283121

C 0 0.1606330581 14.2877426957 10.2041627958

H 0 -0.564477182 15.0556215467 9.9689517407

C 0 1.1705822948 14.0059076593 9.2924018694

Compound 7j

HF/6-311G**

E(RHF) = -1480.01449972

Zero-point correction= 0.502505 (Hartree/Particle)

Thermal correction to Energy= 0.529475

Thermal correction to Enthalpy= 0.530419

Thermal correction to Gibbs Free Energy= 0.444003

Sum of electronic and ZPE= -1479.511995

Sum of electronic and thermal Energies= -1479.485025

Sum of electronic and thermal Enthalpies= -1479.484081

Sum of electronic and thermal Free Energies= -1479.570497

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 332.250 105.483 181.878

O 0 7.2412053669 0.7294956986 4.3579697012

O 0 7.0879797961 2.6579241625 5.4246902017

N 0 11.0885892638 1.422064576 7.1333483671

N 0 10.6282740513 0.606544155 4.4707058471

N 0 10.5447277804 3.2630480693 2.8203500091

N 0 7.1666137701 4.8139422903 2.7679119041

C 0 11.1169529151 -0.264827129 5.4060657346

C 0 11.4004900621 -1.5931320556 5.0277299556

H 0 11.2236963421 -1.8781324218 4.0072888172

C 0 11.8794172394 -2.4767671453 5.9459134146

H 0 12.0935264999 -3.4902007846 5.6585501875

C 0 12.0963773036 -2.0706585495 7.2808698501

H 0 12.474789526 -2.7801732383 7.9945125676

C 0 11.8314164619 -0.7925121086 7.6668220472

H 0 11.991016392 -0.4600477246 8.6755723282

C 0 11.3347188458 0.1409595007 6.7319734957

C 0 10.6383357752 2.2070411983 6.2284186256

C 0 10.3451206514 3.639103592 6.3208897354

C 0 10.5021068198 4.4933206233 7.3995707291

H 0 10.8340810509 4.1123651636 8.3476977036

C 0 10.23884436 5.836410535 7.2128726153

H 0 10.3517320366 6.5252023745 8.0307461067

C 0 9.8467419137 6.3076847578 5.9645399992

H 0 9.6627550307 7.3583566854 5.8290279809

C 0 9.6930382895 5.4484669044 4.8890009325

H 0 9.4013859677 5.8302605317 3.9312206077

C 0 9.9236936041 4.0969437815 5.0789953562

C 0 9.8391586427 2.9658501209 4.0485338599

C 0 10.3860464913 1.7896971615 4.879194472

C 0 8.4038646066 2.6353629197 3.4726749287

C 0 8.7643565591 1.7767172027 2.2212271373

H 0 8.957019348 0.7960307972 2.6216005477

C 0 10.1129320253 2.3609181773 1.7607016876

H 0 10.8190125677 1.5475691455 1.6061194421

H 0 10.0389435463 2.9116747375 0.8317185534

C 0 7.5051624402 1.8753199942 4.4610536441

C 0 6.1752861125 2.1386890198 6.3986453814

H 0 5.4766922499 1.4810538477 5.9016857349

H 0 5.6500535302 3.0112392969 6.7575094936

C 0 6.8997730634 1.4297831746 7.5253164288

H 0 6.1773028244 1.1157593465 8.2731058301

H 0 7.6159012652 2.0928096405 7.9978920275

H 0 7.4183102842 0.5502580002 7.1633204396

C 0 7.7124263359 3.8794747092 3.0874978223

C 0 11.9732545278 3.4761882958 2.8936932333

H 0 12.204877316 4.2217216187 3.6436592803

H 0 12.3178720459 3.8518205115 1.9366418205

H 0 12.5292095661 2.5647836407 3.1205029334

C 0 7.6983760237 1.6184150212 1.1488778242

C 0 6.9682461718 0.4363930933 1.0964741838

H 0 7.1494148844 -0.3273195217 1.8299245683

C 0 6.0036009823 0.2357090411 0.1233593105

H 0 5.4522557609 -0.6875558029 0.1027698499

C 0 5.7517775357 1.2177326412 -0.8174116458

H 0 5.0038192268 1.0648421402 -1.575026903

C 0 6.470004993 2.4005245601 -0.7757142264

H 0 6.280065471 3.1734363515 -1.4989172595

C 0 7.4344730165 2.5978769642 0.196469181

H 0 7.9698834693 3.5284407106 0.2118455977

Compound 7j

B3LYP/6-311G**

E(RB3LYP) = -1489.34918550

Zero-point correction= 0.468433 (Hartree/Particle)

Thermal correction to Energy= 0.497392

Thermal correction to Enthalpy= 0.498336

Thermal correction to Gibbs Free Energy= 0.407883

Sum of electronic and ZPE= -1488.880752

Sum of electronic and thermal Energies= -1488.851794

Sum of electronic and thermal Enthalpies= -1488.850849

Sum of electronic and thermal Free Energies= -1488.941303

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	312.118	114.065	190.375

O 0 7.3485977258 0.6883621452 4.4424091088

O 0 6.9647673984 2.7177759396 5.3472681445

N 0 11.0957226421 1.3643318168 7.1462584734

N 0 10.6725432601 0.5838842461 4.4240458859

N 0 10.5652212154 3.2738393222 2.8105484125

N 0 7.2224606246 4.8545457357 2.7117477533

C 0 11.1692042979 -0.297097282 5.3534567552

C 0 11.4862990692 -1.6146312288 4.956500962

H 0 11.329531869 -1.8831922995 3.9187399204

C 0 11.9705646424 -2.5171850124 5.8757782258

H 0 12.2093109578 -3.5285693929 5.5677688554

C 0 12.1574473118 -2.1366842604 7.2239058289

H 0 12.5390126019 -2.8607680593 7.9346830311

C 0 11.8613227066 -0.8586319574 7.6383459346

H 0 12.0000686888 -0.5407961542 8.6646601301

C 0 11.364195521 0.0921339545 6.717188685

C 0 10.638413564 2.1754545469 6.226274784

C 0 10.337624291 3.6005814113 6.3453504805

C 0 10.4716907484 4.4468127779 7.4437158788

H 0 10.7942359972 4.0494654182 8.3987304707

C 0 10.2013086665 5.8010841035 7.2705701031

H 0 10.2978168623 6.4828773334 8.1079562175

C 0 9.8233678808 6.2935441308 6.0176709712

H 0 9.6322753239 7.3536258536 5.8954768978

C 0 9.6907651874 5.4438628406 4.9176573158

H 0 9.4048386671 5.8371157882 3.9519092034

C 0 9.9289207794 4.085773974 5.0911653487

C 0 9.8584110612 2.9651587133 4.0502735418

C 0 10.4016417666 1.7764993044 4.8702114892

C 0 8.4079716851 2.6478333516 3.4636820107

C 0 8.7805908605 1.7669672442 2.2173890904

H 0 8.9757756438 0.7855465239 2.6459528305

C 0 10.1323415852 2.3517935701 1.7516700364

H 0 10.8465720411 1.529914185 1.6076523882

H 0 10.0564412813 2.8967311435 0.8074098188

C 0 7.5118461533 1.8806859188 4.4614353298

C 0 6.061560487 2.1505235918 6.3393158672

H 0 5.5081847523 1.3356350334 5.8720614751

H 0 5.3825093158 2.9706332119 6.5694951474

C 0 6.8158170428 1.6809947073 7.5703028555

H 0 6.1023271377 1.3421858014 8.3268143118

H 0 7.4089941722 2.4926507977 7.9961651063

H 0 7.4774436739 0.8475912007 7.3294797584

C 0 7.7484243524 3.8906573633 3.0629725003

C 0 12.0019722375 3.4830739239 2.8925947097

H 0 12.2286464694 4.2178720788 3.6671410688

H 0 12.3539395906 3.8847382112 1.9391117651

H 0 12.5649185958 2.5597660485 3.1030642317

C 0 7.7080706099 1.5999948098 1.1577564882

C 0 6.953673771 0.4205323353 1.1355070608

H 0 7.1384170999 -0.3369506732 1.8883288812

C 0 5.9666098357 0.2194911307 0.1740289974

H 0 5.3955492206 -0.7023983067 0.1743672251

C 0 5.7160873429 1.1974906726 -0.7851296881

H 0 4.9497290733 1.0428864849 -1.5364778752

C 0 6.4567963599 2.3771076667 -0.7719686312

H 0 6.2657794058 3.1475590145 -1.5105755542

C 0 7.4440017767 2.5764048769 0.1895550862

H 0 7.9984270978 3.5068143725 0.1888288987

Compound7j

B3LYP/6-311G**

E(RB3LYP) = -1489.34918550

Zero-point correction= 0.468433 (Hartree/Particle)

Thermal correction to Energy= 0.497392

Thermal correction to Enthalpy= 0.498336

Thermal correction to Gibbs Free Energy= 0.407883

Sum of electronic and ZPE= -1488.880752

Sum of electronic and thermal Energies= -1488.851794

Sum of electronic and thermal Enthalpies= -1488.850849

Sum of electronic and thermal Free Energies= -1488.941303

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	312.118	114.065	190.375

O	0	7.3485977266	0.6883621441	4.4424091087
O	0	6.9647673979	2.7177759382	5.3472681445
N	0	11.0957226425	1.3643318174	7.1462584733
N	0	10.672543261	0.5838842469	4.4240458857
N	0	10.5652212147	3.2738393232	2.8105484128
N	0	7.222460623	4.8545457348	2.7117477537
C	0	11.1692042993	-0.2970972811	5.3534567549
C	0	11.4862990715	-1.6146312276	4.9565009614
H	0	11.3295318715	-1.8831922982	3.9187399198
C	0	11.9705646452	-2.517185011	5.8757782251
H	0	12.2093109613	-3.5285693913	5.5677688545
C	0	12.1574473143	-2.1366842592	7.2239058283
H	0	12.5390126049	-2.8607680579	7.9346830303
C	0	11.8613227083	-0.8586319564	7.6383459342
H	0	12.0000686902	-0.5407961533	8.6646601297
C	0	11.3641955222	0.0921339554	6.7171886847
C	0	10.6384135639	2.1754545474	6.2262747841
C	0	10.33762429	3.6005814115	6.3453504808
C	0	10.4716907469	4.446812778	7.4437158792
H	0	10.7942359959	4.0494654184	8.3987304711
C	0	10.2013086642	5.8010841035	7.2705701037
H	0	10.2978168596	6.4828773333	8.1079562183
C	0	9.8233678782	6.2935441308	6.0176709719
H	0	9.6322753208	7.3536258535	5.8954768986
C	0	9.6907651854	5.4438628408	4.9176573163
H	0	9.4048386649	5.8371157883	3.951909204
C	0	9.9289207782	4.0857739743	5.091165349
C	0	9.8584110607	2.9651587137	4.0502735419
C	0	10.4016417668	1.776499305	4.8702114892
C	0	8.4079716847	2.6478333513	3.4636820108
C	0	8.7805908606	1.7669672443	2.2173890903
H	0	8.9757756446	0.785546524	2.6459528302
C	0	10.132341585	2.3517935711	1.7516700364
H	0	10.8465720414	1.5299141864	1.607652388
H	0	10.0564412808	2.8967311447	0.8074098189
C	0	7.5118461533	1.8806859177	4.4614353298
C	0	6.0615604867	2.1505235897	6.3393158671
H	0	5.5081847526	1.3356350309	5.8720614749
H	0	5.382509315	2.9706332093	6.5694951472
C	0	6.8158170427	1.6809947056	7.5703028554
H	0	6.1023271378	1.3421857992	8.3268143116
H	0	7.4089941716	2.4926507963	7.9961651063
H	0	7.4774436743	0.8475911994	7.3294797583
C	0	7.7484243513	3.8906573626	3.0629725005
C	0	12.0019722367	3.4830739256	2.89259471
H	0	12.2286464682	4.2178720804	3.6671410692
H	0	12.3539395896	3.8847382134	1.9391117655
H	0	12.5649185955	2.5597660505	3.1030642318
C	0	7.7080706102	1.5999948094	1.1577564881

C 0 6.9536737722 0.4205323344 1.1355070603

H 0 7.1384171017 -0.3369506743 1.8883288804

C 0 5.966609837 0.2194911294 0.1740289968

H 0 5.3955492226 -0.7023983085 0.1743672242

C 0 5.7160873434 1.1974906715 -0.7851296883

H 0 4.9497290739 1.0428864835 -1.5364778754

C 0 6.4567963594 2.3771076662 -0.7719686308

H 0 6.2657794047 3.1475590141 -1.5105755536

C 0 7.4440017761 2.5764048768 0.1895550866

H 0 7.9984270965 3.5068143728 0.1888288994

Compound7j

M06-2X/6-311G**

E(RM062X) = -1488.78094705

Zero-point correction= 0.475172 (Hartree/Particle)

Thermal correction to Energy= 0.503385

Thermal correction to Enthalpy= 0.504329

Thermal correction to Gibbs Free Energy= 0.416356

Sum of electronic and ZPE= -1488.305775

Sum of electronic and thermal Energies= -1488.277562

Sum of electronic and thermal Enthalpies= -1488.276618

Sum of electronic and thermal Free Energies= -1488.364591

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 315.879 112.288 185.155

O 0 7.0850163846 0.5831167788 4.2491469398

O 0 7.3804791111 2.3510248308 5.6004248702

N 0 11.062382109 1.6482531196 7.176595652

N 0 10.4414893146 0.6005435985 4.5826602478

N 0 10.433514838 3.203968427 2.7620366352

N 0 6.8917622716 4.6038604468 2.8143314527

C 0 10.9430869939 -0.1983088915 5.5836593532

C 0 11.1413107732 -1.5713113411 5.3265630192

H 0 10.8935197498 -1.9399463071 4.3387794282

C 0 11.6272623214 -2.3931584149 6.3116796385

H 0 11.7767311988 -3.4472554434 6.1128512612

C 0 11.9335848049 -1.8743942184 7.5894069701

H 0 12.3160586373 -2.5370261737 8.356197527

C 0 11.748853495 -0.5435489701 7.8646009397

H 0 11.9741084342 -0.1178904248 8.8346466868

C 0 11.2499365335 0.3258400769 6.8691187691

C 0 10.5877348369 2.3701845825 6.205267513

C 0 10.2629471903 3.7968361585 6.2060685994

C 0 10.4254998899 4.7378799883 7.2142424264

H 0 10.8153008178 4.4378605142 8.1795097933

C 0 10.0899823036 6.0573538183 6.936155708

H 0 10.2036433346 6.8162196739 7.7008640684

C 0 9.6229604536 6.4184723158 5.6712337461

H 0 9.3823386402 7.4551082894 5.4684143127

C 0 9.4639490843 5.4712403364 4.661573405

H 0 9.1137486688 5.760309422 3.6794462234

C 0 9.7635883432 4.1477997956 4.9470329202

C 0 9.7163687173 2.9513603855 4.005550729

C 0 10.2796513684 1.8445887881 4.9055669749

C 0 8.3174084313 2.5073886622 3.4432234047

C 0 8.7011534812 1.644986524 2.1947631873

H 0 8.751002375 0.6230094977 2.5670796363

C 0 10.1296750249 2.1068608523 1.8428959623

H 0 10.8233042626 1.2668655323 1.9828542956

H 0 10.2194049939 2.4580390008 0.8135355165

C 0 7.5132107761 1.6813606345 4.4588852249

C 0 6.7072617126 1.656335812 6.6721382207

H 0 5.8503034182 1.1274272318 6.2550681695

H 0 6.3634412787 2.4497265004 7.3325186536

C 0 7.6626317676 0.7090424989 7.3721250206

H 0 7.1363985476 0.1742616801 8.1650871875

H 0 8.493753583 1.2573428549 7.8175813312

H 0 8.0552155388 -0.0272224002 6.6670820173

C 0 7.5232508363 3.684944304 3.0897627889

C 0 11.8559589956 3.4638959952 2.9032327478

H 0 12.0155240501 4.306916643 3.5770474946

H 0 12.2604242418 3.7275284901 1.9246395616

H 0 12.4089390744 2.5901701937 3.28174898

C 0 7.6922432701 1.690302343 1.0705092919

C 0 6.7624605625 0.6601789006 0.9376155299

H 0 6.7768378437 -0.1572852677 1.6497730628

C 0 5.8170968827 0.6887576624 -0.0821608844

H 0 5.102060676 -0.1199476109 -0.1756787521

C 0 5.7894394431 1.7513775926 -0.9772168617

H 0 5.0535915045 1.7748837148 -1.7721133731

C 0 6.7064124429 2.7892880513 -0.8443291257

H 0 6.6821970565 3.6273198481 -1.5304061675

C 0 7.6510562614 2.7585937538 0.1728909994

H 0 8.3485310473 3.5825693425 0.2844210691

3.3.2 Gas-phase calculation

1 ninhydrin

B3LYP/6-311G**

E(RB3LYP) = -647.623606749

Zero-point correction= 0.135169 (Hartree/Particle)

Thermal correction to Energy= 0.145609

Thermal correction to Enthalpy= 0.146553

Thermal correction to Gibbs Free Energy= 0.098804

Sum of electronic and ZPE= -647.488438

Sum of electronic and thermal Energies= -647.477997

Sum of electronic and thermal Enthalpies= -647.477053

Sum of electronic and thermal Free Energies= -647.524802

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	91.371	40.403	100.496

O 0 5.0545681217 2.0498117246 0.7757457593

O 0 4.5216495783 1.9364556232 3.70843499

O 0 3.3468983039 0.3278097169 2.485603991

O 0 1.5801566684 2.18989091 4.0051572326

C 0 0.9173011231 4.2548410272 1.7980795728

C 0 0.9156344577 5.118072229 0.7072101543

C 0 1.972836047 5.1173007142 -0.216899892

C 0 3.0515641762 4.2512558654 -0.0703759999

C 0 3.0527685986 3.3869290784 1.0223851036

C 0 1.9979312949 3.3876490351 1.9443909083

C 0 2.2415676079 2.3908463125 3.0154423835

C 0 3.5862001297 1.689409071 2.6983574236

C 0 4.0673262027 2.3701101335 1.3923127441

H 0 0.1081262853 4.2458508823 2.5184799102

H 0 0.0881710109 5.8036682599 0.5644515667

H 0 1.943270521 5.8033775564 -1.0557555481

H 0 3.8731948473 4.2403042006 -0.7765088672

H 0 4.1086312327 1.6610804568 4.5391448836

H 0 4.1614037928 -0.039862797 2.1145436836

1p

B3LYP/6-311G**

E(RB3LYP) = -571.151266425

Zero-point correction= 0.107508 (Hartree/Particle)

Thermal correction to Energy= 0.116337

Thermal correction to Enthalpy= 0.117281

Thermal correction to Gibbs Free Energy= 0.073021

Sum of electronic and ZPE= -571.043758

Sum of electronic and thermal Energies= -571.034930

Sum of electronic and thermal Enthalpies= -571.033985

Sum of electronic and thermal Free Energies= -571.078245

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 73.002 33.669 93.152

O 0 -1.0135850205 -2.3978745075 -0.2429314488

O 0 -2.7779274726 -0.0063943123 -0.4833781442

O 0 -1.0109699295 2.3907499107 -0.3368958665

C 0 1.9025640655 1.4191101937 0.0011746843

C 0 3.0868762178 0.70553963 0.1448019386

C 0 3.0861105889 -0.6995398777 0.172357558

C 0 1.9010187848 -1.4169024861 0.0567923624

C 0 0.7114483539 -0.7044951157 -0.0873883295

C 0 0.7122151558 0.702893928 -0.1149884686

C 0 -0.6606261628 1.2389518127 -0.2757441561

C 0 -1.5881663967 -0.0044874332 -0.3530878275

C 0 -0.6619788261 -1.2449479473 -0.2270387704

H 0 1.8893316258 2.5022408684 -0.0215774094

H 0 4.0275135769 1.2361847839 0.2372916521

H 0 4.0261713264 -1.2271750974 0.285601334

H 0 1.8866061124 -2.5000773541 0.0765228917

2 o-Phenylenediamine

B3LYP/6-311G**

E(RB3LYP) = -343.042640474

Zero-point correction= 0.130467 (Hartree/Particle)

Thermal correction to Energy= 0.137010

Thermal correction to Enthalpy= 0.137954

Thermal correction to Gibbs Free Energy= 0.100030

Sum of electronic and ZPE= -342.912174

Sum of electronic and thermal Energies= -342.905630

Sum of electronic and thermal Enthalpies= -342.904686

Sum of electronic and thermal Free Energies= -342.942611

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 85.975 25.672 79.820

C 0 -6.2050118715 1.3479609429 -0.3567970391

C 0 -5.6722047431 0.1076331051 -0.0256222561

C 0 -6.5296622669 -0.9533154756 0.2557657184

C 0 -7.9201363337 -0.8091091651 0.2153400805

C 0 -8.4635052334 0.4557999143 -0.1224360167

C 0 -7.5877002659 1.5097038135 -0.4018998345

N 0 -9.8372319506 0.6563394067 -0.177844748

N 0 -8.7428398675 -1.8912888999 0.5024918889

H 0 -5.5573309792 2.1877589493 -0.5795673217

H 0 -4.5996457373 -0.0416526642 0.0157012667

H 0 -6.1197858237 -1.9252513913 0.5152927509

H 0 -8.0106063833 2.4764136042 -0.6600359813

H 0 -10.1989646806 1.5600476728 -0.4195516898

H 0 -10.5055208262 -0.0631639698 0.0122357913

H 0 -9.7416848347 -1.8411050394 0.4877976645

H 0 -8.3358682024 -2.7769708036 0.7389297261

3 sarcosine

B3LYP/6-311G**

E(RB3LYP) = -323.831821053

Zero-point correction= 0.107556 (Hartree/Particle)

Thermal correction to Energy= 0.114371

Thermal correction to Enthalpy= 0.115315

Thermal correction to Gibbs Free Energy= 0.076619

Sum of electronic and ZPE= -323.724265

Sum of electronic and thermal Energies= -323.717450

Sum of electronic and thermal Enthalpies= -323.716506

Sum of electronic and thermal Free Energies= -323.755202

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 71.769 23.064 81.442

C 0 -9.5878755193 -0.1526672164 0.0082933459

N 0 -8.3082616035 0.5009390805 0.2394317147

C 0 -7.1720106034 -0.3873288201 0.1207135595

C 0 -5.8931922234 0.4042949698 -0.0393298107

O 0 -4.8050450947 -0.3378337493 0.2614316169

O 0 -5.8271173973 1.5430125434 -0.4253350804

H 0 -10.38729128 0.5892853053 0.0586872935

H 0 -9.6592345088 -0.6751441799 -0.9626415355

H 0 -9.776017767 -0.8910408509 0.7940681

H 0 -8.1760554606 1.2866758451 -0.3882393023

H 0 -7.0833173318 -1.0326303365 1.0004264946

H 0 -7.2194479539 -1.0665801386 -0.7547610442

H 0 -4.0314332563 0.2191175476 0.0870546479

4 malononitrile

B3LYP/6-311G**

E(RB3LYP) = -225.038398683

Zero-point correction= 0.044641 (Hartree/Particle)

Thermal correction to Energy= 0.049483

Thermal correction to Enthalpy= 0.050427

Thermal correction to Gibbs Free Energy= 0.016956

Sum of electronic and ZPE= -224.993757

Sum of electronic and thermal Energies= -224.988916

Sum of electronic and thermal Enthalpies= -224.987972

Sum of electronic and thermal Free Energies= -225.021443

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	31.051	15.273	70.446

C	0	-8.3728731073	-0.4493493636	-0.0000523818
C	0	-7.0820456049	0.2431219996	0.000078335
N	0	-6.0568517175	0.7655463101	0.0001962236
C	0	-9.5159047497	0.4667452032	0.0000825838
N	0	-10.4287289205	1.167246205	0.0002038616
H	0	-8.4323367871	-1.0965177004	-0.8810129618
H	0	-8.4323591129	-1.0967926539	0.8807043396

5 furfural

B3LYP/6-311G**

E(RB3LYP) = -343.440196195

Zero-point correction= 0.079242 (Hartree/Particle)

Thermal correction to Energy= 0.084791

Thermal correction to Enthalpy= 0.085735

Thermal correction to Gibbs Free Energy= 0.049795

Sum of electronic and ZPE= -343.360954

Sum of electronic and thermal Energies= -343.355406

Sum of electronic and thermal Enthalpies= -343.354462

Sum of electronic and thermal Free Energies= -343.390401

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	53.207	19.903	75.640

C	0	-7.9069318115	0.3976358845	0.2956979707
C	0	-9.2577922925	0.2592664646	0.1165886679
C	0	-9.441127762	-0.8966677405	-0.6896382603
C	0	-8.1904907049	-1.3816142722	-0.9455185751
O	0	-7.2469443063	-0.6129134297	-0.3582702487
C	0	-7.0964385346	1.3705149942	1.0151001197
H	0	-6.0048591384	1.1840956564	0.9546123242
O	0	-7.5582137285	2.3070762938	1.6303985689
H	0	-10.0096320168	0.9168859482	0.5221076053
H	0	-10.372087602	-1.3161788232	-1.0359163431
H	0	-7.8284821026	-2.2281009761	-1.5051618294

6

B3LYP/6-311G**

E(RB3LYP) = -1312.12094582

Zero-point correction= 0.365666 (Hartree/Particle)

Thermal correction to Energy= 0.389883

Thermal correction to Enthalpy= 0.390827

Thermal correction to Gibbs Free Energy= 0.311658

Sum of electronic and ZPE= -1311.755280

Sum of electronic and thermal Energies= -1311.731063

Sum of electronic and thermal Enthalpies= -1311.730118

Sum of electronic and thermal Free Energies= -1311.809288

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 244.655 96.106 166.626

C 0 -9.3570298917 0.3838686802 -0.0870090869

C 0 -9.6539303691 -0.9960170645 -0.017681911

C 0 -8.6451556291 -1.9312529404 -0.0321415445

C 0 -7.2945582834 -1.5213378007 -0.1159396656

C 0 -6.9959273462 -0.1227014573 -0.1816310423

C 0 -8.0521916698 0.8139629398 -0.168136596

N 0 -6.3077521352 -2.4694478704 -0.1396414606

C 0 -5.088750065 -2.0014133881 -0.2165307812

C 0 -4.7853782321 -0.6026340608 -0.2597599292

N 0 -5.6985039533 0.3251478774 -0.2518080995

C 0 -3.8354862247 -2.7473488356 -0.3134941065

C 0 -2.7706415054 -1.8373796007 -0.4326220767

C 0 -3.2600785522 -0.3900008178 -0.3521926783

C 0 -3.621371443 -4.1226503737 -0.3546946398

C 0 -2.3199459289 -4.5831274905 -0.5316601354

C 0 -1.261640649 -3.6817140319 -0.6802241901

C 0 -1.4772655967 -2.3026897143 -0.6383636905

C 0 -2.7371003326 0.4439299976 0.8976245431

C 0 -3.137061813 1.9166991409 0.4505578735

C 0 -2.9522993037 1.8758043604 -1.0822754789

N 0 -2.7708721901 0.4606461067 -1.4311110586

C 0 -2.4561285125 3.0249770672 1.1680411868

H 0 -4.2024915392 1.9861734341 0.6666714726

C 0 -3.1519632971 0.1085783544 -2.7897896239

C 0 -2.8259224532 3.7905541989 2.2330673199

C 0 -1.7386633932 4.6855771644 2.4909360189

C 0 -0.7899421891 4.4016846866 1.562360487

O 0 -1.2081850124 3.3953464992 0.7466600441

C 0 -3.3833083598 0.0713490399 2.1579021875

N 0 -3.9078333274 -0.2007768664 3.1469798459

C 0 -1.2834023373 0.3118936658 1.0523103858

N 0 -0.1434394342 0.220543542 1.1897964316

H 0 -10.1652580225 1.1058348132 -0.0737393321

H 0 -10.6872952541 -1.3165531693 0.0478651619

H 0 -8.8462315771 -2.9943647496 0.0191163011

H 0 -7.7998862231 1.8663538528 -0.2197331696

H 0 -4.4574845278 -4.8048133522 -0.2597514104

H 0 -2.1244728436 -5.6488206163 -0.5654179521

H 0 -0.2561978879 -4.0573707343 -0.8314323101

H 0 -0.6522002025 -1.6145425932 -0.7623185299

H 0 -3.8426872507 2.3075234439 -1.5578483242

H 0 -2.0771478058 2.4452910998 -1.4022474681

H 0 -2.9240288321 -0.9414111535 -2.9796094692

H 0 -2.563405928 0.7094690327 -3.4871514772

H 0 -4.2187378277 0.2844148447 -3.0006134197

H 0 -3.7565147543 3.7180587096 2.7734518175

H 0 -1.6771411696 5.4361502151 3.2624121977

H 0 0.1881110765 4.7987359142 1.3507173829

int-1A

B3LYP/6-311G**

E(RB3LYP) = -914.218227822

Zero-point correction= 0.244621 (Hartree/Particle)

Thermal correction to Energy= 0.261182

Thermal correction to Enthalpy= 0.262127

Thermal correction to Gibbs Free Energy= 0.199787

Sum of electronic and ZPE= -913.973606

Sum of electronic and thermal Energies= -913.957045

Sum of electronic and thermal Enthalpies= -913.956101

Sum of electronic and thermal Free Energies= -914.018441

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 163.894 65.676 131.204

C 0 -9.9637685564 -0.9273836813 -0.7807794313

C 0 -9.4992442213 -0.2948159359 -1.9453941733

C 0 -8.1403553003 -0.2379321673 -2.2372753989

C 0 -7.2530580703 -0.8219183549 -1.3360438077

C 0 -7.7160687564 -1.4521575939 -0.174672793

C 0 -9.0777799659 -1.5157420374 0.1154087555

C 0 -5.7726972898 -0.8909687605 -1.4215139189

C 0 -5.2672307902 -1.6671585038 -0.1725551943

C 0 -6.5776329198 -2.010018644 0.5866268321

O 0 -6.6113919165 -2.6635945301 1.6077068304

O 0 -5.0760633793 -0.459048482 -2.3069355247

O 0 -4.699087117 -2.8777948871 -0.6274264794

N 0 -4.298408345 -0.9053742278 0.5974607454

C 0 -4.6109017973 0.4628499787 0.9408405651

C 0 -3.9629023108 1.4902651272 0.2155757721

C 0 -4.2451317024 2.8246315771 0.5616716749

C 0 -5.1082946536 3.128662456 1.6043211612

C 0 -5.7181446619 2.1133929397 2.3414345402

C 0 -5.4616722519 0.7891745283 1.9988770751

N 0 -3.0342462538 1.1859754282 -0.7595083136

H 0 -11.0291681147 -0.9558618314 -0.5826533846

H 0 -10.2148092266 0.1542455829 -2.6247476442

H 0 -7.7693907215 0.2446123175 -3.1334775917

H 0 -9.423206632 -2.0108120775 1.0151164216

H 0 -4.7562800989 -3.5123549854 0.0991018

H 0 -4.0464156602 -1.4394650287 1.4243248792

H 0 -3.7538226742 3.622047863 0.0131953147

H 0 -5.2981205779 4.1677949488 1.8506118822

H 0 -6.3792257857 2.3479742266 3.1668527788

H 0 -5.9225635357 -0.0152619315 2.5629423028

H 0 -2.9110967086 1.8821415763 -1.4787762291

H 0 -3.0970200043 0.2442951099 -1.1203094466

int-1B

B3LYP/6-311G**

E(RB3LYP) = -837.757107746

Zero-point correction= 0.217098 (Hartree/Particle)

Thermal correction to Energy= 0.231617

Thermal correction to Enthalpy= 0.232561

Thermal correction to Gibbs Free Energy= 0.174709

Sum of electronic and ZPE= -837.540010

Sum of electronic and thermal Energies= -837.525491

Sum of electronic and thermal Enthalpies= -837.524546

Sum of electronic and thermal Free Energies= -837.582398

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	145.342	58.239	121.760

C 0 -10.0693766345 1.34340488 -1.5470844381

C 0 -8.9596452269 1.6996838873 -2.3274640781

C 0 -7.6803498918 1.2583059818 -1.9971723372

C 0 -7.5398658136 0.4574206529 -0.867509479

C 0 -8.6470998497 0.099249454 -0.0913294952

C 0 -9.9243560873 0.5377238312 -0.4187966824

C 0 -6.2945492213 -0.1186834799 -0.3004172435

C 0 -6.6968392347 -0.903535143 0.9149059224

C 0 -8.2095230804 -0.7821745377 1.0286428049

O 0 -8.9189777274 -1.2971299352 1.8591904177

O 0 -5.1833113587 -0.0021558564 -0.8013597087

N 0 -6.0948794914 -1.7141572784 1.7081050875

C 0 -4.8109295682 -2.0624641597 2.0124029555

C 0 -3.6210901514 -1.2555517466 1.9357133137

C 0 -2.4285531121 -1.7858698026 2.477246503

C 0 -2.3693047816 -3.0501307095 3.0244448397

C 0 -3.52111643 -3.8518318533 3.0922667099

C 0 -4.7101482716 -3.3413889624 2.6288389278

N 0 -3.6393336019 0.0309787069 1.4717747938

H 0 -11.053085349 1.6998101907 -1.8311627193

H 0 -9.1039053183 2.3272146885 -3.1995937378

H 0 -6.8144078545 1.5252963759 -2.5910908937

H 0 -10.7734978931 0.2509073473 0.1901433863

H 0 -1.5327735529 -1.1745623438 2.4314840661

H 0 -1.4255419715 -3.420229911 3.4094920234

H 0 -3.4793620927 -4.8409837161 3.5310256141

H 0 -5.6350524628 -3.8978370964 2.7134944692

H 0 -2.7401699193 0.4909593022 1.4803251087

H 0 -4.1593540512 0.1846312332 0.6066838694

int-1C

B3LYP/6-311G**

E(RB3LYP) = -837.761611741

Zero-point correction= 0.218661 (Hartree/Particle)

Thermal correction to Energy= 0.232440

Thermal correction to Enthalpy= 0.233385

Thermal correction to Gibbs Free Energy= 0.178394

Sum of electronic and ZPE= -837.542951

Sum of electronic and thermal Energies= -837.529171

Sum of electronic and thermal Enthalpies= -837.528227

Sum of electronic and thermal Free Energies= -837.583218

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	145.859	57.061	115.738

C 0 4.4515374349 -0.5325583424 -0.5269883651

C 0 3.8422364763 -1.7597389202 -0.2396152878

C 0 2.4886279217 -1.8318616493 0.0927217772

C 0 1.7501513573 -0.6563108658 0.1125865901

C 0 2.3612086923 0.5705320888 -0.1653434859

C 0 3.7143694835 0.6462764511 -0.4863754561

C 0 0.2963863227 -0.4540045917 0.4960645258

C 0 0.0561882049 1.0130049555 0.1570526591

C 0 1.3816299362 1.6903227637 -0.0759635839

O 0 1.5985479894 2.871535056 -0.2113739628

N 0 -0.677317793 -1.2090091839 -0.2453200959

C 0 -1.9832365267 -0.7357363721 -0.2260327794

C 0 -2.1823241749 0.6627363844 -0.0736905971

C 0 -3.0941382953 -1.5699645331 -0.4026122618

C 0 -4.3748145248 -1.0340940684 -0.3983274977

C 0 -4.5786715617 0.3406571368 -0.2283151586

C 0 -3.4854073954 1.1791106548 -0.0832805623

O 0 0.2264653032 -0.6910591017 1.9101957292

H 0 -0.5569275717 -2.2124079318 -0.2705920319

H 0 5.5056365108 -0.5053239436 -0.7780384545

H 0 4.4342312126 -2.6676607365 -0.2679155668

H 0 2.0376755617 -2.7861615796 0.3406426176

H 0 4.1649190902 1.6092067383 -0.6975058892

H 0 -2.9461202204 -2.6372766756 -0.5326389322

H 0 -5.2252221043 -1.6938565785 -0.5282361609

H 0 -5.5828639622 0.7463437592 -0.2270285662

H 0 -3.5979321615 2.2520541879 0.0160955772

H 0 -0.641174927 -0.4013886113 2.2188981764

N 0 -1.0950233388 1.537062719 -0.0370289865

int-1

B3LYP/6-311G**

E(RB3LYP) = -761.326088892

Zero-point correction= 0.191812 (Hartree/Particle)

Thermal correction to Energy= 0.203767

Thermal correction to Enthalpy= 0.204711

Thermal correction to Gibbs Free Energy= 0.153343

Sum of electronic and ZPE= -761.134277

Sum of electronic and thermal Energies= -761.122322

Sum of electronic and thermal Enthalpies= -761.121378

Sum of electronic and thermal Free Energies= -761.172745

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	127.865	49.573	108.112

C	0	-9.2882801005	0.7652631993	0.3882925456
C	0	-8.539269008	1.9057382621	0.0795904726
C	0	-7.1523160852	1.841251875	-0.0747391143
C	0	-6.5333859854	0.6088572566	0.0871897833
C	0	-7.2869700307	-0.5387198746	0.3978268539
C	0	-8.6644138767	-0.4729511122	0.5507395411
C	0	-5.1130935224	0.2274639244	-0.0104746279
C	0	-5.0010741576	-1.1781218201	0.2455003059
C	0	-6.3858409079	-1.7298950541	0.5180872172
O	0	-6.6952671618	-2.8678194412	0.7732366778
N	0	-4.0890158071	0.9921459104	-0.2802959176
C	0	-2.8796246222	0.3443091118	-0.3015908121
C	0	-2.7717072971	-1.0630165086	-0.0447822246
N	0	-3.8739263992	-1.8293073258	0.2347043932
C	0	-1.7080388235	1.080680059	-0.5837195107
C	0	-0.4833349694	0.4522872755	-0.6105911313
C	0	-0.3773076564	-0.934102307	-0.3575597113
C	0	-1.5003174467	-1.6788568425	-0.0796764367
H	0	-10.3630697071	0.8471782906	0.5017690079
H	0	-9.0458398917	2.85659633	-0.0418670397
H	0	-6.5701037999	2.7229022315	-0.313801981
H	0	-9.2295576416	-1.366385627	0.7900132115
H	0	-1.8135310243	2.1418310747	-0.7744664828
H	0	0.4115854716	1.0241234691	-0.8278849809
H	0	0.5963746168	-1.4092373851	-0.3836166675
H	0	-1.4531741657	-2.7428149718	0.1186166284

int-2A

B3LYP/6-311G**

E(RB3LYP) = -1085.15959530

Zero-point correction= 0.302651 (Hartree/Particle)

Thermal correction to Energy= 0.321799

Thermal correction to Enthalpy= 0.322743

Thermal correction to Gibbs Free Energy= 0.254739

Sum of electronic and ZPE= -1084.856945

Sum of electronic and thermal Energies= -1084.837797

Sum of electronic and thermal Enthalpies= -1084.836853

Sum of electronic and thermal Free Energies= -1084.904856

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 201.932 76.609 143.126

C 0 -9.196132899 1.7938864294 0.3830976933

C 0 -8.4922274398 3.0030272035 0.4033218699

C 0 -7.0994537932 3.0149753358 0.3936082803

C 0 -6.4285410357 1.7941261407 0.3651767584

C 0 -7.1334958304 0.5820862173 0.3457878852

C 0 -8.5202773568 0.572191054 0.3537623367

C 0 -4.9917363643 1.5030890416 0.3438812733

C 0 -4.8178820705 0.0800583117 0.3444641749

C 0 -6.1856934364 -0.6262384917 0.380609642

N 0 -3.9943458515 2.3489488619 0.3172782493

C 0 -2.7501297186 1.7752517001 0.2823691387

C 0 -2.5765520408 0.354552578 0.265509649

N 0 -3.6548679438 -0.4987585476 0.2979071122

C 0 -1.6071246895 2.6068611071 0.2555821288

C 0 -0.3472195798 2.0549346636 0.2123914584

C 0 -0.1777555288 0.6525625856 0.1936390959

C 0 -1.271863415 -0.182743634 0.2193439184

O 0 -6.2628657431 -1.3209120712 1.6033991462

N 0 -6.4585744671 -1.5593590276 -0.7184568423

C 0 -6.4006104189 -0.9906240551 -2.0643641645

C 0 -5.7764515543 -2.8459048538 -0.6002447307

C 0 -6.6298474435 -3.8956000645 0.0944444417

O 0 -6.1947225492 -5.1393896789 -0.192781928

O 0 -7.563463675 -3.69202505 0.8333503538

H 0 -6.7407413405 -5.7548666875 0.319336472

H 0 -10.2803348688 1.8072560573 0.3901865189

H 0 -9.0387445425 3.9390455952 0.4268578539

H 0 -6.5416383663 3.9437628983 0.4076954828

H 0 -9.0637419193 -0.3658524868 0.3306670884

H 0 -1.764450911 3.6786432945 0.2700344354

H 0 0.5248512172 2.6985886464 0.1928709763

H 0 0.8219747782 0.2349393762 0.1605413581

H 0 -1.1692269151 -1.2612988508 0.2096512207

H 0 -7.0460405316 -1.8952537143 1.5595838085

H 0 -6.8316017999 -1.7016474008 -2.7723864308

H 0 -7.0005440495 -0.0814201479 -2.105791908

H 0 -5.3794870996 -0.7468747093 -2.3969629792

H 0 -4.8302726723 -2.776081784 -0.0510445214

H 0 -5.529666134 -3.2274358421 -1.5923163164

int-2B

B3LYP/6-311G**

E(RB3LYP) = -1008.67209651

Zero-point correction= 0.255539 (Hartree/Particle)

Thermal correction to Energy= 0.273864

Thermal correction to Enthalpy= 0.274808

Thermal correction to Gibbs Free Energy= 0.206398

Sum of electronic and ZPE= -1008.416557

Sum of electronic and thermal Energies= -1008.398233

Sum of electronic and thermal Enthalpies= -1008.397288

Sum of electronic and thermal Free Energies= -1008.465698

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	171.852	69.712	143.980

C 0 -9.3546569829 -1.4910696607 -0.218123862

C 0 -8.6856866298 -2.7098940544 -0.1143495948

C 0 -7.291705301 -2.7432760626 -0.0569034164

C 0 -6.6008882158 -1.5461289761 -0.12947972

C 0 -7.2629841045 -0.2970424031 -0.2741766353

C 0 -8.6655276166 -0.2782607267 -0.2940828278

C 0 -5.1658714827 -1.3123973126 -0.023109849

C 0 -4.9338654797 0.1050544437 -0.0891562092

C -1 -6.24436 0.772428 -0.301129

N 0 -4.2149954616 -2.193848945 0.1223183308

C 0 -2.9492398155 -1.6804911121 0.215525297

C 0 -2.7086661474 -0.2696924951 0.1487163087

N 0 -3.7344113074 0.6212661919 -0.0086882161

C 0 -1.8556287907 -2.5578686921 0.3815350983

C 0 -0.5762958779 -2.0584228639 0.4771057472

C 0 -0.3388724977 -0.6666883238 0.4109619205

C 0 -1.3840119219 0.2134515699 0.2502195696

N -1 -6.416925 2.043927 -0.58448

C 0 -5.3904765878 3.0697457551 -0.3258692668

C -1 -7.722753 2.579564 -0.813508

C -1 -8.589019 2.813068 0.59746

O 0 -9.7913373132 2.7359091622 0.3588105397

O 0 -7.8795705474 3.0286449202 1.5738560752

H 0 -10.4379026499 -1.4721144722 -0.2278995828

H 0 -9.2515895385 -3.6325546671 -0.0584180099

H 0 -6.7484618369 -3.6737316869 0.05402105

H 0 -9.2432575184 0.6347778415 -0.3155443365

H 0 -2.0628088097 -3.619830318 0.4306921045

H 0 0.2597128214 -2.7361255362 0.6052849466

H 0 0.6755551678 -0.2936797519 0.4890128791

H 0 -1.2264088477 1.2839374985 0.1986967765

H 0 -4.4224930875 2.6157255767 -0.1547945222

H 0 -5.3605135607 3.7448877061 -1.1815773723

H 0 -5.7406862443 3.6053516812 0.5616654234

H 0 -7.6269052849 3.5647609994 -1.2654742593

H 0 -8.3015429898 1.9302847513 -1.4604253942

int-2

B3LYP/6-311G**

E(RB3LYP) = -820.053845713

Zero-point correction= 0.260435 (Hartree/Particle)

Thermal correction to Energy= 0.275128

Thermal correction to Enthalpy= 0.276072

Thermal correction to Gibbs Free Energy= 0.218862

Sum of electronic and ZPE= -819.793411

Sum of electronic and thermal Energies= -819.778718

Sum of electronic and thermal Enthalpies= -819.777773

Sum of electronic and thermal Free Energies= -819.834984

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 172.645 61.229 120.409

C 0 -9.5039820384 1.0554851495 -0.4361699372

C 0 -9.5697850012 -0.3398221091 -0.4135487285

C 0 -8.3965715091 -1.075905155 -0.2802079402

C 0 -7.1848356115 -0.4060387783 -0.1724356536

C 0 -7.0915494118 1.0206309765 -0.1930375609

C 0 -8.293282602 1.7388987915 -0.3288435522

C 0 -5.848346226 -0.9491424373 -0.0266913275

C 0 -4.9201992172 0.1655383902 0.0431596965

C 0 -5.678186099 1.3805905743 -0.0586095496

N 0 -5.1064704809 2.6335565849 -0.0273095199

C 0 -5.9940820611 3.8088960123 -0.1414373747

C 0 -3.8128342533 2.8752621976 0.0977899894

N 0 -5.4797777326 -2.1997204792 0.0367383324

C 0 -4.1336517798 -2.4094513365 0.1764561182

C 0 -3.2069053643 -1.3179315172 0.2466339201

N 0 -3.6161617275 -0.0156823001 0.1781029378

C 0 -3.6486461307 -3.7352556868 0.2531286483

C 0 -2.3021766575 -3.9807143398 0.3936299645

C 0 -1.3868616702 -2.9058269111 0.4630047234

C 0 -1.827951317 -1.6045845993 0.3912859507

H 0 -10.417741879 1.6308266827 -0.5400539197

H 0 -10.5265724666 -0.8410402019 -0.4991623707

H 0 -8.4058600377 -2.1595842193 -0.25842944

H 0 -8.3231528428 2.8176587811 -0.3545137131

H 0 -6.7052850562 3.80751792 0.6827154794

H 0 -5.3880108109 4.7094494435 -0.0995375745

H 0 -6.5270699441 3.7700019263 -1.0898224856

H 0 -3.4914771513 3.903987216 0.1084371128

H 0 -3.1364685418 2.0398903804 0.183382813

H 0 -4.3752250843 -4.5372896142 0.196993128

H 0 -1.9382530242 -5.0001466184 0.4517115273

H 0 -0.3280153 -3.1116590517 0.5737275367

H 0 -1.1403109703 -0.7683956716 0.4428127695

int-3

B3LYP/6-311G**

E(RB3LYP) = -590.761591538

Zero-point correction= 0.143731 (Hartree/Particle)

Thermal correction to Energy= 0.155099

Thermal correction to Enthalpy= 0.156043

Thermal correction to Gibbs Free Energy= 0.103659

Sum of electronic and ZPE= -590.617861

Sum of electronic and thermal Energies= -590.606493

Sum of electronic and thermal Enthalpies= -590.605549

Sum of electronic and thermal Free Energies= -590.657933

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 97.326 39.191 110.252

C 0 -5.0134817952 -0.4261134747 -0.1359135543

N -1 -5.8540847223 0.6252162096 0.4688469755

C -1 -5.1394099898 1.6908263344 1.2458826839

C -1 -3.6509026842 1.4531751705 1.1750269067

O 0 -3.1549110159 0.9456138321 2.1972488009

O 0 -3.1485762432 1.7500961967 0.0682260446

C -1 -7.1519026037 0.6346822855 0.3948434339

C 0 -8.0891499491 -0.2553831705 -0.2064050212

H 0 -7.6288134054 1.4792457103 0.8845136914

C 0 -9.4621281996 -0.1233404784 -0.220329528

C 0 -9.9739656308 -1.2354723958 -0.9319924647

C 0 -8.8875116778 -1.9725431046 -1.3057738518

O 0 -7.7414738639 -1.3979065077 -0.8776456632

H 0 -4.30156805 0.078695544 -0.7906437095

H 0 -4.4369604634 -0.8770575624 0.6744694564

H 0 -5.6227191645 -1.1573629018 -0.649138614

H 0 -5.3943812554 2.6470417566 0.7845795063

H 0 -5.5164228776 1.6370381997 2.2695233673

H 0 -10.0235060233 0.6801784162 0.2302971693

H 0 -11.0059637094 -1.4639869316 -1.141668495

H 0 -8.7716901594 -2.8912574131 -1.8564277062

int-4

B3LYP/6-311G**

E(RB3LYP) = -492.033860474

Zero-point correction= 0.100921 (Hartree/Particle)

Thermal correction to Energy= 0.110048

Thermal correction to Enthalpy= 0.110992

Thermal correction to Gibbs Free Energy= 0.065659

Sum of electronic and ZPE= -491.932940

Sum of electronic and thermal Energies= -491.923812

Sum of electronic and thermal Enthalpies= -491.922868

Sum of electronic and thermal Free Energies= -491.968202

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 69.056 32.927 95.412

C 0 -8.0463541765 -0.4407804785 -0.2878602162

C 0 -7.3318836579 0.5504562032 0.4381275423

H 0 -6.253764789 0.4332563133 0.4244416239

C 0 -7.8316507547 1.6125012972 1.1374530348

C 0 -9.370495854 -0.7194428469 -0.5616536459

C 0 -9.3828856028 -1.8860551994 -1.3647193153

C 0 -8.0758551894 -2.2485999022 -1.5328749619

O 0 -7.2539929364 -1.394203965 -0.8943288028

C 0 -6.9484966668 2.5097297925 1.8092653334

N 0 -6.2311852183 3.2348603162 2.3524369929

C 0 -9.2282897206 1.8801313714 1.2348186093

N 0 -10.3668050521 2.0703189067 1.2949519087

H 0 -10.2213926237 -0.1514654887 -0.2238718055

H 0 -10.2453571316 -2.3925320389 -1.7665647513

H 0 -7.5982906265 -3.057974281 -2.0598215464

TS-1-1

B3LYP/6-311G**=(qst3 maxcycle=300)

E(RB3LYP) = -914.158862259

Zero-point correction= 0.240491 (Hartree/Particle)

Thermal correction to Energy= 0.256533

Thermal correction to Enthalpy= 0.257478

Thermal correction to Gibbs Free Energy= 0.196363

Sum of electronic and ZPE= -913.918371

Sum of electronic and thermal Energies= -913.902329

Sum of electronic and thermal Enthalpies= -913.901385

Sum of electronic and thermal Free Energies= -913.962499

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 160.977 63.708 128.627

O 0 -0.1544798433 1.6859114971 1.8813111311

O 0 -2.2840210488 0.5609745475 -0.1745880276

O 0 -0.9746658165 -2.1471717447 -0.727643267

C 0 1.7093435661 -0.9440472214 -1.6504434478

C 0 2.8797930429 -0.2103862458 -1.8219276526

C 0 3.1111080381 0.964789035 -1.0899601336

C 0 2.1776242262 1.4287575164 -0.1684388562

C 0 1.0012556333 0.7001586739 -0.0061827208

C 0 0.769930858 -0.4747084748 -0.7369815401

C 0 -0.537253076 -1.0845761862 -0.3559034735

C 0 -1.2587674076 -0.014871455 0.5023579094

C 0 -0.124504561 0.9360522542 0.9248461556

H 0 1.5215711198 -1.8560459264 -2.2044546912

H 0 3.6283497083 -0.5490260685 -2.5292977569

H 0 4.0322183725 1.514362756 -1.2469262383

H 0 2.3466147843 2.3315075469 0.4063374562

C 0 -2.1182095364 -4.067549965 2.8354569544

C 0 -1.6099478465 -3.9225833149 4.1259702921

C 0 -1.2315644015 -2.6742446708 4.6026967477

C 0 -1.3573006384 -1.5285183073 3.80249615

C 0 -1.8898517771 -1.6903170305 2.5074874264

C 0 -2.2600991759 -2.9434682204 2.0302005554

N 0 -2.1017114863 -0.509627426 1.6955669357

N 0 -1.0524040025 -0.2595610122 4.2951573015

H 0 -2.4044593669 -5.0423344498 2.4611021605

H 0 -1.4988676318 -4.7904367584 4.766283216

H 0 -0.8280252196 -2.5737359089 5.6051062788

H 0 -2.642432202 -3.0226539617 1.0208711342

H 0 -2.8975294441 -0.2052518632 0.8170674275

H 0 -2.1623493094 0.3136402618 2.3033621947

H 0 -0.6054194211 0.3985615675 3.6676857887

H 0 -0.6277257668 -0.2537897244 5.2102848195

TS-1-2

B3LYP/6-311G**=(qst3 maxcycle=300)

E(RB3LYP) = -914.215390444

Zero-point correction= 0.243845 (Hartree/Particle)

Thermal correction to Energy= 0.260005

Thermal correction to Enthalpy= 0.260949

Thermal correction to Gibbs Free Energy= 0.199354

Sum of electronic and ZPE= -913.971546

Sum of electronic and thermal Energies= -913.955385

Sum of electronic and thermal Enthalpies= -913.954441

Sum of electronic and thermal Free Energies= -914.016036

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 163.156 64.255 129.637

C 0 3.7908669202 1.6942776769 -0.199366391

C 0 3.617802303 1.5073075195 1.1817523454

C 0 2.6461554747 0.6407358332 1.6712006674

C 0 1.8474165208 -0.0350180855 0.7507371799

C 0 2.0201796879 0.1515144368 -0.6264342357

C 0 2.9970272818 1.0158666041 -1.1178223302

C 0 0.7421730874 -0.9866371771 1.0155095096

C 0 0.2464403433 -1.5395201261 -0.3608226304

C 0 1.0742833822 -0.6961816813 -1.3856916112

O 0 0.9941674811 -0.8157265421 -2.5874879814

O 0 0.2714350881 -1.2693814764 2.0914759329

O 0 0.7218092652 -2.8687118137 -0.4573678663

N 0 -1.1766445393 -1.5231590015 -0.5004253331

C 0 -1.9705729611 -0.3376615572 -0.5417203273

C 0 -2.7644174287 -0.0202373422 0.588223069

C 0 -3.5582532735 1.1394626135 0.5414962239

C 0 -3.5670746446 1.9534205109 -0.5827152371

C 0 -2.7939587551 1.635013261 -1.699286779

C 0 -2.0095789436 0.4856325185 -1.6695681879

N 0 -2.7949616498 -0.8718785892 1.6779390361

H 0 4.5551965795 2.3787071023 -0.5494189541

H 0 4.2525397437 2.0501994222 1.8728675263

H 0 2.5024503026 0.4877193765 2.7340804325

H 0 3.1213043471 1.1487392736 -2.1858939487

H 0 0.775891721 -3.0742035843 -1.4011375262

H 0 -1.5821904617 -2.4008893171 -0.7855705509

H 0 -4.1734423627 1.3915714304 1.3996782039

H 0 -4.1877619951 2.8431277814 -0.5881026349

H 0 -2.8099886973 2.2644907966 -2.5808279648

H 0 -1.4135286125 0.2035334163 -2.5293957504

H 0 -3.0839338378 -0.4497060331 2.5475676627

H 0 -1.9728696668 -1.4567192768 1.772474141

TS-1-3

B3LYP/6-311G**=(calcall ts noeigentest)

E(RB3LYP) = -837.745190465

Zero-point correction= 0.216069 (Hartree/Particle)

Thermal correction to Energy= 0.230497

Thermal correction to Enthalpy= 0.231441

Thermal correction to Gibbs Free Energy= 0.173706

Sum of electronic and ZPE= -837.529121

Sum of electronic and thermal Energies= -837.514694

Sum of electronic and thermal Enthalpies= -837.513750

Sum of electronic and thermal Free Energies= -837.571485

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	144.639	57.111	121.513

C	0	4.782820742	0.0148616309	-0.3181138957
C	0	4.3189126582	-1.1986776901	-0.8512178826
C	0	2.9564404042	-1.4647509073	-0.9449583675
C	0	2.0676660193	-0.4945891307	-0.4879405929
C	0	2.5304088097	0.7165606464	0.0420921043
C	0	3.8934429858	0.9855826822	0.13279675
C	0	0.5796797981	-0.5442293277	-0.4786242144
C	0	0.1290273692	0.7771080472	0.1343783363
C	0	1.3851014749	1.5824569538	0.4354995266
O	0	1.4424646461	2.6920258219	0.9079885616
O	0	-0.1090156758	-1.4292150897	-0.9309152288
N	0	-1.0247001314	1.2728040669	0.3179352291
C	0	-2.2293754513	0.578497037	0.1487918894
C	0	-2.5263956887	-0.6250858824	0.823659333
C	0	-3.7904595587	-1.1897923907	0.6489365874
C	0	-4.7417927813	-0.6077449784	-0.1847895746
C	0	-4.4510217861	0.5952640224	-0.8255553778
C	0	-3.2168068584	1.1992043281	-0.6314145095
N	0	-1.5310492541	-1.2094897336	1.6759659354
H	0	5.8504744657	0.194285774	-0.2609410975
H	0	5.0365865332	-1.9353355493	-1.1941642628
H	0	2.5839210502	-2.3951405162	-1.3569023615
H	0	4.2371037966	1.9282892988	0.541786784
H	0	-4.0201282359	-2.1112292659	1.1746376415
H	0	-5.7083209455	-1.0802325708	-0.3166027775
H	0	-5.1894984417	1.070266283	-1.460993493
H	0	-2.9786687035	2.1481454223	-1.096496867
H	0	-1.7489226534	-1.0455435488	2.6544040865
H	0	-1.4841647573	-2.2118838333	1.5300065781

TS-1-4

B3LYP/6-311G**=(qst3 maxcycle=300)

E(RB3LYP) = -837.692609431

Zero-point correction= 0.213133 (Hartree/Particle)

Thermal correction to Energy= 0.227319

Thermal correction to Enthalpy= 0.228263

Thermal correction to Gibbs Free Energy= 0.172313

Sum of electronic and ZPE= -837.479477

Sum of electronic and thermal Energies= -837.465290

Sum of electronic and thermal Enthalpies= -837.464346

Sum of electronic and thermal Free Energies= -837.520296

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 142.645 57.687 117.757

C 0 4.4458236091 -0.3899903543 -0.4633178685

C 0 3.7999151619 -1.6336133781 -0.5304539811

C 0 2.4227530226 -1.7462060057 -0.3658401862

C 0 1.6932945392 -0.5826064556 -0.1392304724

C 0 2.3387689271 0.6668583392 -0.0848259432

C 0 3.7169985971 0.7733236205 -0.2376856351

C 0 0.2530639478 -0.3714452574 0.0615709865

C 0 0.010712938 1.0524943524 0.1060608508

C 0 1.3477386612 1.7599096975 0.1205755076

O 0 1.5522929376 2.9445827332 0.2316805021

N 0 -0.7915078131 -1.1905415155 -0.2058851809

C 0 -2.0630381453 -0.6523834099 -0.2247569714

C 0 -2.2330329058 0.7581676768 -0.1115503891

C 0 -3.1896860849 -1.4813322367 -0.3456658686

C 0 -4.4522687277 -0.920041139 -0.371172167

C 0 -4.6298542305 0.4741565214 -0.2826008843

C 0 -3.5332515515 1.3004169237 -0.1567763373

O 0 0.365464752 -1.7308403775 1.7709326318

H 0 -0.5878776989 -2.0156433408 0.4640649895

H 0 5.5210735185 -0.3400781188 -0.5897209156

H 0 4.3887131562 -2.5267670347 -0.7062192614

H 0 1.9356476366 -2.7115714382 -0.3851646175

H 0 4.1941567551 1.7449057531 -0.1851192484

H 0 -3.0507072627 -2.5532909725 -0.4242741502

H 0 -5.3186275113 -1.5644794414 -0.4661071183

H 0 -5.628342864 0.8928156799 -0.3116726631

H 0 -3.6277472283 2.3765047483 -0.0790041118

H 0 -0.1561100269 -1.4254389682 2.5246545786

N 0 -1.159867119 1.6061333982 0.0416808944

TS-2-1

B3LYP/6-311G**=(qst3 maxcycle=300)

E(RB3LYP) = -1085.09640217

Zero-point correction= 0.297081 (Hartree/Particle)

Thermal correction to Energy= 0.316262

Thermal correction to Enthalpy= 0.317206

Thermal correction to Gibbs Free Energy= 0.248464

Sum of electronic and ZPE= -1084.799321

Sum of electronic and thermal Energies= -1084.780140

Sum of electronic and thermal Enthalpies= -1084.779196

Sum of electronic and thermal Free Energies= -1084.847939

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 198.457 76.037 144.681

C 0 -9.1256506174 0.9481904946 1.1539535363

C 0 -8.4123996208 2.1018966622 0.8101345422

C 0 -7.0890866273 2.0191460807 0.3811249275

C 0 -6.5080577706 0.7580406029 0.2726939203

C 0 -7.2363147578 -0.4037732643 0.5714244364

C 0 -8.5361296515 -0.3136889799 1.050706744

C 0 -5.1212403341 0.3757005742 -0.0117955611

C 0 -5.0018677541 -1.0491861299 0.1279090158

C 0 -6.377585925 -1.6584928149 0.4277523542

O 0 -6.5368124765 -2.6488543344 1.3031480633

N 0 -4.1119039946 1.1621439165 -0.2811122383

C 0 -2.9016097889 0.5308596267 -0.4004120605

C 0 -2.7747299446 -0.884359604 -0.2284437785

N 0 -3.8664789175 -1.6763971401 0.0322091858

C 0 -1.7475748793 1.2949672766 -0.687206625

C 0 -0.5192077645 0.6832463944 -0.7926450285

C 0 -0.393700085 -0.7128222876 -0.615021944

C 0 -1.5003447478 -1.4832294865 -0.3377502014

H 0 -10.1419270999 1.0382330098 1.5208950798

H 0 -8.887726608 3.0716283774 0.9050057249

H 0 -6.5105441203 2.9078771617 0.1587289842

H 0 -9.0669431173 -1.2080164307 1.3579604185

H 0 -1.8694230661 2.3640954663 -0.8129270739

H 0 0.3625156296 1.2750590405 -1.0105738697

H 0 0.5824215366 -1.1767357368 -0.6978345781

H 0 -1.432095647 -2.555064021 -0.195209218

C 0 -5.8437343831 -3.2969658354 -1.6087058044

N 0 -6.9140691848 -2.6021729734 -0.8657402806

C 0 -7.9951815279 -2.1492657067 -1.7405152963

C 0 -8.8916945641 -3.2925136825 -2.1849784316

O 0 -9.8314207324 -2.8341963805 -3.0405978226

O 0 -8.813660437 -4.4389878253 -1.8352419101

H 0 -5.0808775737 -3.6158638539 -0.9027847024

H 0 -6.2755674041 -4.1700952055 -2.0992216734

H 0 -5.3895249196 -2.6390219735 -2.3558574884

H 0 -7.0856536506 -3.1729257658 0.2268572151

H 0 -8.6237964987 -1.4282174745 -1.2162611142

H 0 -7.6066741561 -1.6409599822 -2.6306524534

H 0 -10.3895179282 -3.5898784654 -3.278829234

TS-2-2

B3LYP/6-311G**=(qst3 maxcycle=300)

E(RB3LYP) = -1085.12351825

Zero-point correction= 0.297327 (Hartree/Particle)

Thermal correction to Energy= 0.316227

Thermal correction to Enthalpy= 0.317171

Thermal correction to Gibbs Free Energy= 0.250219

Sum of electronic and ZPE= -1084.826191

Sum of electronic and thermal Energies= -1084.807292

Sum of electronic and thermal Enthalpies= -1084.806348

Sum of electronic and thermal Free Energies= -1084.873299

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	198.435	76.241	140.911

C	0	-1.6928755271	4.3803353222	-0.7837211818
C	0	-0.3875565452	4.8746182758	-0.813214274
C	0	0.6941012841	4.0137141566	-0.6428912539
C	0	0.4425034504	2.6595080757	-0.4644934101
C	0	-0.8691470024	2.1411923052	-0.4731666952
C	0	-1.9455031723	3.0183654732	-0.6083718855
C	0	1.3833367116	1.5741372337	-0.1989289712
C	0	0.645500573	0.3579020324	-0.0298605023
C	0	-0.817188007	0.6633945031	-0.2237069617
N	0	2.6839800704	1.6463526728	-0.1141577712
C	0	3.3174496028	0.4639273671	0.1569511209
C	0	2.5837750053	-0.7555067773	0.3150248386
N	0	1.2178764355	-0.784091967	0.2100658288
C	0	4.7248040904	0.4417224447	0.279668202
C	0	5.3755761452	-0.7407396786	0.5474319482
C	0	4.6502713859	-1.9440866449	0.7021273583
C	0	3.2790304558	-1.954224082	0.5880501706
O	0	-1.1514085284	0.7160973491	1.8041425349
N	0	-1.6875664163	-0.2207903226	-0.6925235404
C	0	-2.9965972185	0.178787707	-1.2215756408
C	0	-1.6231472444	-1.6452651629	-0.3130175286
C	0	-2.5956670165	-2.0003336623	0.8707102579
O	0	-2.7569077436	-1.0916617714	1.7664923539
O	0	-3.0997461883	-3.1073136155	0.829722012
H	0	-1.9187692229	-0.1514190541	1.819833168
H	0	-2.5277688363	5.062731707	-0.8913152106
H	0	-0.2180774694	5.9357388472	-0.9538749269
H	0	1.7143105468	4.3773765028	-0.6342451091
H	0	-2.9688611959	2.6772786452	-0.5571992498
H	0	5.25811628	1.376508168	0.1574480953
H	0	6.4551984695	-0.753558365	0.6423457869
H	0	5.1818397871	-2.8642635365	0.9143756812
H	0	2.700924048	-2.8624314351	0.7069785108
H	0	-1.6249438334	1.5235838336	2.0350413276
H	0	-3.6674182524	0.4738784964	-0.4104856282
H	0	-2.88900495	0.9838497345	-1.9454915424
H	0	-3.4280337067	-0.68738275	-1.7199075625
H	0	-0.6066325488	-1.8944139872	-0.0210611319
H	0	-1.9104736961	-2.2465180608	-1.1741992075

TS-2-3

B3LYP/6-311G**=(qst3 maxcycle=300)

E(RB3LYP) = -1008.67351052

Zero-point correction= 0.273575 (Hartree/Particle)

Thermal correction to Energy= 0.291065

Thermal correction to Enthalpy= 0.292009

Thermal correction to Gibbs Free Energy= 0.227322

Sum of electronic and ZPE= -1008.399936

Sum of electronic and thermal Energies= -1008.382445

Sum of electronic and thermal Enthalpies= -1008.381501

Sum of electronic and thermal Free Energies= -1008.446189

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.646	69.661	136.146

C	0	-9.5632155798	-1.4693880733	0.2691278975
C	0	-8.9231857312	-2.6996051309	0.4242275857
C	0	-7.5299852821	-2.7689891439	0.4416149726
C	0	-6.8082307848	-1.5985044479	0.2731465679
C	0	-7.4431871693	-0.3445239278	0.0674243356
C	0	-8.8439121479	-0.2848819827	0.0959530063
C	0	-5.3680842338	-1.3866984853	0.333695957
C	0	-5.1102589267	0.024882029	0.1823344727
C	0	-6.4062584942	0.6938230812	-0.0490329779
N	0	-4.4302060343	-2.2764115432	0.5108410245
C	0	-3.1532684793	-1.7851744239	0.5508455602
C	0	-2.8871202764	-0.3855005762	0.4019437747
N	0	-3.8964077808	0.5174494179	0.2137424446
C	0	-2.0739382505	-2.6752847089	0.7444590191
C	0	-0.7830839498	-2.1996751564	0.7891673554
C	0	-0.5200791979	-0.8185817745	0.6426258733
C	0	-1.5504461757	0.073124721	0.4531739906
N	0	-6.5877668622	1.959414732	-0.4071397596
C	0	-5.515200643	2.968527511	-0.2594494968
C	0	-7.8190658255	2.5065929015	-0.7773264379
C	0	-8.7522273759	3.1729571418	0.6922079617
O	0	-9.9177382975	2.9014174541	0.5183775164
O	0	-7.9891311942	3.7276120992	1.4475618471
H	0	-10.6455026181	-1.4213941696	0.2945276651
H	0	-9.5116230406	-3.6005014495	0.5535038988
H	0	-7.0093566899	-3.7062923536	0.5960625849
H	0	-9.3896779187	0.6459446476	0.0398352176
H	0	-2.30222254	-3.7283396873	0.8552608034
H	0	0.0415532037	-2.8869439529	0.9384906228
H	0	0.5028825591	-0.4627490772	0.6810612273
H	0	-1.3721148854	1.1356147893	0.339502815
H	0	-5.374674377	3.460725656	-1.2228585662
H	0	-5.8866952135	3.6870356525	0.4748143812
H	0	-4.5935259223	2.5035901859	0.0666138564
H	0	-7.677697147	3.4153141134	-1.3540700137
H	0	-8.4868764672	1.8000423616	-1.2483826832

3.3.3 Solution-phase calculation (using SMD model)

1 ninhydrin

B3LYP/6-311G**

E(RB3LYP) = -647.646037840

Zero-point correction= 0.134798 (Hartree/Particle)

Thermal correction to Energy= 0.145321

Thermal correction to Enthalpy= 0.146265

Thermal correction to Gibbs Free Energy= 0.098018

Sum of electronic and ZPE= -647.511239

Sum of electronic and thermal Energies= -647.500717

Sum of electronic and thermal Enthalpies= -647.499772

Sum of electronic and thermal Free Energies= -647.548019

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 91.190 40.549 101.544

O 0 5.0889910094 2.1007102792 0.8085221679

O 0 4.5401689484 1.9405350249 3.6891218992

O 0 3.3278741093 0.331366682 2.5004638517

O 0 1.5444741911 2.144748282 3.9689464435

C 0 0.9200615388 4.2647173904 1.8048975924

C 0 0.9162604209 5.123416432 0.709759101

C 0 1.9667415883 5.1138326135 -0.2220450284

C 0 3.0443906459 4.2447734362 -0.0802305634

C 0 3.0490472651 3.384445776 1.0158822008

C 0 1.9987262571 3.3942661639 1.9478797998

C 0 2.2357386001 2.3916636137 3.0033202486

C 0 3.5844606001 1.6946060456 2.6949677844

C 0 4.0653101815 2.3846396692 1.3939371997

H 0 0.111270683 4.26774355 2.5261247071

H 0 0.0909981111 5.8121169279 0.5702260911

H 0 1.9340230919 5.7958530216 -1.0638584437

H 0 3.8578453447 4.2343130464 -0.7961245328

H 0 4.1736857647 1.6400816988 4.5350857945

H 0 4.1391316484 -0.0790296536 2.1633236865

1p

B3LYP/6-311G**

E(RB3LYP) = -571.169052290

Zero-point correction= 0.107556 (Hartree/Particle)

Thermal correction to Energy= 0.116365

Thermal correction to Enthalpy= 0.117309

Thermal correction to Gibbs Free Energy= 0.073055

Sum of electronic and ZPE= -571.061496

Sum of electronic and thermal Energies= -571.052688

Sum of electronic and thermal Enthalpies= -571.051743

Sum of electronic and thermal Free Energies= -571.095997

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 73.020 33.548 93.140

O 0 -1.0354792127 -2.3886388256 -0.2455587286

O 0 -2.7653386111 -0.0063710627 -0.4818430791

O 0 -1.0328797189 2.381443167 -0.3391093379

C 0 1.9010476591 1.4220998462 0.0009300132

C 0 3.0838138713 0.705717932 0.1444852071

C 0 3.0830474354 -0.6997270164 0.1720535435

C 0 1.8994977992 -1.4198975425 0.0566770929

C 0 0.7101451462 -0.7078166153 -0.0875143167

C 0 0.7109162963 0.7062092211 -0.1152512876

C 0 -0.6536915829 1.2322168299 -0.2749642867

C 0 -1.5704725742 -0.0044572128 -0.3510553964

C 0 -0.6550390495 -1.2381947399 -0.2265037696

H 0 1.8977412438 2.505432401 -0.0207465004

H 0 4.0248131201 1.2355762226 0.2370577011

H 0 4.0234704225 -1.226573038 0.2853537464

H 0 1.8950097554 -2.5032425632 0.0775013987

2 o-Phenylenediamine

B3LYP/6-311G**

E(RB3LYP) = -343.061649070

Zero-point correction= 0.130037 (Hartree/Particle)

Thermal correction to Energy= 0.136479

Thermal correction to Enthalpy= 0.137423

Thermal correction to Gibbs Free Energy= 0.099731

Sum of electronic and ZPE= -342.931612

Sum of electronic and thermal Energies= -342.925170

Sum of electronic and thermal Enthalpies= -342.924226

Sum of electronic and thermal Free Energies= -342.961918

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 85.642 25.551 79.329

C 0 -6.2025877472 1.3497700567 -0.3572786031

C 0 -5.6691666735 0.1080172647 -0.025713668

C 0 -6.5292202824 -0.9552750464 0.2562982556

C 0 -7.9232292387 -0.8142844874 0.2167195488

C 0 -8.4694817736 0.4573356955 -0.1228561602

C 0 -7.5888260351 1.5113890674 -0.402359597

N 0 -9.8354962803 0.6560898539 -0.1777843096

N 0 -8.7417957198 -1.8899232837 0.5021373911

H 0 -5.5553320673 2.1910520555 -0.5804489092

H 0 -4.5958198261 -0.042607581 0.0159702997

H 0 -6.1225671306 -1.9287015878 0.5162168988

H 0 -8.0150987155 2.476940636 -0.6602038633

H 0 -10.1962117489 1.5631488104 -0.4203711906

H 0 -10.5072469024 -0.064598045 0.0126927375

H 0 -9.7439674322 -1.8412810281 0.4877599568

H 0 -8.3316524264 -2.7772723808 0.7390212126

3 sarcosine

B3LYP/6-311G**

E(RB3LYP) = -323.846220743

Zero-point correction= 0.107102 (Hartree/Particle)

Thermal correction to Energy= 0.113992

Thermal correction to Enthalpy= 0.114937

Thermal correction to Gibbs Free Energy= 0.075898

Sum of electronic and ZPE= -323.739119

Sum of electronic and thermal Energies= -323.732228

Sum of electronic and thermal Enthalpies= -323.731284

Sum of electronic and thermal Free Energies= -323.770323

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 71.531 23.201 82.164

C 0 -9.5864897457 -0.1633546282 0.0408161031

N 0 -8.3164209884 0.5514493644 0.163545832

C 0 -7.175083331 -0.3439253971 0.0749359227

C 0 -5.8762335711 0.4200042088 0.0162706893

O 0 -4.8164157876 -0.3904018604 0.1784536556

O 0 -5.7728982647 1.6103872235 -0.1815807849

H 0 -10.4080977751 0.5565917317 0.048169179

H 0 -9.6684005272 -0.7712805055 -0.8753352219

H 0 -9.7207177745 -0.8323068166 0.8964423717

H 0 -8.245158094 1.2316843244 -0.5878520135

H 0 -7.1451638813 -1.0067107899 0.9456317829

H 0 -7.1877324664 -1.0039928517 -0.8118368441

H 0 -4.0074877932 0.1419559966 0.0921393281

4 malononitrile

B3LYP/6-311G**

E(RB3LYP) = -225.052481572

Zero-point correction= 0.044822 (Hartree/Particle)

Thermal correction to Energy= 0.049603

Thermal correction to Enthalpy= 0.050547

Thermal correction to Gibbs Free Energy= 0.017193

Sum of electronic and ZPE= -225.007659

Sum of electronic and thermal Energies= -225.002879

Sum of electronic and thermal Enthalpies= -225.001935

Sum of electronic and thermal Free Energies= -225.035288

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 31.126 15.133 70.198

C 0 -8.3734106755 -0.4551976855 -0.0000538997

C 0 -7.0900746713 0.2425816895 0.0000803799

N 0 -6.0695632734 0.7740229416 0.0001962015

C 0 -9.5081119765 0.4647469758 0.0000846285

N 0 -10.4146836924 1.1732672152 0.0002039496

H 0 -8.4326164595 -1.0995713552 -0.8833799704

H 0 -8.4326392514 -1.0998497813 0.8830687107

5 furfural

B3LYP/6-311G**

E(RB3LYP) = -343.448370579

Zero-point correction= 0.079200 (Hartree/Particle)

Thermal correction to Energy= 0.084737

Thermal correction to Enthalpy= 0.085681

Thermal correction to Gibbs Free Energy= 0.049773

Sum of electronic and ZPE= -343.369170

Sum of electronic and thermal Energies= -343.363634

Sum of electronic and thermal Enthalpies= -343.362690

Sum of electronic and thermal Free Energies= -343.398598

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 53.173 19.887 75.575

C 0 -7.9051615208 0.4017673833 0.2986540641

C 0 -9.2582246329 0.2599762119 0.1170639663

C 0 -9.4400079775 -0.8940509475 -0.6877741781

C 0 -8.1888519345 -1.3805401173 -0.9446805577

O 0 -7.2436085645 -0.6124107637 -0.3577164587

C 0 -7.0958534873 1.3636995448 1.0104582239

H 0 -6.0073702274 1.181746324 0.9528254899

O 0 -7.5552746113 2.3107061293 1.6330626232

H 0 -10.0184804891 0.9123304892 0.5184504892

H 0 -10.3711212824 -1.3144917386 -1.0347061916

H 0 -7.8290452722 -2.2287325153 -1.5056374707

6

B3LYP/6-311G**

E(RB3LYP) = -1312.14714094

Zero-point correction= 0.365486 (Hartree/Particle)

Thermal correction to Energy= 0.389647

Thermal correction to Enthalpy= 0.390591

Thermal correction to Gibbs Free Energy= 0.311705

Sum of electronic and ZPE= -1311.781655

Sum of electronic and thermal Energies= -1311.757494

Sum of electronic and thermal Enthalpies= -1311.756550

Sum of electronic and thermal Free Energies= -1311.835436

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 244.507 96.127 166.030

C 0 -9.3648457405 0.3662535905 -0.0744453454

C 0 -9.6584839811 -1.0146633996 -0.0102797814

C 0 -8.6469057199 -1.9484116658 -0.0277138549

C 0 -7.2980032301 -1.5340571671 -0.1106518495

C 0 -7.0026634278 -0.1351171051 -0.1721419423

C 0 -8.0602358144 0.8000927924 -0.154357795

N 0 -6.3046234381 -2.4776868973 -0.136568032

C 0 -5.0857146421 -2.007697386 -0.2177269881

C 0 -4.7880576644 -0.6080302759 -0.2595308539

N 0 -5.7054307445 0.314690277 -0.2432514186

C 0 -3.831777668 -2.7510578871 -0.3164953184

C 0 -2.7696612675 -1.8374267966 -0.4367506822

C 0 -3.2629636165 -0.3905195913 -0.3525218497

C 0 -3.6130504831 -4.1264341547 -0.3647513773

C 0 -2.3110370942 -4.5834436935 -0.5509350021

C 0 -1.2564389971 -3.6781121224 -0.7045853676

C 0 -1.4771065615 -2.299465574 -0.6554253807

C 0 -2.7489338096 0.4435593274 0.9046862294

C 0 -3.1344591786 1.9240787595 0.4592456958

C 0 -2.9626623421 1.8797216969 -1.074610821

N 0 -2.7641757781 0.4645808059 -1.424900642

C 0 -2.4386856819 3.0243972996 1.1734823802

H 0 -4.1946130002 2.0125860467 0.6906314001

C 0 -3.1604605989 0.121204894 -2.7861041899

C 0 -2.830347222 3.8482920287 2.1850967789

C 0 -1.7244106334 4.7174358682 2.460453388

C 0 -0.7395657123 4.3631363857 1.5964247813

O 0 -1.154171515 3.3325848161 0.8010445373

C 0 -3.3990798617 0.0764883434 2.1632308784

N 0 -3.9160335478 -0.1942331675 3.1562150925

C 0 -1.2996662642 0.3016589854 1.0802697422

N 0 -0.1636703596 0.2098467095 1.2458638132

H 0 -10.175129804 1.0861782566 -0.0597913392

H 0 -10.6913889087 -1.3379585932 0.0525549005

H 0 -8.8535204067 -3.0115062094 0.0188349216

H 0 -7.8154290402 1.8550053835 -0.2035109372

H 0 -4.4419686728 -4.8184116772 -0.2716845917

H 0 -2.1140734328 -5.648769282 -0.5927885047

H 0 -0.251651318 -4.0498824169 -0.8708857293

H 0 -0.651970911 -1.6140472931 -0.7968662231

H 0 -3.8600865093 2.3005114856 -1.5436689352

H 0 -2.1001880172 2.4595331366 -1.4093080806

H 0 -2.9218102067 -0.922802498 -2.995384202

H 0 -2.5909892775 0.7417606638 -3.4820452829

H 0 -4.2311804688 0.2860290923 -2.9778248971

H 0 -3.7928833144 3.8372917038 2.6733288104

H 0 -1.6758235442 5.502197932 3.1996265316

H 0 0.2612294283 4.7208185728 1.4164173333

int-1A

B3LYP/6-311G**

E(RB3LYP) = -914.246113924

Zero-point correction= 0.244591 (Hartree/Particle)

Thermal correction to Energy= 0.261125

Thermal correction to Enthalpy= 0.262069

Thermal correction to Gibbs Free Energy= 0.200166

Sum of electronic and ZPE= -914.001523

Sum of electronic and thermal Energies= -913.984989

Sum of electronic and thermal Enthalpies= -913.984045

Sum of electronic and thermal Free Energies= -914.045948

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 163.858 65.668 130.286

C 0 -10.2463097245 -1.8048007137 -0.2960458406

C 0 -10.1952908965 -1.1617948796 -1.5433067499

C 0 -8.9852839014 -0.7335974113 -2.0812776948

C 0 -7.824690558 -0.965673357 -1.3462099507

C 0 -7.8754718009 -1.6099255026 -0.098048452

C 0 -9.088406645 -2.0340857167 0.4411483979

C 0 -6.4354064005 -0.5893917809 -1.6844087695

C 0 -5.5109960437 -1.2316045681 -0.6076532788

C 0 -6.5196543608 -1.726240822 0.4758733835

O 0 -6.2062565073 -2.1393633137 1.5724438364

O 0 -6.0516790575 0.0477613137 -2.6407609909

O 0 -4.8700710035 -2.3662639088 -1.1895616804

N 0 -4.4214329741 -0.4182476012 -0.1609392577

C 0 -4.5330543586 0.8437140126 0.450768769

C 0 -3.3186790161 1.4017449517 0.9335122021

C 0 -3.3392981879 2.6509476109 1.5538428288

C 0 -4.5286941173 3.3680316945 1.6944857573

C 0 -5.7126181554 2.8351302255 1.1993124165

C 0 -5.7133855744 1.5771220795 0.5890326089

N 0 -2.1416588799 0.6439018973 0.8280354236

H 0 -11.2050431184 -2.1249413047 0.0955369883

H 0 -11.1155040559 -0.9961513923 -2.091639339

H 0 -8.9414893749 -0.2324955811 -3.0411025552

H 0 -9.1225284941 -2.5289036548 1.4046277976

H 0 -5.5219718194 -3.0579395354 -1.3714617828

H 0 -3.721818215 -1.0033741467 0.2888454268

H 0 -2.403872337 3.0640477586 1.9189168215

H 0 -4.5190773762 4.3391922745 2.1768121907

H 0 -6.6451898579 3.380392962 1.2917161583

H 0 -6.6570857261 1.1845755298 0.2343531058

H 0 -1.3129589121 1.164066861 1.0906175932

H 0 -2.0103225498 0.2245660192 -0.0874653639

int-1B

B3LYP/6-311G**

E(RB3LYP) = -837.780645760

Zero-point correction= 0.216324 (Hartree/Particle)

Thermal correction to Energy= 0.231164

Thermal correction to Enthalpy= 0.232109

Thermal correction to Gibbs Free Energy= 0.174019

Sum of electronic and ZPE= -837.564322

Sum of electronic and thermal Energies= -837.549481

Sum of electronic and thermal Enthalpies= -837.548537

Sum of electronic and thermal Free Energies= -837.606627

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 145.058 59.224 122.260

C 0 -9.874808174 1.4245841806 -1.5926751141

C 0 -8.758488149 1.4943716225 -2.4388891155

C 0 -7.5459283206 0.9071486651 -2.0797747582

C 0 -7.4754024726 0.2593281334 -0.85124596

C 0 -8.5934195518 0.1866155903 -0.0056120949

C 0 -9.805006435 0.7667258177 -0.3654887362

C 0 -6.3146839809 -0.4329015473 -0.23550495

C 0 -6.7869582237 -0.9343656518 1.0998840883

C 0 -8.2497746274 -0.5842775024 1.2120657072

O 0 -8.9909262399 -0.8732510464 2.1335334832

O 0 -5.227655728 -0.6262593589 -0.7510810374

N 0 -6.2337429307 -1.6862489227 1.9844672315

C 0 -4.9072486188 -2.0432503463 2.1166110808

C 0 -3.775083368 -1.1766194837 1.9617416213

C 0 -2.4912090348 -1.7183519074 2.2048928903

C 0 -2.3175284063 -3.032469004 2.5881110114

C 0 -3.4276952106 -3.8702699625 2.7939592505

C 0 -4.6920264335 -3.3582669368 2.5996789095

N 0 -3.8808804846 0.1430542941 1.6381167227

H 0 -10.8048707076 1.8875224827 -1.9021645654

H 0 -8.8432129311 2.0139015265 -3.3865392209

H 0 -6.6818044135 0.9570665836 -2.7320680565

H 0 -10.6667445637 0.7037224384 0.2888654815

H 0 -1.6324937148 -1.0670361807 2.0770744728

H 0 -1.3142542665 -3.4103241706 2.7523899606

H 0 -3.292956543 -4.8955816552 3.1168886028

H 0 -5.5730946528 -3.9647854564 2.7753952963

H 0 -3.0981089972 0.7383194413 1.8698186945

H 0 -4.7803928194 0.598798357 1.670749104

int-1C

B3LYP/6-311G**

E(RB3LYP) = -837.792070216

Zero-point correction= 0.218522 (Hartree/Particle)

Thermal correction to Energy= 0.232253

Thermal correction to Enthalpy= 0.233197

Thermal correction to Gibbs Free Energy= 0.178415

Sum of electronic and ZPE= -837.573548

Sum of electronic and thermal Energies= -837.559817

Sum of electronic and thermal Enthalpies= -837.558873

Sum of electronic and thermal Free Energies= -837.613655

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	145.741	57.014	115.299

C 0 4.4436437613 -0.5258775437 -0.5464140996

C 0 3.8333840248 -1.7572704934 -0.2754833305

C 0 2.4819469871 -1.8358937216 0.0703707212

C 0 1.7485366902 -0.6593073998 0.1211123312

C 0 2.358187203 0.5743173188 -0.1475642811

C 0 3.7098553405 0.6542185717 -0.4819140602

C 0 0.3001601689 -0.4586989877 0.5303277965

C 0 0.0586381739 1.0004617765 0.1830786476

C 0 1.3735866528 1.675745864 -0.0525693922

O 0 1.5706840717 2.87080882 -0.192832348

N 0 -0.6872087912 -1.2226796161 -0.173485794

C 0 -1.982286815 -0.738389079 -0.1924808704

C 0 -2.1816995831 0.6647586687 -0.0696358541

C 0 -3.093615686 -1.5722524019 -0.3862401627

C 0 -4.3701640585 -1.0304162033 -0.4212925681

C 0 -4.5751737811 0.3502370704 -0.2765012369

C 0 -3.4837966457 1.1873345917 -0.1178853851

O 0 0.2716629532 -0.671097401 1.9536205551

H 0 -0.5635185682 -2.2276334506 -0.2150595314

H 0 5.4950798851 -0.4965287694 -0.8083397611

H 0 4.4225417751 -2.6659128415 -0.3308073185

H 0 2.0255609779 -2.7940796566 0.2914204447

H 0 4.1678557856 1.6149786865 -0.6889315504

H 0 -2.9411891667 -2.6408917677 -0.4954579127

H 0 -5.2203047128 -1.6891244321 -0.5612308309

H 0 -5.5786601936 0.7579757303 -0.3032653713

H 0 -3.6031779789 2.2617319013 -0.0329599421

H 0 -0.600634174 -0.4173931179 2.2871445069

N 0 -1.0912573563 1.5313070935 -0.024689432

int-1

B3LYP/6-311G**

E(RB3LYP) = -761.346192596

Zero-point correction= 0.191889 (Hartree/Particle)

Thermal correction to Energy= 0.203814

Thermal correction to Enthalpy= 0.204758

Thermal correction to Gibbs Free Energy= 0.153466

Sum of electronic and ZPE= -761.154304

Sum of electronic and thermal Energies= -761.142379

Sum of electronic and thermal Enthalpies= -761.141435

Sum of electronic and thermal Free Energies= -761.192727

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	127.895	49.487	107.953

C 0 -4.4748691761 -0.5427392282 0.0000411271

C 0 -3.8232715657 -1.7807893631 0.0000237473

C 0 -2.4276220206 -1.8673990375 0.0000118708

C 0 -1.699912612 -0.6855659351 0.0000168693

C 0 -2.3569117573 0.562777803 0.0000310374

C 0 -3.7432734849 0.6462898315 0.0000450929

C 0 -0.2450778937 -0.4499514921 0.0000153037

C 0 -0.0192362677 0.9627364311 0.0000251464

C 0 -1.3544063983 1.6619532336 0.0000258876

O 0 -1.5521439765 2.8608880867 0.0000662332

N 0 0.7243810922 -1.3249547713 0.0000067516

C 0 1.9899075058 -0.7883512937 0.0000098909

C 0 2.2095036043 0.6291964375 0.000022247

N 0 1.1598440312 1.5141619509 0.0000302505

C 0 3.1046546419 -1.6532775879 0.0000015089

C 0 4.3828086681 -1.1375557476 0.0000052088

C 0 4.598315169 0.2584564993 0.0000175945

C 0 3.530606471 1.1281149119 0.0000261786

H 0 -5.5581996734 -0.5092614318 0.0000509879

H 0 -4.4127104033 -2.690756225 0.0000210221

H 0 -1.929957867 -2.8298761977 0.0000011417

H 0 -4.2390891782 1.6103971922 0.0000571107

H 0 2.9238137953 -2.7219359289 -0.0000078452

H 0 5.2346192571 -1.8081772971 -0.000001241

H 0 5.611583368 0.64313926 0.0000203141

H 0 3.6716736709 2.2028118992 0.0000355633

int-2A

B3LYP/6-311G**

E(RB3LYP) = -1085.18882506

Zero-point correction= 0.301862 (Hartree/Particle)

Thermal correction to Energy= 0.321208

Thermal correction to Enthalpy= 0.322153

Thermal correction to Gibbs Free Energy= 0.253532

Sum of electronic and ZPE= -1084.886963

Sum of electronic and thermal Energies= -1084.867617

Sum of electronic and thermal Enthalpies= -1084.866673

Sum of electronic and thermal Free Energies= -1084.935293

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	201.561	77.079	144.425

C	0	-9.1821512255	1.8980592642	0.4848866786
C	0	-8.4639447072	3.0886894014	0.3260906878
C	0	-7.0728804487	3.0745806409	0.2493003644
C	0	-6.4176798613	1.8467600839	0.3344978299
C	0	-7.1377388839	0.6525312835	0.4918929039
C	0	-8.5232235809	0.6689034789	0.5681106855
C	0	-4.9882169333	1.5307809496	0.29430908
C	0	-4.8304241912	0.116879871	0.4671900949
C	0	-6.2051570659	-0.5601970703	0.6110514659
N	0	-3.9792319208	2.3501657778	0.1404623529
C	0	-2.7400259576	1.7615402762	0.1499958848
C	0	-2.5837347867	0.3497383882	0.3207051799
N	0	-3.6734169373	-0.4753883337	0.4843715881
C	0	-1.5891072518	2.5660627015	-0.0111487687
C	0	-0.3361345941	1.9945251602	-0.0027878254
C	0	-0.1834281661	0.6002463488	0.1664082545
C	0	-1.2872192664	-0.2085357687	0.3259052581
O	0	-6.2468244175	-1.1194827056	1.9156537125
N	0	-6.5316342798	-1.595911975	-0.3734039367
C	0	-6.6150687648	-1.1427844783	-1.7651975108
C	0	-5.7415539778	-2.8136535818	-0.2514783475
C	0	-6.5459717231	-4.0568053405	-0.5777791873
O	0	-5.7411241812	-5.1335727758	-0.6363731302
O	0	-7.7420366135	-4.1180434114	-0.7486945009
H	0	-6.2871909233	-5.9180599927	-0.8129925488
H	0	-10.2645861981	1.9303856366	0.5412272596
H	0	-8.9971224525	4.0306542687	0.2624076765
H	0	-6.5109128369	3.9934495447	0.1269275703
H	0	-9.0861082025	-0.2511202546	0.68144097
H	0	-1.7253226732	3.6339765116	-0.1391343981
H	0	0.5428714651	2.6169685045	-0.1267103173
H	0	0.8105476877	0.1676187108	0.1705952814
H	0	-1.1915627288	-1.2803748309	0.4578164348
H	0	-7.1393675905	-1.4691600626	2.054378584
H	0	-7.0158118406	-1.9539772606	-2.3756269795
H	0	-7.2962110895	-0.2972235883	-1.8541436099
H	0	-5.637651343	-0.8535963979	-2.1808154389
H	0	-5.4002938616	-2.9326859363	0.7780582754
H	0	-4.8448476759	-2.8155430381	-0.8855975738

int-2B

B3LYP/6-311G**

E(RB3LYP) = -1008.71567825

Zero-point correction= 0.255069 (Hartree/Particle)

Thermal correction to Energy= 0.273708

Thermal correction to Enthalpy= 0.274652

Thermal correction to Gibbs Free Energy= 0.204232

Sum of electronic and ZPE= -1008.460610

Sum of electronic and thermal Energies= -1008.441971

Sum of electronic and thermal Enthalpies= -1008.441026

Sum of electronic and thermal Free Energies= -1008.511446

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	171.754	70.056	148.212

C	0	2.9488553497	2.7801158031	-0.0205985924
C	0	1.8788359731	3.6572321826	0.1508069661
C	0	0.5691699431	3.1747114652	0.16481764
C	0	0.3651587104	1.8165881895	-0.0083206444
C	0	1.4385729284	0.9091263493	-0.2092057951
C	0	2.7473098677	1.4100585468	-0.1981551007
C	0	-0.8902126005	1.0726244578	0.0122749515
C	0	-0.595029056	-0.31811566	-0.1626161101
C	-1	0.879761	-0.453722	-0.350604
N	0	-2.09894193	1.5383310333	0.1686762068
C	0	-3.0975001691	0.5999454958	0.1632374067
C	0	-2.8074504796	-0.7930831995	-0.0040436669
N	0	-1.5239062645	-1.2355716791	-0.1711217732
C	0	-4.4376708906	1.0086713065	0.3275715338
C	0	-5.4489472667	0.0728306414	0.3276745375
C	0	-5.1626972931	-1.301651362	0.1646661235
C	0	-3.8650345335	-1.7305840224	0.0015274165
N	-1	1.513318	-1.562264	-0.661277
C	0	0.8917037018	-2.8972941052	-0.6612090845
C	-1	2.930705	-1.575673	-0.849379
C	-1	3.780454	-1.535466	0.590094
O	0	5.0035058855	-1.445949286	0.4004646143
O	0	3.1072388956	-1.6053430745	1.6263721879
H	0	3.9630157425	3.1612874845	-0.0123357064
H	0	2.065970428	4.7164504852	0.2840659631
H	0	-0.2727027914	3.8399057291	0.3141399284
H	0	3.6188085872	0.7851904697	-0.3035729671
H	0	-4.6410759195	2.0657330034	0.4528708825
H	0	-6.4774636098	0.3907716762	0.4546051358
H	0	-5.9743736797	-2.019850355	0.1686570929
H	0	-3.6251058169	-2.7798214379	-0.1254897159
H	0	-0.1712667928	-2.8345191579	-0.4714835696
H	0	1.0857955446	-3.3591845182	-1.630370405
H	0	1.385213824	-3.4798941253	0.1196122635
H	0	3.2077850895	-2.5065779616	-1.3395230602
H	0	3.2529974949	-0.7438496111	-1.4692861047

int-2

B3LYP/6-311G**

E(RB3LYP) = -820.076839178

Zero-point correction= 0.260845 (Hartree/Particle)

Thermal correction to Energy= 0.275413

Thermal correction to Enthalpy= 0.276357

Thermal correction to Gibbs Free Energy= 0.219338

Sum of electronic and ZPE= -819.815994

Sum of electronic and thermal Energies= -819.801426

Sum of electronic and thermal Enthalpies= -819.800482

Sum of electronic and thermal Free Energies= -819.857501

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	172.824	60.899	120.006

C	0	-4.0415551649	-1.6647760613	0.0000297964
C	0	-3.2060096905	-2.7883214903	0.0000225942
C	0	-1.8266923583	-2.6094110269	0.0000138645
C	0	-1.3090992878	-1.3171401313	0.0000102174
C	0	-2.144141849	-0.1535346137	0.0000147742
C	0	-3.5369616006	-0.3653745279	0.0000264335
C	0	0.0699587651	-0.8796027504	0.0000084283
C	0	0.0763368385	0.5777569407	0.000019682
C	0	-1.2802462492	1.0264689118	0.0000141981
N	0	-1.6506333749	2.3662322818	0.0000064956
C	0	-3.0927383918	2.7040793176	-0.0001030796
C	0	-0.8075004844	3.3702502461	0.0000855187
N	0	1.1561296226	-1.6062838696	0.0000003066
C	0	2.3383626121	-0.9113607242	0.0000009242
C	0	2.3597265419	0.5214450869	0.0000134851
N	0	1.2134488476	1.2647562383	0.0000278527
C	0	3.5592012842	-1.6250375279	-0.0000091202
C	0	4.7626785226	-0.9555798716	-0.0000087458
C	0	4.7874643855	0.4582153043	0.0000025815
C	0	3.6149002949	1.180071258	0.0000140735
H	0	-5.1179811016	-1.8022693473	0.000039646
H	0	-3.6316450523	-3.7851882159	0.000026242
H	0	-1.1523775832	-3.4592044609	0.0000118009
H	0	-4.2433496782	0.4501318296	0.0000376857
H	0	-3.5591888007	2.2952433805	0.8940825618
H	0	-3.1943602969	3.7852362668	-0.0001980026
H	0	-3.5590897749	2.2950958874	-0.8942714722
H	0	-1.2082086948	4.3720175438	0.0000459551
H	0	0.2514795125	3.1675594486	0.0001760024
H	0	3.513535997	-2.7087650169	-0.0000175177
H	0	5.6943827253	-1.5100022713	-0.0000171029
H	0	5.7401622332	0.9765231022	0.0000023194
H	0	3.6224752511	2.264735863	0.0000226012

int-3

B3LYP/6-311G**

E(RB3LYP) = -590.820459892

Zero-point correction= 0.144388 (Hartree/Particle)

Thermal correction to Energy= 0.155687

Thermal correction to Enthalpy= 0.156631

Thermal correction to Gibbs Free Energy= 0.104993

Sum of electronic and ZPE= -590.676072

Sum of electronic and thermal Energies= -590.664773

Sum of electronic and thermal Enthalpies= -590.663829

Sum of electronic and thermal Free Energies= -590.715467

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 97.695 38.992 108.681

C 0 -5.0406613543 -0.4203899164 -0.1799540598

N -1 -5.8540752868 0.6251563525 0.4688977039

C -1 -5.1394245028 1.6908121566 1.2459208241

C -1 -3.6509005381 1.4532016076 1.1749833272

O 0 -3.0265117186 2.0675820108 0.2734848012

O 0 -3.1748781606 0.6557236133 2.0203778481

C -1 -7.1518996723 0.6347298833 0.3947981449

C 0 -8.0774482409 -0.246133237 -0.2127080276

H 0 -7.6364344772 1.4665173085 0.897814703

C 0 -9.4516601002 -0.1030731468 -0.2330216549

C 0 -9.9691309723 -1.2170017273 -0.9299107387

C 0 -8.8872583279 -1.972417368 -1.2888062265

O 0 -7.7362731308 -1.406781043 -0.8664110284

H 0 -4.2171954805 0.0640496961 -0.7011572901

H 0 -4.6409816214 -1.0909130107 0.580983054

H 0 -5.6405597759 -0.9741187861 -0.8901978951

H 0 -5.4094198691 2.6510023655 0.8061570344

H 0 -5.4925278557 1.6373021153 2.2758887097

H 0 -10.0016049931 0.7145125623 0.2078799139

H 0 -11.002513414 -1.4412364682 -1.1410133161

H 0 -8.7830664976 -2.9030567153 -1.824103826

int-4

B3LYP/6-311G**

E(RB3LYP) = -492.046211573

Zero-point correction= 0.100771 (Hartree/Particle)

Thermal correction to Energy= 0.109911

Thermal correction to Enthalpy= 0.110855

Thermal correction to Gibbs Free Energy= 0.065353

Sum of electronic and ZPE= -491.945441

Sum of electronic and thermal Energies= -491.936301

Sum of electronic and thermal Enthalpies= -491.935356

Sum of electronic and thermal Free Energies= -491.980859

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 68.970 32.894 95.767

C 0 -0.9577284765 -0.3149654432 -0.0000023552

C 0 0.3708387143 -0.7937406747 0.00000458

H 0 0.4651077337 -1.8748422093 0.000008736

C 0 1.5395948309 -0.0754340175 0.0000031607

C 0 -1.5804158942 0.9204504769 -0.0000160973

C 0 -2.9717889946 0.6788108768 0.0000140195

C 0 -3.1251536012 -0.6817718573 -0.0000157898

O 0 -1.9301422725 -1.3007958236 -0.0000074967

C 0 2.790112067 -0.7544599024 0.0000082431

N 0 3.8106930116 -1.298093022 0.0000125103

C 0 1.5953850902 1.3449244379 -0.0000045531

N 0 1.6404039243 2.5002875645 -0.0000120101

H 0 -1.0929927708 1.8819969794 -0.0000198151

H 0 -3.7636868332 1.4112532205 0.0000319419

H 0 -3.9920675288 -1.323799606 -0.0000190743

TS-1-1

B3LYP/6-311G**=(calcall ts noeigentest)

E(RB3LYP) = -914.195917943

Zero-point correction= 0.240022 (Hartree/Particle)

Thermal correction to Energy= 0.256088

Thermal correction to Enthalpy= 0.257032

Thermal correction to Gibbs Free Energy= 0.195272

Sum of electronic and ZPE= -913.955896

Sum of electronic and thermal Energies= -913.939830

Sum of electronic and thermal Enthalpies= -913.938886

Sum of electronic and thermal Free Energies= -914.000645

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	160.698	63.776	129.984

O 0 1.4003796877 2.249095583 -1.8615985511

O 0 0.0948870268 -0.2309156326 -2.8991846287

O 0 0.220662141 -2.1929311531 -0.6588771692

C 0 2.5429764136 -1.3010487859 1.1597988993

C 0 3.6039038957 -0.6507853146 1.7833768066

C 0 3.9730301913 0.6525023332 1.4131255927

C 0 3.2888952187 1.3347879239 0.4113976478

C 0 2.2233555571 0.6862110945 -0.2100580838

C 0 1.8540762221 -0.6169980324 0.1604111322

C 0 0.712454295 -1.083644351 -0.65379359

C 0 0.2924861573 0.0804124875 -1.5855979908

C 0 1.3423770889 1.1810473968 -1.2857940969

H 0 2.2563336318 -2.307931647 1.4397224734

H 0 4.1587530461 -1.1558746041 2.5657461981

H 0 4.8062201239 1.1297815102 1.9161240926

H 0 3.5723858469 2.3392739896 0.1197425804

C 0 -3.8056691769 -1.6109706408 0.0286413153

C 0 -3.9784372791 -1.07537308 1.3071791013

C 0 -3.2066947058 -0.0045042901 1.7381236368

C 0 -2.2340716733 0.5718859924 0.9018595058

C 0 -2.0847114589 0.0329349344 -0.3915890574

C 0 -2.8569405593 -1.0471611504 -0.8158533773

N 0 -1.1524493146 0.6229809332 -1.3238909511

N 0 -1.505516055 1.6826391376 1.3096975251

H 0 -4.4058424618 -2.4479296005 -0.3073412267

H 0 -4.7185797146 -1.4989314072 1.977489689

H 0 -3.341514072 0.4013602671 2.7355868424

H 0 -2.7087301641 -1.4288176672 -1.8193940888

H 0 -1.0878485471 0.2483714476 -2.50897861

H 0 -1.1328111645 1.6429990515 -1.2417795925

H 0 -0.5418902877 1.7276317087 1.0041866401

H 0 -1.5829699093 1.887701566 2.2978213354

TS-1-2

B3LYP/6-311G**=(calcall ts noeigentest)

E(RB3LYP) = -914.246066929

Zero-point correction= 0.243637 (Hartree/Particle)

Thermal correction to Energy= 0.259869

Thermal correction to Enthalpy= 0.260813

Thermal correction to Gibbs Free Energy= 0.199485

Sum of electronic and ZPE= -914.002430

Sum of electronic and thermal Energies= -913.986198

Sum of electronic and thermal Enthalpies= -913.985254

Sum of electronic and thermal Free Energies= -914.046582

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	163.070	64.353	129.076

C	0	-4.1407078738	-1.7953180519	0.1479968841
C	0	-4.2025457897	-1.0562959479	1.3400903522
C	0	-3.2518798861	-0.0821741993	1.6312757423
C	0	-2.2365611845	0.1379802023	0.7029643914
C	0	-2.1745381803	-0.6021242623	-0.4889114276
C	0	-3.1263947811	-1.5770690023	-0.7796941398
C	0	-1.1180138677	1.0972746393	0.7756802967
C	0	-0.3687791973	1.0500333427	-0.5941498188
C	0	-1.0065635659	-0.1918743526	-1.2921123562
O	0	-0.6157936944	-0.6652410663	-2.3379296198
O	0	-0.8049206013	1.8079931132	1.7051160099
O	0	-0.8191109399	2.1984082818	-1.2893869265
N	0	1.0595177422	1.0872019114	-0.5286774173
C	0	1.9323861877	0.1522964958	0.0158509976
C	0	3.3019631058	0.5208812038	0.1212939796
C	0	4.2251908816	-0.4107184858	0.5915847897
C	0	3.8311724982	-1.6920120856	0.985506216
C	0	2.4860441517	-2.0364612869	0.9285364119
C	0	1.5453798381	-1.1215284877	0.449089549
N	0	3.6914346049	1.8050699653	-0.3173598011
H	0	-4.8953363208	-2.5483714045	-0.0480182438
H	0	-5.0042166877	-1.2518109669	2.0430276727
H	0	-3.2954778884	0.4904573351	2.550201092
H	0	-3.0727402406	-2.1460295566	-1.7003846441
H	0	-0.6146451854	2.0799165819	-2.2299601611
H	0	1.4617017855	1.934551937	-0.90160614
H	0	5.2679313497	-0.1146687272	0.6593753243
H	0	4.5697946101	-2.3982809575	1.3476561531
H	0	2.154011795	-3.0181074815	1.2482166253
H	0	0.5067813109	-1.4236672362	0.4056877695
H	0	4.6819389761	1.9694719845	-0.1763684445
H	0	3.1728770476	2.5526165652	0.1372088833

TS-1-3

B3LYP/6-311G**=(calcall ts noeigentest)

E(RB3LYP) = -837.770714004

Zero-point correction= 0.215966 (Hartree/Particle)

Thermal correction to Energy= 0.230370

Thermal correction to Enthalpy= 0.231314

Thermal correction to Gibbs Free Energy= 0.173612

Sum of electronic and ZPE= -837.554748

Sum of electronic and thermal Energies= -837.540344

Sum of electronic and thermal Enthalpies= -837.539400

Sum of electronic and thermal Free Energies= -837.597102

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 144.559 56.973 121.445

C 0 -4.7922275724 -0.1838068389 0.0150364891

C 0 -4.3262213861 -1.4628144676 0.3608261028

C 0 -2.9652813839 -1.7163451907 0.5061202286

C 0 -2.0793758252 -0.6640334799 0.2895310051

C 0 -2.5458513899 0.6164538053 -0.0550240034

C 0 -3.9077067429 0.8702995703 -0.1951306464

C 0 -0.6017186215 -0.6772344921 0.382046978

C 0 -0.1529069296 0.7301213122 0.0208576831

C 0 -1.4095165244 1.547723904 -0.2082038563

O 0 -1.4496187405 2.7320052421 -0.4766471338

O 0 0.0956991802 -1.602590617 0.7454532807

N 0 0.993813108 1.2731888118 -0.0252885959

C 0 2.2111102043 0.5797329112 0.0748945481

C 0 2.5685090904 -0.4697291077 -0.8005756967

C 0 3.8449040845 -1.0252359084 -0.6796871933

C 0 4.7457111775 -0.5853899197 0.2874521853

C 0 4.3916245433 0.4660104378 1.1332531307

C 0 3.1452586896 1.0642311586 1.0044384909

N 0 1.6320004536 -0.9094661443 -1.7960409174

H 0 -5.8586508621 -0.0187942233 -0.0873392893

H 0 -5.0413178511 -2.2624278617 0.5163297699

H 0 -2.6007821499 -2.7009148052 0.7745928261

H 0 -4.2627509017 1.8599389338 -0.4575717767

H 0 4.1221975152 -1.8259200235 -1.3578917237

H 0 5.7223775522 -1.049276441 0.3685253528

H 0 5.0891089832 0.8297334039 1.8793894444

H 0 2.8620605072 1.8989858239 1.6354060013

H 0 1.9585053965 -0.6363771625 -2.7208620386

H 0 1.5876713956 -1.9251366315 -1.7981726453

TS-1-4

B3LYP/6-311G**=(calcall ts noeigentest)

E(RB3LYP) = -837.729493805

Zero-point correction= 0.214715 (Hartree/Particle)

Thermal correction to Energy= 0.228999

Thermal correction to Enthalpy= 0.229944

Thermal correction to Gibbs Free Energy= 0.173968

Sum of electronic and ZPE= -837.514779

Sum of electronic and thermal Energies= -837.500494

Sum of electronic and thermal Enthalpies= -837.499550

Sum of electronic and thermal Free Energies= -837.555526

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 143.699 58.010 117.811

C 0 4.4759342335 -0.3093562973 -0.373123751

C 0 3.8457660668 -1.5591112433 -0.4713778308

C 0 2.4640445775 -1.6887628069 -0.354155442

C 0 1.7158677236 -0.5350943202 -0.1366734922

C 0 2.3468387766 0.7273562134 -0.0679145888

C 0 3.7284305678 0.8480733979 -0.1733044763

C 0 0.2760729031 -0.3198268344 -0.0162549634

C 0 0.0123031289 1.0853964587 0.0442715084

C 0 1.3363073082 1.8008846737 0.0771394112

O 0 1.5093946947 2.9994780522 0.1734604753

N 0 -0.7607768203 -1.1318974662 -0.1702459042

C 0 -2.046949488 -0.6444652605 -0.177327254

C 0 -2.2334050583 0.7676196349 -0.0718448028

C 0 -3.1482970699 -1.5072514203 -0.2743450214

C 0 -4.4195227541 -0.9704911304 -0.2729410611

C 0 -4.6230381992 0.4231289919 -0.1760836352

C 0 -3.5490370024 1.2790025934 -0.0777411902

O 0 0.472340831 -1.8648444951 1.9578442715

H 0 -0.5923423064 -2.118782258 0.0487353006

H 0 5.5541936717 -0.2476701894 -0.4627328585

H 0 4.4485502402 -2.4442314209 -0.6397554451

H 0 1.9906340952 -2.6595782437 -0.4172975638

H 0 4.2014705612 1.821200658 -0.1093352331

H 0 -2.9840175346 -2.5759610317 -0.349352253

H 0 -5.2755823377 -1.630590365 -0.3484341888

H 0 -5.6323509293 0.8165091866 -0.1781023988

H 0 -3.6777894852 2.3517291829 0.0010870071

H 0 -0.3581435056 -1.520596821 2.3087548942

N 0 -1.171696889 1.6255325606 0.0377504859

TS-2-1

B3LYP/6-311G**=(calcall ts noeigentest)

E(RB3LYP) = -1085.13523813

Zero-point correction= 0.297537 (Hartree/Particle)

Thermal correction to Energy= 0.316479

Thermal correction to Enthalpy= 0.317424

Thermal correction to Gibbs Free Energy= 0.249230

Sum of electronic and ZPE= -1084.837701

Sum of electronic and thermal Energies= -1084.818759

Sum of electronic and thermal Enthalpies= -1084.817815

Sum of electronic and thermal Free Energies= -1084.886008

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 198.594 75.544 143.526

C 0 2.4895840401 3.2766949669 -0.4477126877

C 0 1.4757700504 3.9293416527 0.2624202557

C 0 0.2774877426 3.2783069199 0.5495836133

C 0 0.1269460848 1.9563495502 0.1345144767

C 0 1.1580155026 1.2861734422 -0.5435869844

C 0 2.333157114 1.9529004782 -0.8655063199

C 0 -1.0469894677 1.0819351363 0.1744046033

C 0 -0.7296031061 -0.1384882098 -0.5103460176

C 0 0.7436191614 -0.1322193836 -0.9366195641

O 0 1.0658653284 -0.537801901 -2.2072685188

N 0 -2.2335321339 1.3457511218 0.6581280128

C 0 -3.1810627769 0.3761382223 0.4493888201

C 0 -2.8777619592 -0.818928177 -0.2754774346

N 0 -1.6121075862 -1.0611027571 -0.7563101267

C 0 -4.4916757113 0.5686237234 0.9414208065

C 0 -5.4625627841 -0.3826742826 0.7188784249

C 0 -5.1640778154 -1.5587759708 -0.0047231655

C 0 -3.8946423479 -1.773547853 -0.4949851557

H 0 3.4042766713 3.808633371 -0.6847956801

H 0 1.6172512134 4.9583998005 0.5732183401

H 0 -0.5270923572 3.7910489995 1.0641048025

H 0 3.1139202751 1.457446693 -1.4320162772

H 0 -4.7041757465 1.4799308398 1.4888756441

H 0 -6.4665556218 -0.2296405701 1.0984033338

H 0 -5.9415576034 -2.2954544589 -0.1720558725

H 0 -3.6451083483 -2.6703294447 -1.0507548514

C 0 0.9001798356 -2.5068784231 0.1054172655

N 0 1.623529496 -1.2593071666 -0.2294560676

C 0 2.6078548006 -0.9216515475 0.8062661137

C 0 3.8766176195 -1.7344282935 0.6408414217

O 0 4.6732142069 -1.5766698152 1.7053773896

O 0 4.160652434 -2.410063839 -0.3202546334

H 0 0.2503228997 -2.777068989 -0.7226927585

H 0 1.6383870723 -3.2963446254 0.2503862142

H 0 0.3109075672 -2.3898966802 1.017595259

H 0 1.8635548463 -1.2607310101 -1.4646684063

H 0 2.8980909407 0.1264266822 0.735888005

H 0 2.201308608 -1.0817169217 1.8087717788

H 0 5.4980918551 -2.0699812798 1.5556459409

TS-2-2

B3LYP/6-311G**=(calcall ts noeigentest)

E(RB3LYP) = -1085.16853679

Zero-point correction= 0.297334 (Hartree/Particle)

Thermal correction to Energy= 0.316098

Thermal correction to Enthalpy= 0.317042

Thermal correction to Gibbs Free Energy= 0.250175

Sum of electronic and ZPE= -1084.871202

Sum of electronic and thermal Energies= -1084.852439

Sum of electronic and thermal Enthalpies= -1084.851494

Sum of electronic and thermal Free Energies= -1084.918362

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 198.355 75.788 140.734

C 0 -2.6852974318 -3.5617853828 -0.1123773879

C 0 -1.49631213 -4.2908204083 -0.038796978

C 0 -0.2712076009 -3.6338455115 0.0498728346

C 0 -0.2655597237 -2.2434898266 0.0820711518

C 0 -1.4624784537 -1.5011136378 0.0493302031

C 0 -2.6806699984 -2.1653693969 -0.0742004032

C 0 0.8673407816 -1.3227426948 0.0887290461

C 0 0.3700947607 0.019441997 0.0500488097

C 0 -1.146583919 -0.0245461937 0.0805041033

N 0 2.141898083 -1.6134076414 0.0939848434

C 0 2.9926695601 -0.5407812731 0.0492900248

C 0 2.4964819686 0.7998863947 -0.0056281305

N 0 1.1481640778 1.0588712814 -0.0055460542

C 0 4.3887343282 -0.7583073593 0.0501787396

C 0 5.2542493689 0.3112424925 -0.0027552827

C 0 4.7622260585 1.6349958234 -0.0594821331

C 0 3.4068085933 1.8776887994 -0.0617810446

O 0 -1.430106792 0.4475836784 -1.6942338653

N 0 -1.8432432959 0.8406009983 0.8460563396

C 0 -3.2463895752 0.5868525141 1.2027151541

C 0 -1.4592003946 2.2569631312 0.9281632397

C 0 -2.0936958772 3.1637674341 -0.1463314498

O 0 -2.3234118572 2.6584443595 -1.3120369932

O 0 -2.314537313 4.337354428 0.1545990912

H 0 -1.874141432 1.517268392 -1.5333799261

H 0 -3.6302690254 -4.0842097216 -0.2066370791

H 0 -1.5274384131 -5.373981303 -0.0666108444

H 0 0.6605836144 -4.186005176 0.0804383568

H 0 -3.6158710651 -1.6307394599 -0.1600504499

H 0 4.7486012726 -1.7798130044 0.09198474

H 0 6.324761827 0.1402823938 -0.0021082471

H 0 5.4604558577 2.4630558367 -0.1016916762

H 0 3.0102632023 2.8855011844 -0.1054910447

H 0 -2.1491701007 -0.1099441793 -2.0250069003

H 0 -3.9003828934 0.6317741762 0.3270892944

H 0 -3.3507447514 -0.3796587084 1.6919659948

H 0 -3.5559213956 1.3579735666 1.9062310575

H 0 -0.3789971246 2.3521305976 0.830601697

H 0 -1.7525027911 2.6355813992 1.9061911689

TS-2-3

B3LYP/6-311G**=(calcall ts noeigentest)

E(RB3LYP) = -1008.69808261

Zero-point correction= 0.272314 (Hartree/Particle)

Thermal correction to Energy= 0.290362

Thermal correction to Enthalpy= 0.291306

Thermal correction to Gibbs Free Energy= 0.224787

Sum of electronic and ZPE= -1008.425769

Sum of electronic and thermal Energies= -1008.407721

Sum of electronic and thermal Enthalpies= -1008.406777

Sum of electronic and thermal Free Energies= -1008.473296

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.205	70.835	140.000

C 0 2.8203885039 2.9685454024 -0.1331510767

C 0 1.7210348211 3.7988784789 0.0901701789

C 0 0.438210124 3.2548133295 0.1370184334

C 0 0.2849082511 1.8893707418 -0.056499039

C 0 1.3898026611 1.0281671678 -0.3113577184

C 0 2.6734572198 1.5937365714 -0.3318608338

C 0 -0.9254897246 1.0858016617 -0.0124181841

C 0 -0.5613939681 -0.2953414567 -0.2336091708

C 0 0.8874347348 -0.3476551441 -0.4439224208

N 0 -2.1517569301 1.4857274758 0.1930202862

C 0 -3.1045495296 0.5011529749 0.1895034493

C 0 -2.7537810712 -0.8684601686 -0.0349359641

N 0 -1.458980041 -1.2546534594 -0.2496525394

C 0 -4.4576821142 0.8426037577 0.4098650154

C 0 -5.4291027235 -0.1336374399 0.4082844744

C 0 -5.0848973398 -1.486652893 0.1856821799

C 0 -3.774524266 -1.8485349768 -0.0319116439

N 0 1.5877718739 -1.4487331139 -0.7527738903

C 0 0.9188440325 -2.7723458263 -0.6857224794

C 0 2.926601847 -1.4869449709 -0.9940503379

C 0 3.9217375844 -1.5866818746 0.9047094202

O 0 5.0477671233 -1.8130940692 0.5908758306

O 0 3.0871043668 -1.383807246 1.7271538136

H 0 3.8175486354 3.3938368277 -0.1519514919

H 0 1.8665637268 4.8630567703 0.2358036867

H 0 -0.4281123953 3.8778821228 0.3274378126

H 0 3.5673668722 1.0095819116 -0.4788180031

H 0 -4.7007156684 1.8857359223 0.5781002967

H 0 -6.4659932472 0.1333890162 0.5781686847

H 0 -5.8619343919 -2.2427655733 0.1874518309

H 0 -3.4935718352 -2.8815314282 -0.203324328

H 0 1.6682854975 -3.537231954 -0.8633589702

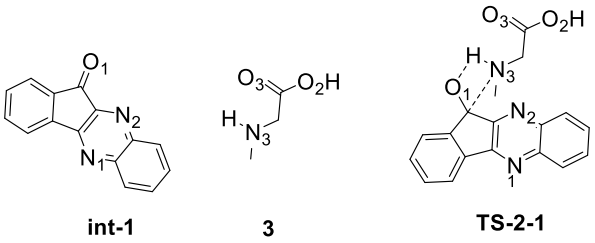
H 0 0.471380509 -2.907428606 0.2960856729

H 0 0.1411775353 -2.8252369217 -1.4440826243

H 0 3.2848551222 -2.4206600552 -1.4016371663

H 0 3.3916442041 -0.5865829549 -1.361693184

3.4 Hydrogen bonding investigation



int-1 **3** **TS-2-1**

The hydrogen bonding was assessed on the nitrogen and oxygen atoms in the figure above, in which the alphabetic numbers indicate the atom label only.

3.4.1 Gas-phase calculation results for liquid-air interface simulation

3_methylglycine_1etoh_oh.log

opt

E(RB3LYP) = -478.941639528

Zero-point correction= 0.189941 (Hartree/Particle)

Thermal correction to Energy= 0.202108

Thermal correction to Enthalpy= 0.203052

Thermal correction to Gibbs Free Energy= 0.149692

Sum of electronic and ZPE= -478.751699

Sum of electronic and thermal Energies= -478.739531

Sum of electronic and thermal Enthalpies= -478.738587

Sum of electronic and thermal Free Energies= -478.791947

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	126.825	40.337	112.306

C	0	2.6176351875	-0.1438114864	0.8308960092
N	0	1.1771748014	-0.3443425341	0.7777412595
C	0	0.714840357	-0.9042251438	-0.4747319921
C	0	-0.6838934329	-1.4630257887	-0.3350982455
O	0	-1.3047087101	-1.5963721661	-1.5038783848
O	0	-1.165648173	-1.792257898	0.7343115817
H	0	2.8959715624	0.2242751334	1.8205602974
H	0	3.208416713	-1.0534569162	0.6198283873
H	0	2.9148512566	0.6173995888	0.1026241192
H	0	0.8597116153	-0.9389817271	1.5356560034
H	0	0.7147854572	-0.1494697729	-1.2672919689
H	0	1.3368926842	-1.7426500018	-0.8493131706
H	0	-2.1911259025	-2.0127965164	-1.3358937946
C	0	-5.5781420578	-1.9899366739	-1.5125663899
H	0	-5.8510325293	-3.0373806636	-1.6590712359
H	0	-5.0467069186	-1.646077287	-2.4035415145
H	0	-6.4950853455	-1.4032181202	-1.413020608
C	0	-4.7142376356	-1.8372348431	-0.2752199341
H	0	-4.4316089022	-0.786984235	-0.1280335903
H	0	-5.2645193819	-2.1650054994	0.6143827092
O	0	-3.5416144881	-2.6500207178	-0.4361757061
H	0	-2.9694556073	-2.5396172807	0.3433098184

3_methylglycine_1etoh_o.log

opt

E(RB3LYP) = -478.934578372

Zero-point correction= 0.189661 (Hartree/Particle)

Thermal correction to Energy= 0.202102

Thermal correction to Enthalpy= 0.203046

Thermal correction to Gibbs Free Energy= 0.149130

Sum of electronic and ZPE= -478.744917

Sum of electronic and thermal Energies= -478.732477

Sum of electronic and thermal Enthalpies= -478.731533

Sum of electronic and thermal Free Energies= -478.785449

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	126.821	41.188	113.476

C	0	2.284629413	0.5589171126	-0.2685631289
N	0	0.8426048223	0.4480343757	-0.4437966956
C	0	0.3228468969	-0.8256263656	-0.001582826

C 0 -1.1817580204 -0.9071004055 -0.1209122555

O 0 -1.6077475045 -2.1846993874 -0.1139865123

O 0 -1.9517757184 0.02406003 -0.1774268486

H 0 2.6061381993 1.5586842551 -0.5657654493

H 0 2.6280092212 0.3807355238 0.7658278845

H 0 2.7972062486 -0.1599036254 -0.9162912753

H 0 0.3668264826 1.216431167 0.0249947736

H 0 0.7516381393 -1.6365007919 -0.5990692194

H 0 0.5552623371 -1.0777924231 1.0539251242

H 0 -2.5764424647 -2.1595749355 -0.1380682557

C 0 -0.3938346678 4.7300547178 -0.8164004342

H 0 0.6425460067 4.5616159607 -0.5122051669

H 0 -0.8793599066 5.3335183814 -0.0456324311

H 0 -0.3910177306 5.2968104328 -1.7516350865

C 0 -1.1231228908 3.4096726675 -0.989302302

H 0 -2.1562413092 3.594117166 -1.3142720462

H 0 -0.6342463445 2.7998430653 -1.7609327621

O 0 -1.1133190239 2.7232634506 0.2635361712

H 0 -1.5985410955 1.892465778 0.1473418221

3_methylglycine_2etoh_oh-nh.log

opt

3_methylglycine_2etoh_oh-o.log

opt

E(RB3LYP) = -634.044011017

Zero-point correction= 0.271908 (Hartree/Particle)

Thermal correction to Energy= 0.289791

Thermal correction to Enthalpy= 0.290736

Thermal correction to Gibbs Free Energy= 0.222044

Sum of electronic and ZPE= -633.772103

Sum of electronic and thermal Energies= -633.754220

Sum of electronic and thermal Enthalpies= -633.753275

Sum of electronic and thermal Free Energies= -633.821967

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	181.847	58.541	144.575

C 0 2.2641368026 0.8806141556 -1.0140925633

N 0 0.8331977244 0.6452537455 -0.8719665293

C 0 0.5206946824 -0.7412827851 -0.6058540789

C 0 -0.9584030563 -0.9867865176 -0.4067880775

O 0 -1.2866345433 -2.2583437745 -0.5890288915

O 0 -1.7683452809 -0.1316499801 -0.0745574866

H 0 2.4403942607 1.9484854565 -1.1556462174

H 0 2.8642288103 0.5448087155 -0.1499223247

H 0 2.6424621928 0.3619691887 -1.9011187438

H 0 0.4467809079 1.2481118991 -0.1489911697

H 0 0.8506268176 -1.3674785259 -1.4405396102

H 0 1.0168233885 -1.1591707828 0.2944688251

H 0 -2.2570922645 -2.3650186058 -0.3923401196

C 0 -5.3127439907 -3.3980306295 -1.3220780483

H 0 -5.7302134089 -3.8331605743 -0.4114560868

H 0 -4.4729577519 -4.0180531645 -1.6456422333

H 0 -6.078221085 -3.4249652694 -2.101837368

C 0 -4.866168264 -1.9710496862 -1.0694877411

H 0 -4.4382542776 -1.5316079654 -1.9793312113

H 0 -5.7187327586 -1.3537322652 -0.7647495376

O 0 -3.8876816114 -1.9812106468 -0.0160537214

H 0 -3.5832421934 -1.072970393 0.1440059972

C 0 -0.7885531063 4.752202933 -0.0679916869

H 0 0.3008848699 4.6802427677 -0.0151540658

H 0 -1.1488467896 5.1422676178 0.8870350034

H 0 -1.0497089413 5.4645440429 -0.8556219255

C 0 -1.4018753183 3.3914694337 -0.3468231134

H 0 -2.4948387921 3.483794416 -0.4177635305

H 0 -1.0377817046 2.9957573018 -1.3044973

O 0 -1.0464317233 2.510794036 0.7193885079

H 0 -1.448651815 1.6479842164 0.534572149

3_methylglycine_3etoh.log

opt

E(RB3LYP) = -789.153069710

Zero-point correction= 0.354183 (Hartree/Particle)

Thermal correction to Energy= 0.377524

Thermal correction to Enthalpy= 0.378468

Thermal correction to Gibbs Free Energy= 0.295800

Sum of electronic and ZPE= -788.798887

Sum of electronic and thermal Energies= -788.775546

Sum of electronic and thermal Enthalpies= -788.774602

Sum of electronic and thermal Free Energies= -788.857270

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 236.900 76.012 173.989

C 0 2.5159188184 -1.7109411145 -0.3227163227

N 0 1.4810986867 -0.6762438829 -0.3118596886

C 0 0.507980685 -0.8381217397 0.762968792

C 0 -0.3250977859 0.4164120375 0.9305605033

O 0 -1.3072424672 0.2543014079 1.8006139711

O 0 -0.0718108459 1.4574726795 0.3500122323

H 0 3.2338334223 -1.4962894478 -1.1162144345

H 0 3.0594834707 -1.7932123732 0.6306112675

H 0 2.0608909602 -2.6812306255 -0.5372909139

H 0 1.893567567 0.2486463428 -0.228336634

H 0 -0.1673399699 -1.6689746153 0.542207543

H 0 0.9729785543 -1.0562963618 1.7386333018

H 0 -1.8554537101 1.0889434958 1.8044157433

C 0 -3.782157295 3.8778842504 -0.2963955514

H 0 -2.9265540527 4.1246199486 -0.9324498638

H 0 -3.9183523824 4.6874718006 0.4246535279

H 0 -4.668750907 3.828489098 -0.9357565714

C 0 -3.5674905067 2.5513900766 0.416456311

H 0 -4.4315612679 2.3094593201 1.0389176398

H 0 -3.4177570077 1.7345420524 -0.2965820468

O 0 -2.449254575 2.6138327168 1.3276286142

H 0 -1.6370082217 2.7051802024 0.8018479969

C 0 -4.3974774997 -1.6449459822 -0.5593705809

H 0 -5.0649512643 -0.7923032681 -0.7093584855

H 0 -4.0432638308 -1.6221512316 0.4742618399

H 0 -4.9735318598 -2.5623374315 -0.711055993

C 0 -3.222425944 -1.5782089574 -1.5203740781

H 0 -2.5848189081 -2.4647174216 -1.3863868113

H 0 -3.5876887248 -1.5981784644 -2.5577529541

O 0 -2.488366143 -0.3880167047 -1.2658312119

H 0 -1.6870208508 -0.3918352844 -1.8282243257

C 0 -0.8437165896 1.0296630465 -4.4030656128

H 0 -1.841523502 1.1007026487 -3.962938867

H 0 -0.8419424082 0.201644312 -5.1163318805

H 0 -0.6392764145 1.9556836077 -4.9476912423

C 0 0.1984151686 0.7997941574 -3.3224005619

H 0 1.1994295568 0.7481818528 -3.7730097075

H 0 0.1959132551 1.6306845778 -2.6055564579

O 0 -0.0987368802 -0.4290928402 -2.6556281358

H 0 0.5194085999 -0.5330494956 -1.8942137505

int-1_1etoh_co.log

opt

E(RB3LYP) = -916.428343841

Zero-point correction= 0.273551 (Hartree/Particle)

Thermal correction to Energy= 0.291430

Thermal correction to Enthalpy= 0.292374

Thermal correction to Gibbs Free Energy= 0.224868

Sum of electronic and ZPE= -916.154793

Sum of electronic and thermal Energies= -916.136914

Sum of electronic and thermal Enthalpies= -916.135970

Sum of electronic and thermal Free Energies= -916.203476

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 182.875 67.809 142.079

C 0 2.346415604 -5.0900887123 -0.7907840332

C 0 3.3414966595 -4.128375252 -0.9959541635

C 0 3.067448487 -2.7640797665 -0.8721055716

C 0 1.774316163 -2.3852054125 -0.5378384114

C 0 0.7724360655 -3.3534961215 -0.3310626663

C 0 1.0465205598 -4.7082846413 -0.4551520286

C 0 1.1872481573 -1.0474937943 -0.3379928609

C 0 -0.1936977208 -1.2103570915 -0.000771089

C 0 -0.5218024255 -2.6867316362 0.0133955488

O 0 -1.5896863296 -3.2012480101 0.2441448795

N 0 1.7687248441 0.1182090453 -0.4344623902

C 0 0.9510674362 1.1929920651 -0.1891571098

C 0 -0.4341343079 1.0313312341 0.1497656749

N 0 -0.9975793726 -0.216498915 0.2428160243

C 0 1.4835461788 2.4976876359 -0.2707509353

C 0 0.679432165 3.5893008313 -0.0287539415

C 0 -0.6842566577 3.4250283178 0.303048332

C 0 -1.2383109901 2.1681699994 0.3917818683

H 0 2.5904400103 -6.1409531071 -0.8941420437

H 0 4.343859435 -4.4493362284 -1.2559708298

H 0 3.836616452 -2.0181227399 -1.0308322304

H 0 0.2639946832 -5.4403892037 -0.2929332839

H 0 2.5308299685 2.6012151283 -0.5268291793

H 0 1.0951339385 4.5884023728 -0.0929547733

H 0 -1.297682958 4.2987748238 0.4890715413

H 0 -2.2804381951 2.0062013949 0.6448331607

C 0 -6.1236904707 -0.0567479709 0.4600573495

H 0 -6.2332094256 1.0309355136 0.4713129773

H 0 -6.3684701523 -0.4322247232 1.4566038651

H 0 -6.8419112854 -0.469920968 -0.2540370484

C 0 -4.70336408 -0.4447349493 0.0869785001

H 0 -4.6043765056 -1.5385713126 0.0731217191

H 0 -4.4715024439 -0.0823256438 -0.9261990301

O 0 -3.8164796511 0.1235219496 1.0445270046

H 0 -2.9235575659 -0.2084158521 0.8576051145

int-1_1etoh_n1.log

opt

E(RB3LYP) = -916.428343851

Zero-point correction= 0.273550 (Hartree/Particle)

Thermal correction to Energy= 0.291429

Thermal correction to Enthalpy= 0.292373

Thermal correction to Gibbs Free Energy= 0.224871

Sum of electronic and ZPE= -916.154794

Sum of electronic and thermal Energies= -916.136915

Sum of electronic and thermal Enthalpies= -916.135971

Sum of electronic and thermal Free Energies= -916.203473

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.875	67.809	142.071

C	0	1.1021121657	-4.6987472373	-0.5884193976
C	0	2.3953146717	-4.1651021573	-0.5853773768
C	0	2.6110506161	-2.7884499075	-0.485172137
C	0	1.5021538105	-1.9587912587	-0.3878192291
C	0	0.2000603161	-2.496075575	-0.3907252389
C	0	-0.0121778749	-3.8638737435	-0.4909202485
C	0	1.4079766822	-0.4919561584	-0.2713565751
C	0	0.0239176729	-0.1364560564	-0.1990109498
C	0	-0.8084576436	-1.3968082963	-0.2774925316
O	0	-2.0126489079	-1.4858953622	-0.259461387
N	0	2.3758823813	0.3844194995	-0.2335523451
C	0	1.9680246233	1.6901061069	-0.1207096141
C	0	0.5801847959	2.0482964524	-0.0474095412
N	0	-0.400023339	1.0887209618	-0.0870281731
C	0	2.9381716022	2.7143550624	-0.0743360002
C	0	2.5493265492	4.0307597108	0.0381849204
C	0	1.1815284517	4.3785106856	0.1084638709
C	0	0.2074857481	3.4069185764	0.0661382977
H	0	0.9675245317	-5.7712252722	-0.6673100576
H	0	3.2452570626	-4.8337062902	-0.6623254999
H	0	3.6116106771	-2.3735543235	-0.4828607522
H	0	-1.0206229185	-4.260949238	-0.4918917598
H	0	3.9807224534	2.4261064723	-0.1300083602
H	0	3.2998305655	4.8121889615	0.0734761813
H	0	0.8993370546	5.4210679137	0.1966080595
H	0	-0.8507561398	3.6385971046	0.1185902678
C	0	-5.0760010823	3.0758971218	-0.8191898207
H	0	-4.7864108983	4.1300089521	-0.8059852764
H	0	-5.6150457099	2.8610214226	0.1067020256
H	0	-5.75341739	2.9132106942	-1.6624693326
C	0	-3.8485273122	2.1881908123	-0.9303192412
H	0	-4.1495331268	1.1319782982	-0.9481359581
H	0	-3.32308223	2.3946602379	-1.875263597
O	0	-3.004781287	2.4468788711	0.186585436
H	0	-2.2724722615	1.8101228284	0.1608153817

int-1_1etoh_n2.log

opt

E(RB3LYP) = -916.428497425

Zero-point correction= 0.273672 (Hartree/Particle)

Thermal correction to Energy= 0.291470

Thermal correction to Enthalpy= 0.292415

Thermal correction to Gibbs Free Energy= 0.225371

Sum of electronic and ZPE= -916.154825

Sum of electronic and thermal Energies= -916.137027

Sum of electronic and thermal Enthalpies= -916.136083

Sum of electronic and thermal Free Energies= -916.203126

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 182.900 67.565 141.105

C 0 0.9063762622 -4.5109429633 -0.5372016564

C 0 2.2019987862 -3.9912324631 -0.4443798791

C 0 2.4303058433 -2.6171185583 -0.334768464

C 0 1.3224550858 -1.7762745784 -0.3197473362

C 0 0.017303585 -2.2986236286 -0.4108486077

C 0 -0.2028209727 -3.6641508016 -0.5204959469

C 0 1.2293214025 -0.3098385853 -0.2115823538

C 0 -0.1545263398 0.065437506 -0.2319138691

C 0 -0.9891540202 -1.1927100899 -0.3643622349

O 0 -2.1912136999 -1.2803484109 -0.4192901179

N 0 2.195713114 0.5657986527 -0.11057488

C 0 1.797434526 1.8772654325 -0.0132788398

C 0 0.4109441749 2.2381810301 -0.0354557095

N 0 -0.5766247526 1.2931075488 -0.1508684268

C 0 2.7717793861 2.8902216752 0.1132804519

C 0 2.3861454231 4.2091183516 0.210568019

C 0 1.0202114659 4.567183422 0.1846747902

C 0 0.0487118738 3.5995717055 0.0643446502

H 0 0.7656760037 -5.5823979928 -0.621071043

H 0 3.0477717953 -4.6693450837 -0.4566441106

H 0 3.435448243 -2.2157630059 -0.2592147125

H 0 -1.2135203947 -4.0494044162 -0.589137436

H 0 3.8150742985 2.5986562252 0.1391726794

H 0 3.1385490632 4.982946725 0.309823532

H 0 0.7395652194 5.6109658583 0.2621133504

H 0 -1.0068827826 3.8412450787 0.0437697988

C 0 6.8244522962 -0.6181218323 -1.7816100925

H 0 6.8843242081 -1.6867261576 -1.5599861301

H 0 7.4719570655 -0.0902723707 -1.0773117978

H 0 7.2022999913 -0.4525663493 -2.7944679663

C 0 5.3931952822 -0.126735291 -1.6493068486

H 0 5.3452063346 0.9445484501 -1.8939219834

H 0 4.7484516899 -0.6523467991 -2.3697056157

O 0 4.9592093586 -0.3593220937 -0.3137890365

H 0 4.0639282143 0.01105468 -0.2097154966

int-1_2etoh_co-n1.log

opt

E(RB3LYP) = -1071.52602501

Zero-point correction= 0.354815 (Hartree/Particle)

Thermal correction to Energy= 0.378811

Thermal correction to Enthalpy= 0.379755

Thermal correction to Gibbs Free Energy= 0.295230

Sum of electronic and ZPE= -1071.171210

Sum of electronic and thermal Energies= -1071.147214

Sum of electronic and thermal Enthalpies= -1071.146270

Sum of electronic and thermal Free Energies= -1071.230795

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 237.707 86.609 177.898

C 0 1.2287461727 -4.7971097968 0.0146300189

C 0 2.4644086357 -4.2299038455 -0.3142954241

C 0 2.6185180436 -2.8463235923 -0.4377097292

C 0 1.506478363 -2.0444233904 -0.2240813902

C 0 0.2619868684 -2.6155281261 0.1066392861

C 0 0.110455307 -3.9899708813 0.2288899228

C 0 1.3525006415 -0.5788576471 -0.2775349033

C 0 -0.008015806 -0.2580400248 0.0291399833

C 0 -0.7600182312 -1.5426374133 0.280266337

O 0 -1.9320446034 -1.676530377 0.5561974047

N 0 2.2572085434 0.3220716215 -0.5492379552

C 0 1.8075198126 1.6183918278 -0.5192360169

C 0 0.4431605357 1.9427087348 -0.208785994

N 0 -0.4718215271 0.9580326689 0.0695406252

C 0 2.7105117559 2.6657171846 -0.7995300137

C 0 2.2812504617 3.9741563959 -0.7721607158

C 0 0.9387849978 4.2891589186 -0.464563767

C 0 0.0286910508 3.2943895132 -0.1870459176

H 0 1.1421059622 -5.8736157414 0.1035374085

H 0 3.3186538436 -4.877496035 -0.4760489927

H 0 3.5749734921 -2.4062662375 -0.6919577399

H 0 -0.8535434393 -4.4135945314 0.4850738213

H 0 3.7349483818 2.4015967486 -1.0313974411

H 0 2.9802705896 4.7741687615 -0.9877748426

H 0 0.6243842961 5.3260473705 -0.4468024389

H 0 -1.0075913163 3.5027456692 0.0574337471

C 0 -6.666497398 -2.2976466764 -0.6076454379

H 0 -7.0604363525 -1.3306977883 -0.9302971998

H 0 -7.1361247166 -2.5539730639 0.3450530479

H 0 -6.9472993734 -3.0513456422 -1.3489978592

C 0 -5.1574976604 -2.2305515539 -0.4483971539

H 0 -4.7714637588 -3.2136075319 -0.1418210615

H 0 -4.6900986294 -1.9821104183 -1.4129855961

O 0 -4.8574546738 -1.2460420676 0.5331778724

H 0 -3.9032547154 -1.252489529 0.6785569729

C 0 -5.1833425023 3.1650617694 0.0453470611

H 0 -4.8330129421 4.1942121538 -0.0733716771

H 0 -5.543025872 3.0432236657 1.0697461703

H 0 -6.022276486 3.0034652016 -0.6375815985

C 0 -4.0631214728 2.1793303034 -0.2356889462

H 0 -4.4277446204 1.1534185479 -0.1113335946

H 0 -3.717537492 2.2931514202 -1.2749263971

O 0 -2.9967243767 2.4442433818 0.678793868

H 0 -2.3320773793 1.7462382022 0.5796205168

int-1_solvated.log

opt

E(RB3LYP) = -1226.66245581

Zero-point correction= 0.434811 (Hartree/Particle)

Thermal correction to Energy= 0.464809

Thermal correction to Enthalpy= 0.465753

Thermal correction to Gibbs Free Energy= 0.365562

Sum of electronic and ZPE= -1226.227645

Sum of electronic and thermal Energies= -1226.197647

Sum of electronic and thermal Enthalpies= -1226.196702

Sum of electronic and thermal Free Energies= -1226.296894

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	291.672	105.157	210.870

C 0 -4.4965751968 -1.0543409964 -0.0023711718

C 0 -3.7268349708 -2.2164673786 0.1150288316

C 0 -2.3294661426 -2.1648659798 0.1486087149
C 0 -1.7224388261 -0.9200874007 0.0612897363
C 0 -2.4987668586 0.2530838677 -0.0593306742
C 0 -3.8863408771 0.1978735928 -0.0915502186
C 0 -0.2996068979 -0.5394968858 0.0620158326
C 0 -0.215411496 0.8819337597 -0.0670661235
C 0 -1.6119177282 1.4391717362 -0.1404832928
O 0 -1.9281713663 2.6097913402 -0.2438629408
N 0 0.7595641734 -1.298845338 0.1540946955
C 0 1.9685051724 -0.6456307475 0.1082233905
C 0 2.0439728419 0.7800788471 -0.0263805907
N 0 0.9051228209 1.5407242565 -0.1117488702
C 0 3.1632383898 -1.3897963963 0.190462221
C 0 4.3809067012 -0.7452872807 0.1424242965
C 0 4.45364358 0.6591766015 0.0122215088
C 0 3.3047159552 1.4132347296 -0.0717528676
H 0 -5.5774238202 -1.1294275718 -0.0255241791
H 0 -4.2238870443 -3.1776197248 0.1807498474
H 0 -1.7383236444 -3.0689091771 0.2345447099
H 0 -4.4740558332 1.1037352883 -0.1848578516
H 0 3.0958110964 -2.4671994731 0.2849842112
H 0 5.2964530049 -1.322270204 0.204708052
H 0 5.4223537863 1.143645022 -0.0221465833
H 0 3.3342016735 2.4919745843 -0.1701883964
C 0 -3.7043137325 7.0394826975 0.1930809077
H 0 -3.1445172165 7.7120205706 -0.4638009266
H 0 -3.5328753881 7.348155587 1.2286743852
H 0 -4.769637136 7.1537015954 -0.0272811455
C 0 -3.2725436953 5.6011608523 -0.0145282837
H 0 -3.8533051023 4.9361692583 0.6377233532
H 0 -3.4595566132 5.2961935432 -1.0522867429
O 0 -1.8749029233 5.4969013388 0.2918826355
H 0 -1.6208582947 4.5694626781 0.1863847081
C 0 1.1832417926 6.3384845663 -1.7994239496
H 0 2.2161205384 6.5950785436 -1.5446438392
H 0 0.5160024355 6.8720454331 -1.1167564281
H 0 0.9841190855 6.685596081 -2.8175740202
C 0 0.9609428125 4.842318623 -1.6923236142
H 0 -0.0795770938 4.5992710414 -1.9418743408
H 0 1.6072639125 4.3113942107 -2.4044849177
O 0 1.2566801812 4.4341184179 -0.3513336205
H 0 1.0734207116 3.4789479346 -0.2762283518
C 0 0.7315105815 -5.8827881291 2.3000135582
H 0 1.6056210218 -6.3427371436 1.8291190803
H 0 -0.1667029732 -6.3594417766 1.8956310006
H 0 0.7733169245 -6.0852864807 3.3741505003
C 0 0.709686564 -4.3887394128 2.0400041912
H 0 -0.1627041997 -3.9336893301 2.5278856859
H 0 1.6071417951 -3.9200631742 2.4648388636
O 0 0.6589402178 -4.1721318211 0.6239134049
H 0 0.6866511308 -3.2092123759 0.4600542184

TS-2-1, with 1 EtOH on N1

Gas B3LYP/6-311G**

E(RB3LYP) = -1240.19919263

Zero-point correction= 0.378979 (Hartree/Particle)

Thermal correction to Energy= 0.404001

Thermal correction to Enthalpy= 0.404945

Thermal correction to Gibbs Free Energy= 0.320592

Sum of electronic and ZPE= -1239.820213

Sum of electronic and thermal Energies= -1239.795191

Sum of electronic and thermal Enthalpies= -1239.794247

Sum of electronic and thermal Free Energies= -1239.878601

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	253.515	93.982	177.537

C	0	-2.3624823783	3.0619816887	0.8929723238
C	0	-1.2883321938	3.7170960234	0.2805950689
C	0	-0.1142268762	3.0327384165	-0.0286982432
C	0	-0.056420913	1.6690227386	0.260196009
C	0	-1.152341034	0.9973609931	0.8259677577
C	0	-2.2966628933	1.697453987	1.1823142735
C	0	1.0644135	0.7279745244	0.1806258478
C	0	0.6422655033	-0.5404080258	0.7084436245
C	0	-0.8442804186	-0.4756987324	1.0822931593
O	0	-1.3161180155	-1.0480323437	2.1880639055
N	0	2.2891145217	0.9558611299	-0.2232380184
C	0	3.1638218133	-0.093594793	-0.1001379034
C	0	2.7451597253	-1.341758246	0.4575945163
N	0	1.4477496878	-1.5498536044	0.8578220403
C	0	4.5034701115	0.0629649962	-0.5205747422
C	0	5.3946377624	-0.9773601488	-0.3828864963
C	0	4.9855594973	-2.2070591296	0.1788499462
C	0	3.6845855725	-2.3872505	0.5917784753
H	0	-3.2503956855	3.6249401369	1.1582060528
H	0	-1.3610205342	4.7774156008	0.067253921
H	0	0.7383359667	3.5423097456	-0.465251126
H	0	-3.1082097941	1.1913358804	1.6932676662
H	0	4.7978451372	1.0131492193	-0.9506495288
H	0	6.4215783463	-0.8533464374	-0.7066620333
H	0	5.7033758679	-3.01237223	0.2828011606
H	0	3.3437897807	-3.3196314175	1.0254161803
C	0	-1.0801748118	-2.6877009267	-0.384180594
N	0	-1.7641800656	-1.4613004843	0.0736241753
C	0	-2.6379341684	-0.8953398426	-0.9547284663
C	0	-3.9256554781	-1.6867814736	-1.1102018408
O	0	-4.6674196688	-1.1653709761	-2.1109459493
O	0	-4.2681208046	-2.6290470503	-0.4486219536
H	0	-0.4628236868	-3.0652280639	0.4271501699
H	0	-1.83809848	-3.4285809321	-0.6407894287
H	0	-0.448628743	-2.4870778369	-1.2549240525
H	0	-2.0826253804	-1.6003455344	1.2687556789
H	0	-2.913624379	0.1265699528	-0.6913247162
H	0	-2.1355433764	-0.8464583521	-1.9276882916
H	0	-5.4836795421	-1.6856320499	-2.1598437572
C	0	4.2234753773	5.6198792498	-0.2858370684
H	0	3.3647474265	6.2349396798	-0.5668617963
H	0	4.9006852654	5.5740936039	-1.1422513749
H	0	4.7426911169	6.1075671239	0.5440651135
C	0	3.771583876	4.2223536981	0.102471263
H	0	4.642654404	3.6205257751	0.400768188
H	0	3.1012171723	4.2741325632	0.9735081546
O	0	3.1109862188	3.6369238976	-1.0137070329
H	0	2.8735919004	2.7185785564	-0.7873116179

TS-2-1, with 1 EtOH on O1

Gas B3LYP/6-311G**

E(RB3LYP) = -1240.20021850

Zero-point correction= 0.379075 (Hartree/Particle)

Thermal correction to Energy= 0.404104

Thermal correction to Enthalpy= 0.405048

Thermal correction to Gibbs Free Energy= 0.319157

Sum of electronic and ZPE= -1239.821144

Sum of electronic and thermal Energies= -1239.796114

Sum of electronic and thermal Enthalpies= -1239.795170

Sum of electronic and thermal Free Energies= -1239.881061

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	253.579	93.820	180.772

C 0 2.5408826797 -1.6626944722 2.7866802698

C 0 1.6891495771 -2.7718925676 2.7528614195

C 0 0.5842494124 -2.7948676707 1.9041122384

C 0 0.3700258925 -1.7016574261 1.0685856079

C 0 1.2496899413 -0.608132656 1.0662610007

C 0 2.3178317946 -0.5649074645 1.9525532076

C 0 -0.7630192495 -1.3889855471 0.1916441707

C 0 -0.5706629237 -0.0755866918 -0.3512276001

C 0 0.7793513986 0.4866879612 0.1096202384

O 0 0.8792828985 1.7687004757 0.5442997253

N 0 -1.8259449558 -2.1146367143 -0.0386137126

C 0 -2.7756248721 -1.5175113189 -0.8248346718

C 0 -2.5977686854 -0.1937567332 -1.3409872207

N 0 -1.4520919191 0.5206706019 -1.0966168399

C 0 -3.9661199895 -2.2179209713 -1.1250844597

C 0 -4.9409300453 -1.627601227 -1.8962875639

C 0 -4.7683934298 -0.317014895 -2.3962128849

C 0 -3.618277386 0.3882143784 -2.1244953544

H 0 3.3729301633 -1.6485589588 3.4814962649

H 0 1.8768587904 -3.6096182169 3.4147864085

H 0 -0.1113008815 -3.6255442584 1.9038536429

H 0 2.9486934269 0.3152804559 2.0088921373

H 0 -4.0782854355 -3.2177525439 -0.7234573108

H 0 -5.8536663245 -2.1679224758 -2.1201405915

H 0 -5.5512943666 0.1337385706 -2.9950590722

H 0 -3.46328416 1.3968963036 -2.4874457902

C 0 1.1892501951 1.1060136 -2.403545196

N 0 1.8196322233 0.7249129906 -1.1189877011

C 0 2.9729049173 -0.1591188433 -1.3130728041

C 0 4.1922429616 0.6069258889 -1.7971660536

O 0 5.2020989301 -0.2513158364 -2.0505572778

O 0 4.2776434796 1.7977583088 -1.9272828302

H 0 0.354962791 1.7720273562 -2.2006045421

H 0 1.9364642822 1.6241786593 -3.0044043699

H 0 0.8237907393 0.2250186223 -2.9378893424

H 0 1.8216376703 1.7231723262 -0.3809770656

H 0 3.240207274 -0.640823542 -0.3724584164

H 0 2.7483645688 -0.9588458694 -2.0272154188

H 0 5.9630981915 0.2787795246 -2.3322926058

C 0 -2.6497275715 3.3690359196 3.4909070821

H 0 -3.5003208024 2.7664005254 3.1614983574

H 0 -2.8320439583 4.4032407171 3.187386572

H 0 -2.5970716427 3.3304067503 4.5832730257

C 0 -1.365495337 2.8552939203 2.8597094695

H 0 -0.5149884959 3.462135191 3.2089173557

H 0 -1.1785490099 1.8223745427 3.195346077

O 0 -1.5012509745 2.9220500394 1.4532045812

H 0 -0.6666047828 2.6083572704 1.0602198443

TS-2-1, with 1 EtOH on O3

Gas B3LYP/6-311G**

E(RB3LYP) = -1240.19528214

Zero-point correction= 0.378403 (Hartree/Particle)

Thermal correction to Energy= 0.403654

Thermal correction to Enthalpy= 0.404598

Thermal correction to Gibbs Free Energy= 0.318983

Sum of electronic and ZPE= -1239.816879

Sum of electronic and thermal Energies= -1239.791628

Sum of electronic and thermal Enthalpies= -1239.790684

Sum of electronic and thermal Free Energies= -1239.876300

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 253.297 94.730 180.193

C 0 -2.181117865 3.892225446 -0.2732641091

C 0 -0.960788142 4.2904407933 -0.8296258424

C 0 0.1259041103 3.4181340715 -0.8608283044

C 0 -0.0448145986 2.1324938568 -0.3539992884

C 0 -1.2814415 1.7152003678 0.1625626763

C 0 -2.345389427 2.6038103962 0.2407880386

C 0 0.9347976544 1.0641138477 -0.1311733999

C 0 0.2808204031 -0.0218459473 0.5441960518

C 0 -1.2132029311 0.289051082 0.7015774489

O 0 -1.8812436606 -0.0035460795 1.819237847

N 0 2.2114238944 1.0754575332 -0.4132223241

C 0 2.9068973596 -0.0281356029 0.0062387344

C 0 2.2637947369 -1.0958766486 0.709936546

N 0 0.9146485691 -1.0756755079 0.9671817271

C 0 4.2947221924 -0.110134462 -0.2487882879

C 0 5.0153415402 -1.2011733473 0.1807170633

C 0 4.3810383578 -2.2511846653 0.8818327645

C 0 3.0303236917 -2.2003729162 1.1425326829

H 0 -3.0021217629 4.5987742916 -0.2253370022

H 0 -0.8534321672 5.2976819369 -1.2159418396

H 0 1.0898721287 3.730039129 -1.2448431999

H 0 -3.2736120104 2.302392203 0.7136379544

H 0 4.7585112666 0.7104511427 -0.7828370695

H 0 6.0798775731 -1.2574543967 -0.0161375402

H 0 4.9654657096 -3.1008879577 1.2154535572

H 0 2.5193222073 -2.9908873187 1.6789116834

C 0 -1.5974224084 -2.1080804903 -0.4305268132

N 0 -2.1495613335 -0.7518434534 -0.2346648685

C 0 -2.8840047936 -0.2793390998 -1.4074363144

C 0 -4.3403892531 -0.7075489797 -1.3734110087

O 0 -4.9305667613 -0.4614591021 -2.5570442851

O 0 -4.9276282035 -1.1708209189 -0.4287067115

H 0 -1.0679569055 -2.404666772 0.4702607289

H 0 -2.4239686501 -2.8018454818 -0.5874242241

H 0 -0.9123902064 -2.132247794 -1.2836854708

H 0 -2.5944313179 -0.6447879235 0.9223384135

H 0 -2.8789126322 0.8124796868 -1.4430198888

H 0 -2.4324032386 -0.6288488672 -2.3413385955

H 0 -5.8620244309 -0.7168679142 -2.4723994275

C 0 -3.2206152595 -4.0715855242 3.6158672966

H 0 -2.261748763 -4.3445133464 3.1678241982

H 0 -3.9019787288 -4.9193087504 3.5065932543

H 0 -3.0610237465 -3.8860885026 4.6817115078

C 0 -3.7908585374 -2.8394026071 2.9362284337

H 0 -4.7485521718 -2.5676051809 3.4027282745

H 0 -3.104855455 -1.9916403443 3.0510335874

O 0 -3.98075947 -3.1485978514 1.5521939652

H 0 -4.4131626236 -2.40270637 1.1187840698

TS-2-1, with 2 EtOHs on O1 and O2

Gas B3LYP/6-311G**

E(RB3LYP) = -1395.31076561

Zero-point correction= 0.461253 (Hartree/Particle)

Thermal correction to Energy= 0.491748

Thermal correction to Enthalpy= 0.492692

Thermal correction to Gibbs Free Energy= 0.391947

Sum of electronic and ZPE= -1394.849513

Sum of electronic and thermal Energies= -1394.819017

Sum of electronic and thermal Enthalpies= -1394.818073

Sum of electronic and thermal Free Energies= -1394.918818

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 308.577 111.152 212.036

C 0 -2.0469515692 3.4917708837 0.8024060709

C 0 -0.7619216828 3.7352678359 0.3060839526

C 0 0.130414578 2.685690009 0.0975037082

C 0 -0.301100088 1.3886738428 0.3635790759

C 0 -1.6054862364 1.1370165752 0.8159421071

C 0 -2.4728637672 2.1899836672 1.0750553889

C 0 0.4463037632 0.1272141365 0.3742173109

C 0 -0.4206519402 -0.9123940911 0.8482153906

C 0 -1.8276658108 -0.350665723 1.0869058064

O 0 -2.5125758675 -0.6732627548 2.2159507874

N 0 1.7059493033 -0.0635360627 0.0804150433

C 0 2.1613660596 -1.3393499662 0.2842477153

C 0 1.3045154485 -2.3697406317 0.7883903591

N 0 -0.0197055196 -2.1304698817 1.056975654

C 0 3.5124188943 -1.6454735038 0.0032103858

C 0 3.9943244107 -2.915850433 0.2210076136

C 0 3.1499925022 -3.9290629863 0.7286992744

C 0 1.828973387 -3.6623725007 1.0076272436

H 0 -2.7129467604 4.3255872044 0.9935597593

H 0 -0.4499725972 4.754470094 0.1083533258

H 0 1.1446689999 2.8641995235 -0.2390249668

H 0 -3.4516484167 2.0017421605 1.5020687991

H 0 4.1413847834 -0.8497643627 -0.3773434156

H 0 5.0323161421 -3.1439910702 0.0072393022

H 0 3.5502249074 -4.9214684025 0.9010599142

H 0 1.1616931596 -4.4174029448 1.4049786188

C 0 -2.6972806784 -2.4098355689 -0.2739797926

N 0 -2.9456707585 -1.0014574495 0.1088378027

C 0 -3.5320852853 -0.2293678601 -0.9915673545

C 0 -5.0135378258 -0.5242110023 -1.1678656742

O 0 -5.5032343891 0.119711557 -2.2202038773

O 0 -5.6606437031 -1.241320654 -0.432105311

H 0 -2.291226707 -2.9410734986 0.5825963241

H 0 -3.650869957 -2.8508350152 -0.5635170336

H 0 -1.9888708978 -2.4719826838 -1.1044169612

H 0 -3.3799141845 -0.9888997276 1.2739623451

H 0 -3.4327417943 0.838369469 -0.7974389995

H 0 -3.0185599356 -0.4291456083 -1.9381818582

H 0 -6.4777751628 -0.0873172866 -2.283227602

C 0 -9.6709986752 0.866235854 -2.553905343

H 0 -10.062977073 0.17326799 -3.3014833982

H 0 -8.9303231494 1.5094303442 -3.0357855883

H 0 -10.4917571876 1.4956283071 -2.2007222145

C 0 -9.0559589591 0.1036766094 -1.3966966631

H 0 -8.6534617212 0.7948589011 -0.6457077156

H 0 -9.8103698851 -0.5233711526 -0.9091325615

O 0 -8.0062433478 -0.7348998984 -1.9113946724

H 0 -7.5995200732 -1.2253463532 -1.1785972604

C 0 -0.0422067566 -0.6659142677 6.4048725633

H 0 0.9633189691 -0.9356178088 6.0711729216

H 0 -0.4445046616 -1.5070639592 6.9755092343

H 0 0.0312177745 0.2017812408 7.0676770021

C 0 -0.9317267805 -0.3703624686 5.2077079663

H 0 -1.937515255 -0.0873698126 5.557194724

H 0 -0.5309330861 0.496199199 4.657226269

O 0 -0.9772355333 -1.523051121 4.3895025488

H 0 -1.5630030727 -1.3273938524 3.6353837046

TS-2-1, with 2 EtOHs on O1 and N1

Gas B3LYP/6-311G**

E(RB3LYP) = -1395.30299832

Zero-point correction= 0.460967 (Hartree/Particle)

Thermal correction to Energy= 0.491841

Thermal correction to Enthalpy= 0.492785

Thermal correction to Gibbs Free Energy= 0.391201

Sum of electronic and ZPE= -1394.842032

Sum of electronic and thermal Energies= -1394.811158

Sum of electronic and thermal Enthalpies= -1394.810214

Sum of electronic and thermal Free Energies= -1394.911797

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	308.635	111.777	213.801

C	0	-1.7111636609	3.6566556816	0.7224466544
C	0	-0.4117549338	3.8022925713	0.225396638
C	0	0.3993635807	2.6907031592	0.0044043066
C	0	-0.1355918302	1.4282160368	0.2610012678
C	0	-1.457515901	1.2754659543	0.7100432871
C	0	-2.2394821871	2.3901874052	0.9813697067
C	0	0.5025810698	0.1083641825	0.257348197
C	0	-0.4497147688	-0.8659741452	0.7063885927
C	0	-1.8033694769	-0.1912798018	0.9583756613
O	0	-2.5108304702	-0.4767572114	2.0814573486
N	0	1.743694761	-0.1957448426	-0.028694547
C	0	2.0910886986	-1.511116363	0.1434732146
C	0	1.1428751198	-2.4694505338	0.6213791803
N	0	-0.1551022683	-2.117175433	0.8911262339
C	0	3.4097342822	-1.9273528377	-0.1462859491
C	0	3.7736129986	-3.2412787928	0.0430246539
C	0	2.8415133639	-4.1854864005	0.5285062889
C	0	1.5487129158	-3.8080705907	0.81221634
H	0	-2.30915991	4.5384781472	0.9228960143
H	0	-0.0212600801	4.7952810412	0.0344588355
H	0	1.4228490243	2.7971165504	-0.3396830032
H	0	-3.2305499955	2.2750262438	1.4059958077
H	0	4.1107836757	-1.1892352135	-0.5177906807
H	0	4.7865997992	-3.5567245569	-0.1786884387
H	0	3.1509847275	-5.2132146876	0.6783791966
H	0	0.8150217486	-4.5090279936	1.1907795522
C	0	-2.8538851295	-2.1505479689	-0.4258810256
N	0	-2.9754229291	-0.7287049365	-0.0296231288
C	0	-3.4814076966	0.1051137301	-1.1247908014
C	0	-4.978755576	-0.0688596484	-1.3146204646
O	0	-5.3907890404	0.6423963651	-2.3839577886
O	0	-5.710800555	-0.7216121064	-0.6214691968
H	0	-2.4974942117	-2.722628771	0.4263969495
H	0	-3.8427598395	-2.5033519205	-0.7180761568
H	0	-2.1535788936	-2.267989544	-1.257094532
H	0	-3.4071056707	-0.6928624747	1.1343820704
H	0	-3.2972593925	1.1582333265	-0.9125132207
H	0	-2.9737164552	-0.1226486526	-2.068295685
H	0	-6.350091143	0.5229098874	-2.4547359924
C	0	5.3947238416	3.2926990659	0.2064405996
H	0	4.8747108567	4.2012430449	-0.1080381209
H	0	6.0607779078	2.9870160011	-0.6041511285
H	0	6.0005175058	3.5269561819	1.0863327417
C	0	4.3977498911	2.1881588936	0.5126504202
H	0	4.9331954022	1.2871874124	0.8459358692
H	0	3.7387365505	2.4960317571	1.3381005991
O	0	3.6456094373	1.9214253233	-0.6662605698
H	0	3.0474969315	1.1721290349	-0.4893814475

C 0 0.2230608271 -0.4313653779 6.1129050262

H 0 1.2043317363 -0.6500216697 5.6833279791

H 0 -0.0870229999 -1.2978599919 6.7026914393

H 0 0.3192636375 0.429151395 6.7819451011

C 0 -0.7861267691 -0.1591821186 5.008988833

H 0 -1.7666571002 0.0708280326 5.4548902696

H 0 -0.477997119 0.7324047829 4.439587878

O 0 -0.8562988326 -1.3012988611 4.1759632853

H 0 -1.5147878349 -1.1212397221 3.4806549787

TS-2-1, with 2 EtOHs on N1 and O3

Gas B3LYP/6-311G**

E(RB3LYP) = -1395.30950798

Zero-point correction= 0.461236 (Hartree/Particle)

Thermal correction to Energy= 0.491700

Thermal correction to Enthalpy= 0.492644

Thermal correction to Gibbs Free Energy= 0.393538

Sum of electronic and ZPE= -1394.848272

Sum of electronic and thermal Energies= -1394.817808

Sum of electronic and thermal Enthalpies= -1394.816864

Sum of electronic and thermal Free Energies= -1394.915970

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 308.547 111.282 208.586

C 0 -1.7458696479 3.4071236412 0.7530157218

C 0 -0.5141093734 3.6452787069 0.1332281056

C 0 0.3550658427 2.5957333767 -0.1583636988

C 0 -0.055379771 1.2996702544 0.1555919987

C 0 -1.3132288054 1.0522895563 0.7287539708

C 0 -2.1486645917 2.1077115272 1.0675391376

C 0 0.6776040193 0.0321088427 0.0978950166

C 0 -0.150211612 -1.0067917751 0.6467085555

C 0 -1.5253875921 -0.4330371043 1.0158442597

O 0 -2.1479915285 -0.7827494735 2.1424206164

N 0 1.9061599716 -0.1775752356 -0.3042595587

C 0 2.3718763811 -1.4595386355 -0.1587067718

C 0 1.5544620713 -2.4802202019 0.4191050107

N 0 0.2645540175 -2.2269945874 0.8177307976

C 0 3.6842321697 -1.7757119137 -0.5756065178

C 0 4.1684944621 -3.0545009712 -0.4156266396

C 0 3.366215054 -4.0612473293 0.1655730815

C 0 2.0822723188 -3.7803964499 0.5756886778

H 0 -2.3880454507 4.2440127182 1.0039365469

H 0 -0.221322919 4.6626124886 -0.0999943153

H 0 1.3293624836 2.7754646111 -0.6005175171

H 0 -3.0829876674 1.9185831652 1.584296525

H 0 4.2835539711 -0.9902067587 -1.0209208209

H 0 5.1758036337 -3.2931759197 -0.7368797648

H 0 3.7671803421 -5.0608376761 0.2867250596

H 0 1.4451676186 -4.5332094183 1.0239174853

C 0 -2.5090253598 -2.4624660093 -0.3867711697

N 0 -2.729167318 -1.0661655071 0.0420662293

C 0 -3.3763976671 -0.263112326 -0.9972586075

C 0 -4.8648737347 -0.5534650034 -1.1104987722

O 0 -5.4110380833 0.1438548426 -2.1005233231

O 0 -5.4739047325 -1.3113594204 -0.3826799178

H 0 -2.052059279 -3.0111287199 0.4329679536

H 0 -3.4773811395 -2.9024969012 -0.6266869538

H 0 -1.8542423654 -2.5091669002 -1.2620737083

H 0 -3.0681165559 -1.0647431471 1.238504834

H 0 -3.2698419793 0.7984743088 -0.7719529927

H 0 -2.9143266882 -0.4260021497 -1.9775222677

H 0 -6.3861092554 -0.0641314649 -2.1234641751

C 0 5.3151049664 3.5423684431 -0.4212837135

H 0 4.7204281142 4.4077714451 -0.7248257037

H 0 5.94244993 3.2504404833 -1.2670929198

H 0 5.9633299994 3.8403644002 0.4076938193

C 0 4.4097052721 2.3915349513 -0.016317245

H 0 5.0202020598 1.5345653935 0.3044518936

H 0 3.7907127049 2.6871157175 0.8440929057

O 0 3.5975355743 2.0444674273 -1.1318866846

H 0 3.0574775961 1.2682824274 -0.8930854828

C 0 -9.6024118452 0.8835173098 -2.1329668552

H 0 -10.0489670762 0.2257737307 -2.8818022489

H 0 -8.8989418654 1.5508906828 -2.6371734901

H 0 -10.3944481796 1.4930194267 -1.6904856483

C 0 -8.9034661553 0.0683108931 -1.0623847842

H 0 -8.4463756938 0.7244716935 -0.3111002449

H 0 -9.6204863702 -0.582947805 -0.5504079463

O 0 -7.8957157557 -0.7412396425 -1.6927645821

H 0 -7.4330868058 -1.2613220182 -1.0151195505

TS-2-1, with 3 EtOHs on N1, O1 and O2

Gas B3LYP/6-311G**

E(RB3LYP) = -1550.41357315

Zero-point correction= 0.543135 (Hartree/Particle)

Thermal correction to Energy= 0.579475

Thermal correction to Enthalpy= 0.580419

Thermal correction to Gibbs Free Energy= 0.464142

Sum of electronic and ZPE= -1549.870438

Sum of electronic and thermal Energies= -1549.834098

Sum of electronic and thermal Enthalpies= -1549.833154

Sum of electronic and thermal Free Energies= -1549.949431

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	363.626	129.109	244.725

C 0 -1.9508979704 3.4350840629 0.6591684086

C 0 -0.6703691119 3.6490296738 0.1383671081

C 0 0.2087597765 2.5859892767 -0.0593874496

C 0 -0.2390047982 1.3003997291 0.2452042354

C 0 -1.542126907 1.0761603051 0.7183305177

C 0 -2.3916878498 2.1460536082 0.9656363803

C 0 0.4844479017 0.0259007642 0.273758357

C 0 -0.3958971921 -0.9934484809 0.7679402593

C 0 -1.7883785652 -0.4014398729 1.0177197781

O 0 -2.4561213037 -0.6925271658 2.1658822926

N 0 1.7393182433 -0.2052300051 -0.020517835

C 0 2.175076752 -1.4885777644 0.1884117553

C 0 1.2985741998 -2.490563825 0.7112505997

N 0 -0.0163397968 -2.2155297675 0.9891512645

C 0 3.5144928202 -1.8267331835 -0.1077470553

C 0 3.9668912363 -3.106946315 0.1182233723

C 0 3.1056400804 -4.0936089387 0.6480416814

C 0 1.7945348502 -3.7925293198 0.9391138822

H 0 -2.6029525469 4.2821506789 0.8401685477

H 0 -0.3484632818 4.6585822464 -0.0900321691

H 0 1.2184134185 2.7473647153 -0.4223605449

H 0 -3.36785266 1.9802744034 1.4075384707

H 0 4.1602130418 -1.0568906046 -0.5136126966

H 0 4.9954953005 -3.3624409285 -0.1087727429

H 0 3.4841893181 -5.0933407537 0.82614971

H 0 1.1137009294 -4.5271258976 1.3511718021

C 0 -2.7248606398 -2.4687610689 -0.2801564565

N 0 -2.933888645 -1.0462400695 0.0739525241

C 0 -3.5212210412 -0.2868094391 -1.0354185153

C 0 -5.0135299669 -0.5465431662 -1.1729413499

O 0 -5.5080388067 0.0797326163 -2.2329699276

O 0 -5.6626300928 -1.2249196649 -0.4029662291

H 0 -2.3207203198 -2.9905738117 0.5830252543

H 0 -3.6931610634 -2.8919815373 -0.5463642799

H 0 -2.0305531213 -2.567313045 -1.1188452276

H 0 -3.3492888315 -1.0026860488 1.2458382003

H 0 -3.3892601655 0.7825058333 -0.8722439268

H 0 -3.0327010285 -0.5258813343 -1.9860192217

H 0 -6.4892089489 -0.1024054649 -2.270151647

C 0 5.1614517366 3.5127479427 0.0509475323

H 0 4.5834162818 4.3751482511 -0.2909743773

H 0 5.8385402839 3.2190762778 -0.7549404478

H 0 5.7586959376 3.816344191 0.9153776247

C 0 4.2374322458 2.3607913477 0.4073744587

H 0 4.8304411668 1.5074347727 0.7675219769

H 0 3.5674780581 2.6577043264 1.2280630429

O 0 3.493665206 2.0051909073 -0.7530392167

H 0 2.9451174674 1.2268860371 -0.5432864054

C 0 -9.6521080477 0.9370421447 -2.5185259926

H 0 -10.0751866342 0.2342684496 -3.2395005537

H 0 -8.9002689025 1.5436444105 -3.029656065

H 0 -10.4488266832 1.6005546542 -2.1728709078

C 0 -9.0426129722 0.1911315903 -1.34768048

H 0 -8.6088012755 0.8918512736 -0.6234765921

H 0 -9.8075194834 -0.3988274849 -0.8311261595

O 0 -8.0254229662 -0.6931519274 -1.8517344348

H 0 -7.6229423018 -1.1745814287 -1.1108634926

C 0 0.2710563568 -0.4209479129 6.1886717521

H 0 1.2623365491 -0.6246688877 5.7750371268

H 0 -0.018542478 -1.2756982301 6.8054450336

H 0 0.3354169456 0.4645583251 6.8283333365

C 0 -0.7353990256 -0.2174513111 5.0674802482

H 0 -1.7264603033 -0.0013651341 5.4970598846

H 0 -0.4484633282 0.663184639 4.4704860368

O 0 -0.7638564913 -1.3887700133 4.2741544319

H 0 -1.4225162262 -1.2528876107 3.5686202621

3.4.2 SMD calculation results for liquid-air interface simulation

int-1 with **3** EtOHs on N1, N2, O1.

SMD B3LYP/6-311G**

E(RB3LYP) = -1226.66245581

Zero-point correction= 0.434811 (Hartree/Particle)

Thermal correction to Energy= 0.464809

Thermal correction to Enthalpy= 0.465753

Thermal correction to Gibbs Free Energy= 0.365562

Sum of electronic and ZPE= -1226.227645

Sum of electronic and thermal Energies= -1226.197647

Sum of electronic and thermal Enthalpies= -1226.196702

Sum of electronic and thermal Free Energies= -1226.296894

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 291.672 105.157 210.870

C 0 -4.4965751968 -1.0543409964 -0.0023711718

C 0 -3.7268349708 -2.2164673786 0.1150288316

C 0 -2.3294661426 -2.1648659798 0.1486087149

C 0 -1.7224388261 -0.9200874007 0.0612897363

C 0 -2.4987668586 0.2530838677 -0.0593306742

C 0 -3.8863408771 0.1978735928 -0.0915502186

C 0 -0.2996068979 -0.5394968858 0.0620158326

C 0 -0.215411496 0.8819337597 -0.0670661235

C 0 -1.6119177282 1.4391717362 -0.1404832928

O 0 -1.9281713663 2.6097913402 -0.2438629408

N 0 0.7595641734 -1.298845338 0.1540946955

C 0 1.9685051724 -0.6456307475 0.1082233905

C 0 2.0439728419 0.7800788471 -0.0263805907

N 0 0.9051228209 1.5407242565 -0.1117488702

C 0 3.1632383898 -1.3897963963 0.190462221

C 0 4.3809067012 -0.7452872807 0.1424242965

C 0 4.45364358 0.6591766015 0.0122215088

C 0 3.3047159552 1.4132347296 -0.0717528676

H 0 -5.5774238202 -1.1294275718 -0.0255241791

H 0 -4.2238870443 -3.1776197248 0.1807498474

H 0 -1.7383236444 -3.0689091771 0.2345447099

H 0 -4.4740558332 1.1037352883 -0.1848578516

H 0 3.0958110964 -2.4671994731 0.2849842112

H 0 5.2964530049 -1.322270204 0.204708052

H 0 5.4223537863 1.143645022 -0.0221465833

H 0 3.3342016735 2.4919745843 -0.1701883964

C 0 -3.7043137325 7.0394826975 0.1930809077

H 0 -3.1445172165 7.7120205706 -0.4638009266

H 0 -3.5328753881 7.348155587 1.2286743852

H 0 -4.769637136 7.1537015954 -0.0272811455

C 0 -3.2725436953 5.6011608523 -0.0145282837

H 0 -3.8533051023 4.9361692583 0.6377233532

H 0 -3.4595566132 5.2961935432 -1.0522867429

O 0 -1.8749029233 5.4969013388 0.2918826355

H 0 -1.6208582947 4.5694626781 0.1863847081

C 0 1.1832417926 6.3384845663 -1.7994239496

H 0 2.2161205384 6.5950785436 -1.5446438392

H 0 0.5160024355 6.8720454331 -1.1167564281

H 0 0.9841190855 6.685596081 -2.8175740202

C 0 0.9609428125 4.842318623 -1.6923236142

H 0 -0.0795770938 4.5992710414 -1.9418743408

H 0 1.6072639125 4.3113942107 -2.4044849177

O 0 1.2566801812 4.4341184179 -0.3513336205

H 0 1.0734207116 3.4789479346 -0.2762283518

C 0 0.7315105815 -5.8827881291 2.3000135582

H 0 1.6056210218 -6.3427371436 1.8291190803

H 0 -0.1667029732 -6.3594417766 1.8956310006

H 0 0.7733169245 -6.0852864807 3.3741505003

C 0 0.709686564 -4.3887394128 2.0400041912

H 0 -0.1627041997 -3.9336893301 2.5278856859

H 0 1.6071417951 -3.9200631742 2.4648388636

O 0 0.6589402178 -4.1721318211 0.6239134049

H 0 0.6866511308 -3.2092123759 0.4600542184

3 with 1 EtOH on O2

SMD B3LYP/6-311G**

E(RB3LYP) = -478.956594982

Zero-point correction= 0.188328 (Hartree/Particle)

Thermal correction to Energy= 0.200884

Thermal correction to Enthalpy= 0.201828

Thermal correction to Gibbs Free Energy= 0.146859

Sum of electronic and ZPE= -478.768267

Sum of electronic and thermal Energies= -478.755711

Sum of electronic and thermal Enthalpies= -478.754767

Sum of electronic and thermal Free Energies= -478.809736

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 126.057 41.188 115.692

C 0 2.5334145393 0.116067054 0.3828866099

N 0 1.1433558592 -0.2621979386 0.6328145719

C 0 0.5607637235 -0.9788999576 -0.4900677636

C 0 -0.7876963921 -1.5656940414 -0.1433752572

O 0 -1.4368673511 -2.0008791159 -1.2214157885

O 0 -1.2201713786 -1.6594677415 0.9905175833

H 0 2.9469437844 0.5883564782 1.2770987661

H 0 3.182891441 -0.7320636678 0.1089294414

H 0 2.5803062453 0.8455738344 -0.4316714194

H 0 1.105680627 -0.86859895 1.4471230645

H 0 0.4341979873 -0.3062384018 -1.3442639865

H 0 1.1800303298 -1.8203361199 -0.8524433606

H 0 -2.3025796624 -2.4315432677 -0.9548545053

C 0 -5.1294851234 -1.3803802717 -1.31903302

H 0 -5.537944121 -2.0211320622 -2.1056290556

H 0 -4.2711833264 -0.8365290781 -1.7234131515

H 0 -5.8942930893 -0.6512084569 -1.0377282812

C 0 -4.7301422774 -2.2008915946 -0.1114327619

H 0 -4.3181113882 -1.5630686406 0.6777116585

H 0 -5.5913859551 -2.740452968 0.2945430495

O 0 -3.7299318937 -3.1637392731 -0.5249899789

H 0 -3.5152920282 -3.7218663692 0.2341672352

3 with 1 EtOH on O3

SMD B3LYP/6-311G**

E(RB3LYP) = -478.952176863

Zero-point correction= 0.188851 (Hartree/Particle)

Thermal correction to Energy= 0.201411

Thermal correction to Enthalpy= 0.202355

Thermal correction to Gibbs Free Energy= 0.147870

Sum of electronic and ZPE= -478.763326

Sum of electronic and thermal Energies= -478.750766

Sum of electronic and thermal Enthalpies= -478.749821

Sum of electronic and thermal Free Energies= -478.804306

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 126.387 41.404 114.673

C 0 2.3751916737 0.3928656984 -0.2699381055

N 0 0.9247809322 0.3775857978 -0.4611832207

C 0 0.3348167832 -0.8676457507 -0.0008350411

C 0 -1.1684820395 -0.8720274803 -0.1114987179

O 0 -1.6676232651 -2.1079128362 0.0063868089

O 0 -1.8771580678 0.1055948909 -0.2573456594

H 0 2.7671102279 1.3693218463 -0.5629489916

H 0 2.6874863368 0.1936878078 0.76839235

H 0 2.8438259528 -0.3618420469 -0.9090442295

H 0 0.5158223447 1.1515340927 0.0565911107

H 0 0.7183736692 -1.70440802 -0.5923398477

H 0 0.5619007007 -1.1109871209 1.0538267482

H 0 -2.6385112075 -2.0567002886 -0.0145716301

C 0 -0.5377582071 4.8478924636 -0.8496885766

H 0 0.5039957093 4.7791931202 -0.5219537279

H 0 -1.0929552507 5.43293625 -0.1102370232

H 0 -0.5630637333 5.3861942299 -1.8015495058

C 0 -1.1461651281 3.4682126635 -1.0050633792

H 0 -2.183405466 3.5502595121 -1.3555273947

H 0 -0.5883248494 2.8859659666 -1.749124487

O 0 -1.108799852 2.8050114401 0.2676664751

H 0 -1.470756174 1.9122939138 0.1397691251

3 with 2 EtOHs on O2 and N3

SMD B3LYP/6-311G**

E(RB3LYP) = -634.065649035

Zero-point correction= 0.269583 (Hartree/Particle)

Thermal correction to Energy= 0.287890

Thermal correction to Enthalpy= 0.288835

Thermal correction to Gibbs Free Energy= 0.215505

Sum of electronic and ZPE= -633.796066

Sum of electronic and thermal Energies= -633.777759

Sum of electronic and thermal Enthalpies= -633.776814

Sum of electronic and thermal Free Energies= -633.850144

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 180.654 59.089 154.335

C 0 3.0470325481 -0.5091848703 0.1512149079

N 0 1.5886581599 -0.3885325331 0.0679470564

C 0 0.9284789126 -1.6661619591 -0.1705684812

C 0 -0.573394362 -1.5462689411 -0.0468284234

O 0 -1.196610742 -2.6321167307 -0.4905736177

O 0 -1.1405495216 -0.5807845255 0.4315431208

H 0 3.4749199924 0.4696391476 0.3770430194

H 0 3.3776982064 -1.2228822371 0.9196056669

H 0 3.44417942 -0.8385459068 -0.8128838127

H 0 1.2284247206 0.0058171864 0.9327534574

H 0 1.1681085646 -2.0284622524 -1.174391843

H 0 1.2431927759 -2.454737945 0.532777055

H 0 -2.1866031205 -2.5622842688 -0.3350693054

C 0 -4.493422336 -1.7016496306 -2.1704679289

H 0 -4.9891798054 -2.6498683594 -2.3966404703

H 0 -3.4693302455 -1.7444438195 -2.5518218754

H 0 -5.0212165743 -0.9027110029 -2.6985469993

C 0 -4.5060439493 -1.4313134012 -0.6812986738

H 0 -4.0118726271 -0.4820382934 -0.4504967247

H 0 -5.5315733863 -1.3896649717 -0.3018568809

O 0 -3.8080651523 -2.5128967934 -0.0162252176

H 0 -3.8885777554 -2.38501173 0.9381382551

C 0 -0.311885633 3.2425708527 -2.7308972266

H 0 -0.8786096125 2.6706669468 -3.4721717624

H 0 0.5681556903 3.6654420022 -3.2253796455

H 0 -0.9388795978 4.0683116502 -2.3813355775

C 0 0.1017983908 2.3522777958 -1.5735124109

H 0 0.6507039915 2.9459279724 -0.8273382525

H 0 -0.7908532442 1.9491825134 -1.0754105954

O 0 0.918062698 1.2952499223 -2.0762278246

H 0 1.1544426136 0.7017066822 -1.3203976293

3 with 2 EtOHs on O2 and O3

SMD B3LYP/6-311G**

E(RB3LYP) = -634.062898081

Zero-point correction= 0.269805 (Hartree/Particle)

Thermal correction to Energy= 0.288091

Thermal correction to Enthalpy= 0.289036

Thermal correction to Gibbs Free Energy= 0.218971

Sum of electronic and ZPE= -633.793093

Sum of electronic and thermal Energies= -633.774807

Sum of electronic and thermal Enthalpies= -633.773862

Sum of electronic and thermal Free Energies= -633.843927

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 180.780 59.413 147.464

C 0 2.3006422943 0.5667426892 -1.0589702007

N 0 0.8478833062 0.4768504004 -0.9142287362

C 0 0.4277504674 -0.8519123638 -0.5010178687

C 0 -1.0568280038 -0.945489266 -0.2408741505

O 0 -1.4756469841 -2.2010960776 -0.1825122624

O 0 -1.7972978186 0.0126041794 -0.0700518247

H 0 2.5768289687 1.5950252669 -1.3030689864

H 0 2.8559451489 0.2663558845 -0.1550229111

H 0 2.6341114164 -0.0735174589 -1.881582255

H 0 0.5438178106 1.153144652 -0.2184800222

H 0 0.6791541784 -1.5803461257 -1.2777372365

H 0 0.9206188216 -1.2097938327 0.4221847745

H 0 -2.4527923351 -2.2387371928 0.0554592602

C 0 -4.8207228581 -3.0212614096 -1.6905881402

H 0 -5.1105622128 -3.9984281365 -1.2941666797

H 0 -3.8008043227 -3.0914012526 -2.0790467268

H 0 -5.4868411404 -2.7760044535 -2.5223508628

C 0 -4.9204103436 -1.9563179656 -0.6196742459

H 0 -4.6296202559 -0.9760771772 -1.0118484232

H 0 -5.9421251056 -1.8856455756 -0.2345851148

O 0 -4.0374877744 -2.3207964045 0.4703017267

H 0 -4.1544408718 -1.6785846196 1.1829275746

C 0 -0.9212431814 4.8591459597 -0.4130828281

H 0 0.1682550564 4.8709232482 -0.3117489256

H 0 -1.35477113 5.3105961175 0.4844777697

H 0 -1.1926287013 5.4780470428 -1.2731819712

C 0 -1.4298771534 3.4428955297 -0.5970716529

H 0 -2.5211935359 3.447147894 -0.7187370296

H 0 -0.996627094 2.9957515478 -1.5005990666

O 0 -1.0666710953 2.6712697892 0.5569294049

H 0 -1.3815637707 1.7626974707 0.408084711

3 with 3 EtOHs on O2, O3 and N3

SMD B3LYP/6-311G**

E(RB3LYP) = -789.172734702

Zero-point correction= 0.351019 (Hartree/Particle)

Thermal correction to Energy= 0.374890

Thermal correction to Enthalpy= 0.375834

Thermal correction to Gibbs Free Energy= 0.293148

Sum of electronic and ZPE= -788.821716

Sum of electronic and thermal Energies= -788.797845

Sum of electronic and thermal Enthalpies= -788.796901

Sum of electronic and thermal Free Energies= -788.879586

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 235.247 77.877 174.026

C 0 2.9566672156 -1.3205753742 -1.1305783074

N 0 1.6153776849 -0.8615102766 -0.7555935404

C 0 0.6089675218 -1.9083266091 -0.8790924764

C 0 -0.7480705145 -1.4338803421 -0.4150175867

O 0 -1.7058877625 -2.3018376901 -0.6949760757

O 0 -0.9276120383 -0.3787807406 0.1742788835

H 0 3.670662733 -0.5112588182 -0.9655687719

H 0 3.2869657448 -2.2008209732 -0.5604956714

H 0 2.972580692 -1.5764612799 -2.1934498692

H 0 1.6273748544 -0.5348529627 0.2069862775

H 0 0.5235777422 -2.218140677 -1.9248812579

H 0 0.8490173579 -2.8158835755 -0.3017478881

H 0 -2.5968968422 -1.9842217561 -0.3560414541

C 0 -3.8102587889 2.3745490832 -2.7063776245

H 0 -3.2565762934 3.3172615032 -2.663288722

H 0 -4.7757167981 2.519802969 -2.212044825

H 0 -3.9970533689 2.1343898305 -3.7571699559

C 0 -3.0268802344 1.2600886937 -2.040820688

H 0 -3.5840205336 0.3168061925 -2.1035959726

H 0 -2.0650524078 1.1159631456 -2.5482092013

O 0 -2.8072106011 1.6109753528 -0.6661684718

H 0 -2.2426974166 0.9220153304 -0.2788134843

C 0 -5.3975633752 -0.1349753727 1.671902807

H 0 -6.3521209665 -0.5516028734 1.3357457981

H 0 -5.1872619975 0.7700321824 1.0961791706

H 0 -5.500783724 0.141630506 2.7259152204

C 0 -4.2735892209 -1.1401041593 1.5061173494

H 0 -3.321413633 -0.7164755364 1.8279775877

H 0 -4.4598577225 -2.0457280009 2.0924808239

O 0 -4.0805984268 -1.4988203873 0.1183044845

H 0 -4.8247479739 -2.0420733411 -0.1725451723

C 0 0.839784766 3.7005690776 -2.5367722215

H 0 -0.0325758342 3.6834267637 -3.1975847638

H 0 1.7399966293 3.7057918098 -3.1590916968

H 0 0.8129309926 4.6311729609 -1.961748396

C 0 0.8374830286 2.4980072422 -1.6105265562

H 0 1.7107488833 2.5405448488 -0.9451576042

H 0 -0.0599134195 2.5169684408 -0.9772696798

O 0 0.871181694 1.3033514763 -2.3961020291

H 0 1.1093892835 0.5518357267 -1.7981618383

int-1 with 1 EtOH on O1.

SMD B3LYP/6-311G**

E(RB3LYP) = -916.450430837

Zero-point correction= 0.272753 (Hartree/Particle)

Thermal correction to Energy= 0.290743

Thermal correction to Enthalpy= 0.291687

Thermal correction to Gibbs Free Energy= 0.223674

Sum of electronic and ZPE= -916.177678

Sum of electronic and thermal Energies= -916.159688

Sum of electronic and thermal Enthalpies= -916.158744

Sum of electronic and thermal Free Energies= -916.226757

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	182.444	68.200	143.144

C 0 1.9541199401 -4.9805434554 -0.6586884375

C 0 2.9979225181 -4.1185765046 -1.0112819732

C 0 2.8505679681 -2.7293821829 -0.939784069

C 0 1.6336609944 -2.223669159 -0.5069283904

C 0 0.5804984061 -3.0935659503 -0.1510024973

C 0 0.728980739 -4.4729210939 -0.2228387988

C 0 1.1755345207 -0.8339986576 -0.3259902391

C 0 -0.1750288612 -0.8670447066 0.1439926566

C 0 -0.6011167205 -2.3030328017 0.2723771323

O 0 -1.6850385268 -2.7180498918 0.6460935917

N 0 1.8267323789 0.2778243034 -0.5359762168

C 0 1.1168871179 1.4250402664 -0.2699026942

C 0 -0.2379057798 1.3837885109 0.2008401279

N 0 -0.8843630929 0.191282292 0.4067199452

C 0 1.7341298326 2.6784009797 -0.4639611215

C 0 1.0405167113 3.8407450701 -0.2025866471

C 0 -0.2929826794 3.7986228952 0.2613802915

C 0 -0.9233375359 2.5906619185 0.4602843124

H 0 2.1004833839 -6.0522751946 -0.7252093565

H 0 3.940527416 -4.5362277712 -1.3467728731

H 0 3.664106367 -2.0688441312 -1.2151260053

H 0 -0.086132504 -5.132059173 0.0532267098

H 0 2.7577051699 2.6964789373 -0.8197022236

H 0 1.5217930599 4.800312817 -0.3536462565

H 0 -0.8192483692 4.7248269052 0.4610044222

H 0 -1.9452374588 2.5308410578 0.8165322855

C 0 -6.0689026073 -0.4977403045 0.2197282415

H 0 -5.9274201538 0.5667921197 0.4299492887

H 0 -6.6244417318 -0.941256113 1.0516502159

H 0 -6.6747394705 -0.5910488492 -0.6862809577

C 0 -4.731733205 -1.19000012 0.0408571082

H 0 -4.8862324762 -2.2546672492 -0.181829035

H 0 -4.1910273501 -0.749626058 -0.8080553004

O 0 -3.9747757731 -1.037092676 1.2465799195

H 0 -3.1391259578 -1.5158277695 1.1247267842

int-1 with 1 EtOH on N1

SMD B3LYP/6-311G**

E(RB3LYP) = -916.452781246

Zero-point correction= 0.273030 (Hartree/Particle)

Thermal correction to Energy= 0.290929

Thermal correction to Enthalpy= 0.291873

Thermal correction to Gibbs Free Energy= 0.224113

Sum of electronic and ZPE= -916.179751

Sum of electronic and thermal Energies= -916.161852

Sum of electronic and thermal Enthalpies= -916.160908

Sum of electronic and thermal Free Energies= -916.228668

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 182.561 67.849 142.614

C 0 0.9400774201 -4.6145378514 -0.5975848161

C 0 2.2493327799 -4.1235696856 -0.6419406664

C 0 2.5163773893 -2.754373316 -0.543465529

C 0 1.4417758286 -1.8885365804 -0.3995644586

C 0 0.1210731667 -2.3838012316 -0.3547003625

C 0 -0.1416545969 -3.7441484648 -0.4529132403

C 0 1.398238628 -0.4205805803 -0.2727863874

C 0 0.029815702 -0.0252485334 -0.1518241132

C 0 -0.836248958 -1.2572531951 -0.2015865487

O 0 -2.0487930325 -1.2993036068 -0.1339345628

N 0 2.3879528013 0.4314857944 -0.2613678014

C 0 2.0217466318 1.7488407309 -0.1244694247

C 0 0.6481654643 2.1439682803 -0.0039345989

N 0 -0.3573789916 1.209755223 -0.0195334338

C 0 3.0206605971 2.7447609299 -0.0997411377

C 0 2.6734251055 4.071523614 0.0374559391

C 0 1.3193182157 4.4568130238 0.1541445583

C 0 0.3198108866 3.5101307519 0.1333815404

H 0 0.7664875776 -5.6813635348 -0.6767658866

H 0 3.0733645522 -4.8189280736 -0.755428527

H 0 3.5332156641 -2.3819541182 -0.5794425567

H 0 -1.159922954 -4.1143895413 -0.4174906648

H 0 4.0552604275 2.4352032155 -0.1904343104

H 0 3.4466563828 4.8310347863 0.0563135888

H 0 1.0689510407 5.5058649404 0.2605667764

H 0 -0.7262276899 3.7793199465 0.2214407546

C 0 -5.1304838321 2.6969133086 -0.8737372685

H 0 -5.0422306905 3.7736778504 -0.699445787

H 0 -5.7024462461 2.2612855298 -0.0488661572

H 0 -5.6927347123 2.5440522635 -1.799596461

C 0 -3.7599924948 2.0548535975 -0.9699633517

H 0 -3.8613198048 0.9772401138 -1.154291728

H 0 -3.2022142153 2.4836968865 -1.8137635691

O 0 -3.0605364393 2.2831133834 0.2588763469

H 0 -2.1960072936 1.8348800129 0.1974078848

int-1 with 1 EtOH on N2

SMD B3LYP/6-311G**

E(RB3LYP) = -916.452548853

Zero-point correction= 0.273118 (Hartree/Particle)

Thermal correction to Energy= 0.290939

Thermal correction to Enthalpy= 0.291883

Thermal correction to Gibbs Free Energy= 0.224751

Sum of electronic and ZPE= -916.179431

Sum of electronic and thermal Energies= -916.161610

Sum of electronic and thermal Enthalpies= -916.160665

Sum of electronic and thermal Free Energies= -916.227798

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 182.567 67.707 141.292

C 0 0.8013794706 -4.5511228632 -0.535151428

C 0 2.1080563348 -4.0610063962 -0.4380745813

C 0 2.365199424 -2.6910315958 -0.3271109378

C 0 1.2810401681 -1.8235737509 -0.31537589

C 0 -0.0373287782 -2.3178810944 -0.409569702

C 0 -0.2886731461 -3.6790462112 -0.5206582416

C 0 1.2215373478 -0.3556954759 -0.2089428892

C 0 -0.1521753092 0.0437603705 -0.2299836087

C 0 -1.0065809736 -1.1908992566 -0.3615400023

O 0 -2.2191846127 -1.2373684872 -0.4144277007

N 0 2.2006801849 0.5042234413 -0.1094657487

C 0 1.8247755768 1.8241695404 -0.0174277489

C 0 0.4440871379 2.2101731675 -0.0385132765

N 0 -0.5568991465 1.2777428893 -0.150782923

C 0 2.8159726714 2.8201063816 0.1026905776

C 0 2.4529998145 4.1467446267 0.1957904105

C 0 1.093646965 4.5285971601 0.1718349769

C 0 0.1046721395 3.5771976878 0.0570390866

H 0 0.6365769194 -5.6188937496 -0.6206263127

H 0 2.9385134145 -4.7578797115 -0.4487363483

H 0 3.3792553487 -2.3173083607 -0.2477875379

H 0 -1.3051095426 -4.0490925979 -0.592759572

H 0 3.8556755434 2.5152113435 0.1252154824

H 0 3.2189774789 4.9080147493 0.2895754097

H 0 0.8313139753 5.5775270285 0.2456068354

H 0 -0.9451483421 3.8456473218 0.0376976856

C 0 6.8846678142 -0.3976958096 -1.7646256746

H 0 7.0923766989 -1.4215034826 -1.4387071684

H 0 7.4677268513 0.2860368287 -1.1401848895

H 0 7.2235416088 -0.2917947922 -2.7992825344

C 0 5.4037241838 -0.0891249923 -1.6546331669

H 0 5.2066982965 0.9345853399 -1.9992635514

H 0 4.828037346 -0.7697828683 -2.2962032753

O 0 5.0060457731 -0.2379085328 -0.2856988501

H 0 4.0629883931 0.0099330222 -0.2128202244

int-1 with 2 EtOHs on O1 and N1

SMD B3LYP/6-311G**

E(RB3LYP) = -1071.55643196

Zero-point correction= 0.353599 (Hartree/Particle)

Thermal correction to Energy= 0.376787

Thermal correction to Enthalpy= 0.377731

Thermal correction to Gibbs Free Energy= 0.296565

Sum of electronic and ZPE= -1071.202833

Sum of electronic and thermal Energies= -1071.179645

Sum of electronic and thermal Enthalpies= -1071.178701

Sum of electronic and thermal Free Energies= -1071.259867

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 236.438 84.909 170.829

C 0 1.0236625885 -4.6659717654 -0.6883406852

C 0 2.3143979199 -4.1303889138 -0.7501789888

C 0 2.5380011296 -2.7545897474 -0.6326101195

C 0 1.438961455 -1.9283153736 -0.4508863396

C 0 0.1365442296 -2.4686724345 -0.3874835865

C 0 -0.0831873428 -3.8354409026 -0.5054504684

C 0 1.3492036534 -0.465403711 -0.2940168049

C 0 -0.0283402195 -0.1199220005 -0.1300518868

C 0 -0.8504875248 -1.3795731726 -0.1853924806

O 0 -2.0605660772 -1.469124587 -0.0884143861

N 0 2.3085701662 0.4201408319 -0.2960943394

C 0 1.9018512063 1.7214327852 -0.1259145902

C 0 0.519459856 2.0667716358 0.0407613832

N 0 -0.4538119011 1.0991951673 0.0331799294

C 0 2.8666248437 2.7503187774 -0.1140120925

C 0 2.478961179 4.0619211434 0.0565140534

C 0 1.1169161245 4.3982061138 0.221311321

C 0 0.1497418557 3.4182829104 0.2135544922

H 0 0.8842889287 -5.7364889676 -0.7831114014

H 0 3.1585883284 -4.7956849214 -0.8919736525

H 0 3.5408530362 -2.347524143 -0.6813339027

H 0 -1.0870581983 -4.2411438341 -0.4559885972

H 0 3.9078383452 2.4780620845 -0.2410283219

H 0 3.2260470519 4.8472805287 0.0647840392

H 0 0.834414942 5.4358932808 0.3549056665

H 0 -0.9010460694 3.6513202803 0.340000433

C 0 -6.7468641951 -2.3385460252 0.5301839848

H 0 -7.3182360988 -1.5662602331 0.0064856887

H 0 -6.9419329644 -2.2434871318 1.6025933988

H 0 -7.1102258982 -3.3162708411 0.2007240425

C 0 -5.2647914725 -2.1998523556 0.2425062153

H 0 -4.7057393642 -2.9915976991 0.7580451084

H 0 -5.076814098 -2.3061058631 -0.8337538574

O 0 -4.832217538 -0.9112296968 0.6996045515

H 0 -3.8816774618 -0.8449778393 0.5338882715

C 0 -5.2155323538 2.5289352871 -0.906342789

H 0 -5.2039872171 3.5553611509 -0.5268957372

H 0 -5.8181882591 1.9167691444 -0.2296514213

H 0 -5.6960391758 2.5317118212 -1.8892127574

C 0 -3.8060978428 1.9778663143 -1.0031435057

H 0 -3.8315829496 0.9469797328 -1.3782528891

H 0 -3.2135774801 2.575709692 -1.7089512566

O 0 -3.2116291152 2.0141575842 0.3001583045

H 0 -2.311763612 1.6430240432 0.2297202341

int-1 with 2 EtOHs on O1 and N2

SMD B3LYP/6-311G**

E(RB3LYP) = -1071.55661423

Zero-point correction= 0.353884 (Hartree/Particle)

Thermal correction to Energy= 0.377838

Thermal correction to Enthalpy= 0.378782

Thermal correction to Gibbs Free Energy= 0.294572

Sum of electronic and ZPE= -1071.202731

Sum of electronic and thermal Energies= -1071.178777

Sum of electronic and thermal Enthalpies= -1071.177832

Sum of electronic and thermal Free Energies= -1071.262042

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 237.097 86.481 177.235

C 0 1.8158291853 -5.1735667393 0.0510042687

C 0 2.9483417626 -4.3784134748 -0.1533176361

C 0 2.871072323 -2.9818481613 -0.1365129925

C 0 1.6310882035 -2.4012537132 0.089760152

C 0 0.4882136568 -3.2036061763 0.2985181327

C 0 0.5686191533 -4.5901731986 0.2808275203

C 0 1.2275632793 -0.986504735 0.1690366366

C 0 -0.1767417342 -0.9334301219 0.4352832874

C 0 -0.6973041287 -2.3415980779 0.5223291416

O 0 -1.8467516089 -2.6875252462 0.7334918638

N 0 1.9556400334 0.0898803715 0.0339800424

C 0 1.2848007412 1.2826280056 0.1764075709

C 0 -0.1235193056 1.3199007094 0.4451005439

N 0 -0.8562049145 0.1670679561 0.5706355597

C 0 1.9940152435 2.4955216488 0.0587162529

C 0 1.3328166991 3.69703817 0.2011463864

C 0 -0.054302493 3.734578644 0.4640176024

C 0 -0.7724647235 2.565841016 0.5842996301

H 0 1.9103092909 -6.2529675057 0.0318227802

H 0 3.9065567263 -4.8545060849 -0.3275566645

H 0 3.7523225647 -2.370657952 -0.2915166685

H 0 -0.3145078727 -5.1974890424 0.4425661992

H 0 3.0590003345 2.4556811889 -0.1380115059

H 0 1.8833146346 4.6264596379 0.1111509493

H 0 -0.5524167625 4.6909413083 0.571905662

H 0 -1.8370934112 2.5663115228 0.7871587127

C 0 -6.003420769 -0.3148059349 -0.4496445946

H 0 -5.837313071 0.7540708601 -0.2843648671

H 0 -6.6964049087 -0.6771641553 0.3157491475

H 0 -6.4757071237 -0.4413215646 -1.428192588

C 0 -4.6933341916 -1.0757023953 -0.3876039818

H 0 -4.8704563592 -2.144926229 -0.5673112073

H 0 -4.012640505 -0.7168614335 -1.1717214963

O 0 -4.1117249911 -0.8767510454 0.9058904707

H 0 -3.2939989517 -1.3985374257 0.9376096243

C 0 6.274823503 0.1464716719 -2.5942369331

H 0 6.7646455363 -0.7846121928 -2.2931116417

H 0 6.8121048239 0.9811652855 -2.1338562161

H 0 6.3578325834 0.2421061466 -3.6807546275

C 0 4.8190472657 0.149253879 -2.1687586146

H 0 4.334873093 1.0801851748 -2.4923240509

H 0 4.2850448891 -0.6834809367 -2.6457950692

O 0 4.7599752052 0.0281172649 -0.7419256674

H 0 3.8209766041 0.0522903207 -0.4712018348

TS-2-1 with 1 EtOH on N1

SMD B3LYP/6-311G**

E(RB3LYP) = -1240.24192809

Zero-point correction= 0.378522 (Hartree/Particle)

Thermal correction to Energy= 0.403421

Thermal correction to Enthalpy= 0.404365

Thermal correction to Gibbs Free Energy= 0.320026

Sum of electronic and ZPE= -1239.863406

Sum of electronic and thermal Energies= -1239.838507

Sum of electronic and thermal Enthalpies= -1239.837563

Sum of electronic and thermal Free Energies= -1239.921902

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	253.150	93.866	177.506

C	0	-2.4193537424	3.019026732	0.8760279299
C	0	-1.342879068	3.7060437915	0.3038295367
C	0	-0.1618993058	3.0390327263	-0.0157382869
C	0	-0.0926834516	1.6672853416	0.2260629762
C	0	-1.1880828298	0.9669074453	0.7578466942
C	0	-2.3461005632	1.6448689833	1.1158907784
C	0	1.0378825806	0.7435346919	0.1237902312
C	0	0.6262939371	-0.5414709369	0.6124910511
C	0	-0.8664494663	-0.5132566491	0.9612295101
O	0	-1.2807841304	-1.0792767512	2.1398315389
N	0	2.2660178452	0.9971769279	-0.252870452
C	0	3.1556376085	-0.0424478415	-0.1404933042
C	0	2.7496538504	-1.3048913242	0.3932135664
N	0	1.4479641799	-1.5358883338	0.7713596269
C	0	4.49836149	0.1413268456	-0.5387869509
C	0	5.4040495926	-0.8879378073	-0.4045943683
C	0	5.0065120179	-2.1320831461	0.1330744077
C	0	3.7024217331	-2.3379048656	0.5265669355
H	0	-3.319247842	3.5620746942	1.1425269521
H	0	-1.4223558401	4.7726282383	0.1263895985
H	0	0.6881432646	3.5707047712	-0.4275193815
H	0	-3.1769084669	1.1188625793	1.5729209427
H	0	4.7890466185	1.1019861375	-0.9481203706
H	0	6.4335546274	-0.743430322	-0.7119999057
H	0	5.7347991162	-2.9286647737	0.2332660896
H	0	3.3761669735	-3.286221606	0.9380193687
C	0	-1.0822863543	-2.7004080472	-0.4242703811
N	0	-1.7579369101	-1.471775316	0.0512187666
C	0	-2.6596632758	-0.9315642842	-0.9740483281
C	0	-3.9895702011	-1.6588295923	-0.9703381345
O	0	-4.7199854548	-1.2959161159	-2.0320221925
O	0	-4.3669177167	-2.4351473929	-0.1244051992
H	0	-0.5050733358	-3.1297598815	0.3904348801
H	0	-1.8508246618	-3.4119022825	-0.7283658825
H	0	-0.4284125266	-2.4890045947	-1.2732696405
H	0	-2.0713883268	-1.637213165	1.2597898759
H	0	-2.8772854282	0.1190095768	-0.7832770854
H	0	-2.2131598143	-0.9957099936	-1.9703252346
H	0	-5.5835586476	-1.7409356941	-1.9864996957

C 0 4.3911157792 5.5715859286 -0.2000289658

H 0 3.6210369218 6.2230531498 -0.6244601264

H 0 5.1853201346 5.4503018571 -0.9429861589

H 0 4.8148172516 6.0680520541 0.6778183269

C 0 3.8052779877 4.2251157449 0.1802798018

H 0 4.583248868 3.58786661 0.6213202241

H 0 3.019210169 4.3560081991 0.9360612326

O 0 3.2676786943 3.6108363499 -0.9974057013

H 0 2.9169323485 2.7302913913 -0.7519464561

TS-2-1 with 1 EtOH on O1

SMD B3LYP/6-311G**

E(RB3LYP) = -1240.24384607

Zero-point correction= 0.378399 (Hartree/Particle)

Thermal correction to Energy= 0.403261

Thermal correction to Enthalpy= 0.404205

Thermal correction to Gibbs Free Energy= 0.319519

Sum of electronic and ZPE= -1239.865447

Sum of electronic and thermal Energies= -1239.840585

Sum of electronic and thermal Enthalpies= -1239.839641

Sum of electronic and thermal Free Energies= -1239.924327

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 253.050 93.772 178.238

C 0 2.994985397 -2.502349841 2.3112740904

C 0 2.1684145773 -3.6121578859 2.1038733119

C 0 0.9654688954 -3.4831013926 1.4124444744

C 0 0.6208061969 -2.228053062 0.9144836088

C 0 1.4651248196 -1.1205153908 1.0908841674

C 0 2.6444081919 -1.2446918011 1.8145905013

C 0 -0.6099756185 -1.7743281716 0.2646902747

C 0 -0.5229318024 -0.3565784197 0.0589711592

C 0 0.8552203869 0.1479023215 0.4980365446

O 0 0.9369758704 1.2707172812 1.3103727437

N 0 -1.6707954473 -2.4780811854 -0.0353424958

C 0 -2.7207179878 -1.7659085905 -0.55610946

C 0 -2.6474124543 -0.347821918 -0.7277658076

N 0 -1.508549788 0.3521873421 -0.4051223855

C 0 -3.9083607092 -2.4420188184 -0.9153196398

C 0 -4.9796880766 -1.7396028506 -1.4210005731

C 0 -4.9078991122 -0.3382341277 -1.5854996504

C 0 -3.7627668855 0.3473014441 -1.2442185304

H 0 3.9157510595 -2.618646873 2.8718274938

H 0 2.4596653313 -4.5778029636 2.5015701837

H 0 0.303704606 -4.3311529549 1.2793653242

H 0 3.2814116526 -0.3853659646 1.9917302255

H 0 -3.9472438355 -3.5165683365 -0.7776175712

H 0 -5.8886555472 -2.263393706 -1.6946502503

H 0 -5.761617015 0.1977636265 -1.984244156

H 0 -3.6873530901 1.4217413364 -1.366743092

C 0 0.9599714988 1.5269031648 -1.6812065159

N 0 1.7242260284 0.7818712559 -0.6522789839

C 0 2.8495674556 0.0512967064 -1.2495094516

C 0 4.0615866527 0.9482775153 -1.4054186961

O 0 5.0107460226 0.3252549103 -2.1144829043

O 0 4.1826922773 2.0574763305 -0.94111488

H 0 0.1944100943 2.127234082 -1.196684344

H 0 1.6564698138 2.1882841561 -2.1978990209

H 0 0.501423125 0.8473741568 -2.4022282189

H 0 1.7921544862 1.5336365006 0.3737327404

H 0 3.1524502025 -0.7812480081 -0.6152822784

H 0 2.5796474411 -0.3640852328 -2.2242134191

H 0 5.7920921893 0.9018829849 -2.1684750192

C 0 -2.7322485397 4.5263275682 1.9393264242

H 0 -3.0607084003 4.7309630846 0.9155776221

H 0 -2.1469207909 5.382505825 2.288544956

H 0 -3.6196881305 4.4357619926 2.5727379498

C 0 -1.9044143289 3.2558498716 1.9908992563

H 0 -1.5901721306 3.05630223 3.0252651461

H 0 -2.5115011291 2.4012608079 1.6628343771

O 0 -0.7636147069 3.4164808421 1.1465260732

H 0 -0.2076117456 2.6107541575 1.2220606955

TS-2-1 with 2 EtOHs on O3 and N1

SMD B3LYP/6-311G**

E(RB3LYP) = -1395.35303046

Zero-point correction= 0.459815 (Hartree/Particle)

Thermal correction to Energy= 0.490348

Thermal correction to Enthalpy= 0.491293

Thermal correction to Gibbs Free Energy= 0.392376

Sum of electronic and ZPE= -1394.893216

Sum of electronic and thermal Energies= -1394.862682

Sum of electronic and thermal Enthalpies= -1394.861738

Sum of electronic and thermal Free Energies= -1394.960654

	E	CV	S
	KCal/Mol	Cal/Mol-K	Cal/Mol-K
Total	307.698	111.732	208.187

C 0 -1.9707938151 3.3439511496 0.443250396

C 0 -0.7228166719 3.6104350543 -0.1310666658

C 0 0.191757882 2.583127824 -0.3542743488

C 0 -0.1808987053 1.2825580295 -0.0149762905

C 0 -1.4505260325 1.0060692575 0.519165894

C 0 -2.3399577634 2.0400295229 0.7817211684

C 0 0.6016109275 0.0457458951 -0.004856856

C 0 -0.2030904778 -1.0012830939 0.5573289953

C 0 -1.6158934865 -0.4785350483 0.8426803149

O 0 -2.1981753656 -0.7859245817 2.0472467883

N 0 1.8530033928 -0.1304089571 -0.3478660387

C 0 2.3659027265 -1.3844126232 -0.1260701354

C 0 1.5733545578 -2.4078175998 0.4805537503

N 0 0.2598751588 -2.1866279646 0.8218138773

C 0 3.7034433611 -1.6650968399 -0.4832910765

C 0 4.2345125341 -2.912745963 -0.2403202751

C 0 3.4557376259 -3.921048739 0.3694383768

C 0 2.1480456149 -3.6737024236 0.7253456796

H 0 -2.6568448087 4.1615609391 0.6344533974

H 0 -0.4576759097 4.6303938555 -0.3855884554

H 0 1.1738494461 2.78700951 -0.7654062721

H 0 -3.3014632229 1.840113166 1.2414084158

H 0 4.2892181013 -0.8808792131 -0.9488409044

H 0 5.2610516085 -3.1246288327 -0.5170649202

H 0 3.8926276617 -4.8955363786 0.5551259499

H 0 1.5325608081 -4.4349356254 1.1908972951

C 0 -2.4786197756 -2.5912532861 -0.3975505909

N 0 -2.7508899788 -1.1858666538 -0.0209698855

C 0 -3.4517572299 -0.4729171952 -1.0973924497

C 0 -4.9424957298 -0.7660558542 -1.0747972831

O 0 -5.5397789832 -0.2631061332 -2.1460638715

O 0 -5.5139531125 -1.3578374101 -0.1808375972

H 0 -2.0619724297 -3.1180398887 0.4570454632

H 0 -3.4261756429 -3.0548574785 -0.6733306188

H 0 -1.788426878 -2.6484514888 -1.2424268467

H 0 -3.1073608637 -1.1556105654 1.1885700919

H 0 -3.3417253076 0.6045872332 -0.9816280377

H 0 -3.0465649917 -0.7377457093 -2.0780000464

H 0 -6.5304233675 -0.4440860634 -2.1139394316

C 0 5.3166344476 3.5272403072 -0.4394034094

H 0 4.8024253702 4.3639631594 -0.9221308758

H 0 6.0482974449 3.1213958716 -1.1446746819

H 0 5.8556275156 3.912091586 0.4312363546

C 0 4.326166383 2.4567578585 -0.0224867327

H 0 4.8522172045 1.6327379475 0.4776554294

H 0 3.6043363242 2.870023067 0.6947420265

O 0 3.6498548479 1.9781259225 -1.1914404639

H 0 3.0309907997 1.2702130126 -0.9188795949

C 0 -8.7934781755 1.4546989373 -1.333994341

H 0 -9.2691962015 1.6868082085 -2.2909492398

H 0 -7.7613748409 1.8153239666 -1.3615601064

H 0 -9.3234626804 1.9964455925 -0.5457157487

C 0 -8.8412562415 -0.0326768486 -1.0575968307

H 0 -8.3673569572 -0.2703510876 -0.0995663046

H 0 -9.8746288155 -0.3909168566 -1.0314201007

O 0 -8.1399996116 -0.7181060716 -2.1254649116

H 0 -8.2486999606 -1.6700723991 -1.9990938145

TS-2-1 with 3 EtOHs on O1, O2 and N1

SMD B3LYP/6-311G**

E(RB3LYP) = -1550.46177419

Zero-point correction= 0.541036 (Hartree/Particle)

Thermal correction to Energy= 0.577459

Thermal correction to Enthalpy= 0.578403

Thermal correction to Gibbs Free Energy= 0.462921

Sum of electronic and ZPE= -1549.920738

Sum of electronic and thermal Energies= -1549.884315

Sum of electronic and thermal Enthalpies= -1549.883371

Sum of electronic and thermal Free Energies= -1549.998853

E CV S

KCal/Mol Cal/Mol-K Cal/Mol-K

Total 362.361 129.745 243.053

C 0 -2.2424579509 3.2975854318 0.3895249142

C 0 -0.9666434479 3.5764785324 -0.1124564016

C 0 -0.0194945625 2.5639686897 -0.2523066112

C 0 -0.3859163181 1.2648067774 0.0972861457

C 0 -1.6802312037 0.9753378389 0.5607708584

C 0 -2.6064014975 1.9948224884 0.7382189892

C 0 0.4175573912 0.0445351376 0.1835148229

C 0 -0.4004445982 -1.0052522908 0.7184655069

C 0 -1.8351703533 -0.50373301 0.9021974005

O 0 -2.4771666529 -0.782045122 2.1017530823

N 0 1.6903175674 -0.1162784004 -0.0781321268

C 0 2.209983677 -1.3552467373 0.2040560751

C 0 1.3986937723 -2.380359902 0.7833556524

N 0 0.0632939628 -2.1762769173 1.0355750616

C 0 3.5722240284 -1.6183274708 -0.0611133147

C 0 4.1086198667 -2.8492288197 0.2465246647

C 0 3.3109204539 -3.8579608984 0.8308989756

C 0 1.9787491315 -3.6286758506 1.0957479809

H 0 -2.9560950708 4.1041319704 0.514957574

H 0 -0.7066567131 4.5951295232 -0.3771918687

H 0 0.9814508353 2.7782681705 -0.6085697437

H 0 -3.5921765583 1.7857193441 1.1381561945

H 0 4.1732284627 -0.8344709635 -0.5074092555

H 0 5.1545253824 -3.0474840089 0.0417274527

H 0 3.7534676988 -4.818249843 1.0694956122

H 0 1.3485383134 -4.3892145246 1.5420292858

C 0 -2.6102373548 -2.6663553205 -0.2845281203

N 0 -2.9113177667 -1.2505732953 0.0301417324

C 0 -3.5706771271 -0.5853327807 -1.1024938962

C 0 -5.0701042524 -0.8310573052 -1.0869820326

O 0 -5.6322374084 -0.3909567139 -2.2037140754

O 0 -5.6744329765 -1.3368015951 -0.1626929239

H 0 -2.2317735798 -3.1641377945 0.6043751174

H 0 -3.5420271052 -3.1439516944 -0.5890137785

H 0 -1.8813300826 -2.7454087411 -1.0941971486

H 0 -3.3308578168 -1.1935430494 1.2358411545

H 0 -3.4270324396 0.4933034311 -1.0574344369

H 0 -3.1581540878 -0.9276376373 -2.0553996417

H 0 -6.63054201 -0.5219721829 -2.1700228366

C 0 5.0977406091 3.5983809311 -0.0698127511

H 0 4.5919740027 4.4202148417 -0.5859158032

H 0 5.8653039898 3.1949572893 -0.7373136277

H 0 5.5926087379 4.0034331238 0.8176867594

C 0 4.1069297269 2.5176702693 0.3189862229

H 0 4.6236839646 1.7083246951 0.8516351501

H 0 3.3489688255 2.9284044359 0.9994786936

O 0 3.4883578453 2.0140818969 -0.871303047

H 0 2.8721921017 1.2974580337 -0.616659912

C 0 -8.7273409916 1.6435501635 -1.7533852038

H 0 -9.1861693063 1.7481588418 -2.740540376

H 0 -7.6695112458 1.9099353459 -1.8308093812

H 0 -9.2088436555 2.3515917433 -1.0732520445

C 0 -8.8946448003 0.2330544445 -1.2306519015

H 0 -8.4373638843 0.122543142 -0.2417913565

H 0 -9.9536306084 -0.0305768467 -1.1536641957

O 0 -8.2569343312 -0.6779562563 -2.1609733692

H 0 -8.4408052916 -1.582224922 -1.8738701295

C 0 0.0128651429 -0.5928378307 6.2228626051

H 0 0.9854811872 -1.0289334248 5.9746881458

H 0 -0.5213368206 -1.294655206 6.8707838725

H 0 0.1838830367 0.3305690296 6.7841174121

C 0 -0.7853468586 -0.316138924 4.9626287927

H 0 -1.7541130968 0.1328998623 5.2245252878

H 0 -0.249832234 0.4097755351 4.3339579517

O 0 -0.9760962139 -1.5441592042 4.2588131155

H 0 -1.5232971103 -1.3436854363 3.4692577986