Mechanistic Insights into the Dearomative Diborylation of Pyrazines: A Radical or non-Radical Process?

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1. Computational Investigations

1.1 DFT calculations on the intramolecular migration pathway of the pyrazine dearomatization reaction

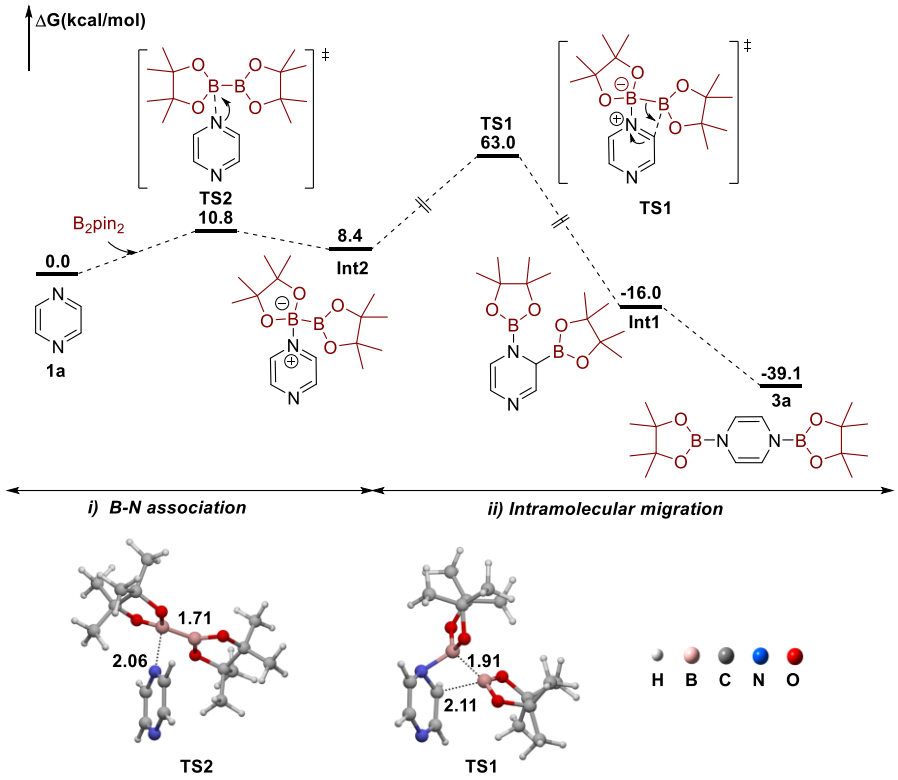


Figure S1. Gibbs free energy profile and 3D structures of the formation of *N, N'*-diboryl-1,4-dihydropyrazine *via* 1,3-boryl migration. Selected distances were shown in Å.

In the previous work, the authors proposed a possible mechanism for the directly diborylation of pyrazine. First, one nitrogen atom of pyrazine coordinates with one boron atom of B_2pin_2 to form a four-coordinated boron intermediate, making the Bpin group and the C_2 carbon of pyrazine nucleophilic and electrophilic, respectively. Then, the intramolecular nucleophilic attack of Bpin on the C_2 carbon takes place to give the 1,2-adduct. Finally, the dearomatization product are formed *via* rearrangement of α-boryl intermediates.

We have carried out density theory (DFT) calculations to investigate whether the proposed mechanism is kinetically or thermodynamically feasible. The results are presented in Figure S1. A pyrazine molecule approaches the B atom of B_2pin_2, leading to the formation of a stable intermediate **Int2**, which is endothermic by 8.4 kcal/mol

with a barrier of 10.8 kcal/mol. Then, intramolecular nucleophilic attack of Bpin on the C_2 position of pyrazine takes place to give the 1,2-adduct **Int1** (*via* **TS1**), being exothermic by 16.0 kcal/mol with a barrier of 63.0 kcal/mol. Thus, the formation of intermediate **Int1** from **Int2** is kinetically very difficult. The very high energy barrier for intramolecular nucleophilic attack is not consistent with the mild experimental conditions. Thus, this reaction pathway is unlikely to occur for the studied reaction.

1.2 DFT calculations on the potential pathway of the pyrazine dearomatization reaction

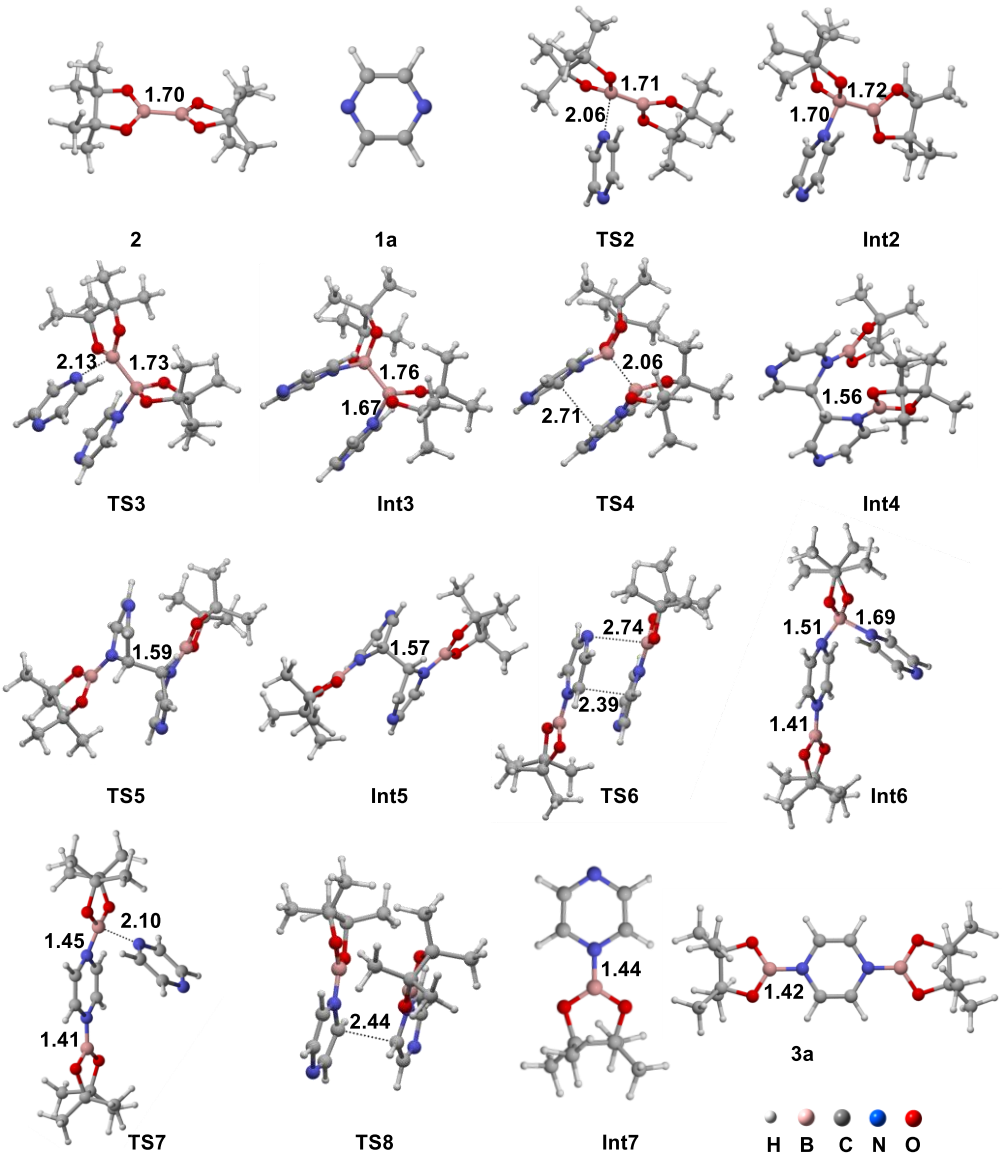


Figure S2. 3D structures of the species involved in the dearomative diborylation of pyrazine (**1a**). Selected distances were shown in Å.

1.3 DFT calculations on the dearomative diborylation of 2,3-dimethylpyrazine catalyzed by 2,6-dichloro-4,4′-bipyridine

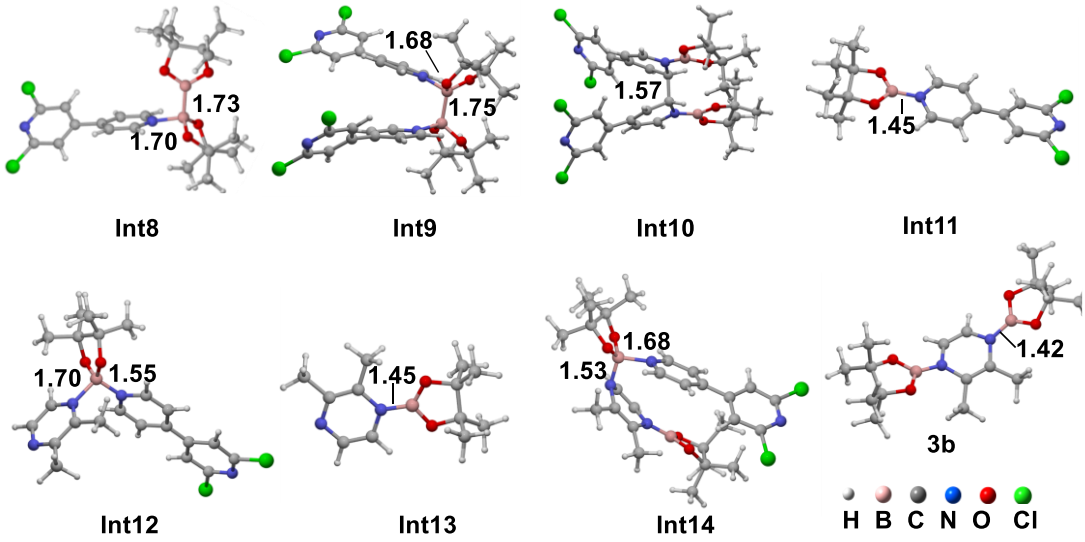


Figure S3. 3D structures of the intermediates involved in the dearomative diborylation of 2,3-dimethylpyrazine catalyzed by 2,6-dichloro-4,4′-bipyridine. Selected distances were shown in Å.

1.4 DFT calculations on dearomatization reaction of 2,3-dimethylpyrazine, in which only B_2pin_2 is used as a reducing agent.

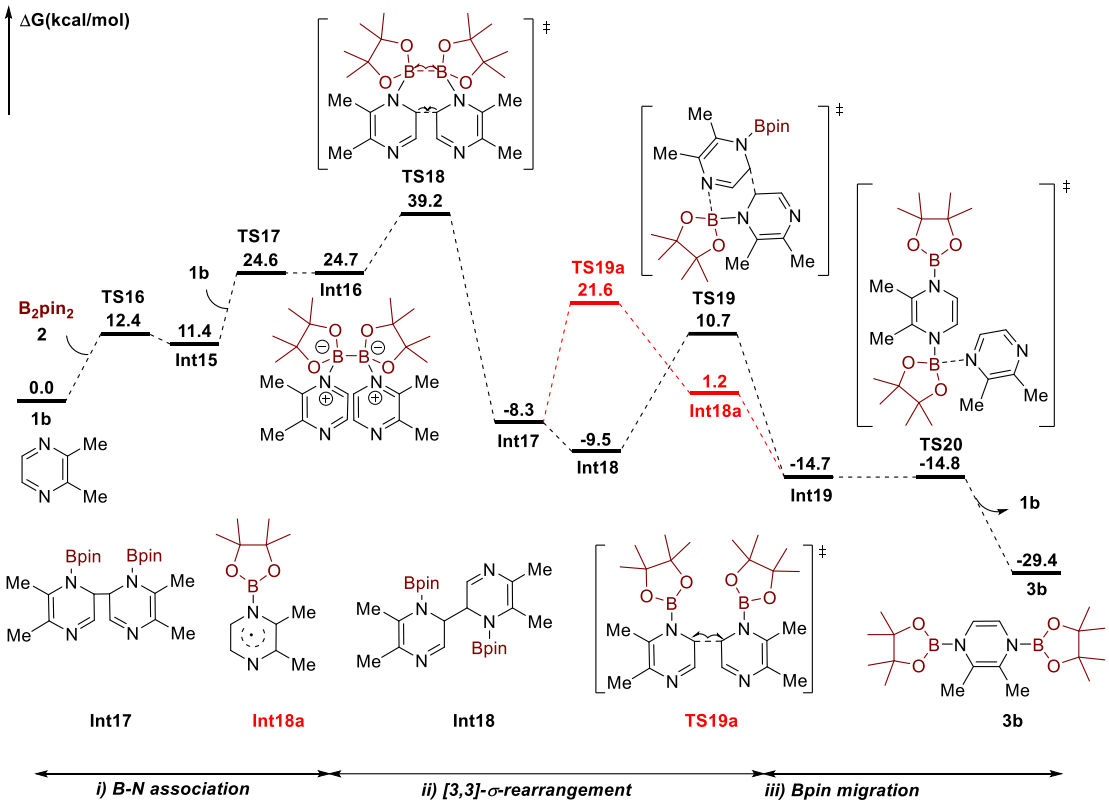


Figure S4. Gibbs free energy profile of 2,3-dimethylpyrazine dearomatization without catalyst.

As shown in Figure S4, in the absence of 2,6-dichloro-4,4'-bipyridine as the catalyst, the rate-determining step of the dearomatization process in this reaction is the [3,3]-σ-rearrangement of **Int16**, which involved a barrier of 39.2 kcal/mol (**TS18**, relative to the starting reactants **1b**-2,3-dimethylpyrazine and **2**-B_2pin_2). Thus, this mechanism can be ruled out because of the involvement of a high-energy transition state **TS18** in this pathway.

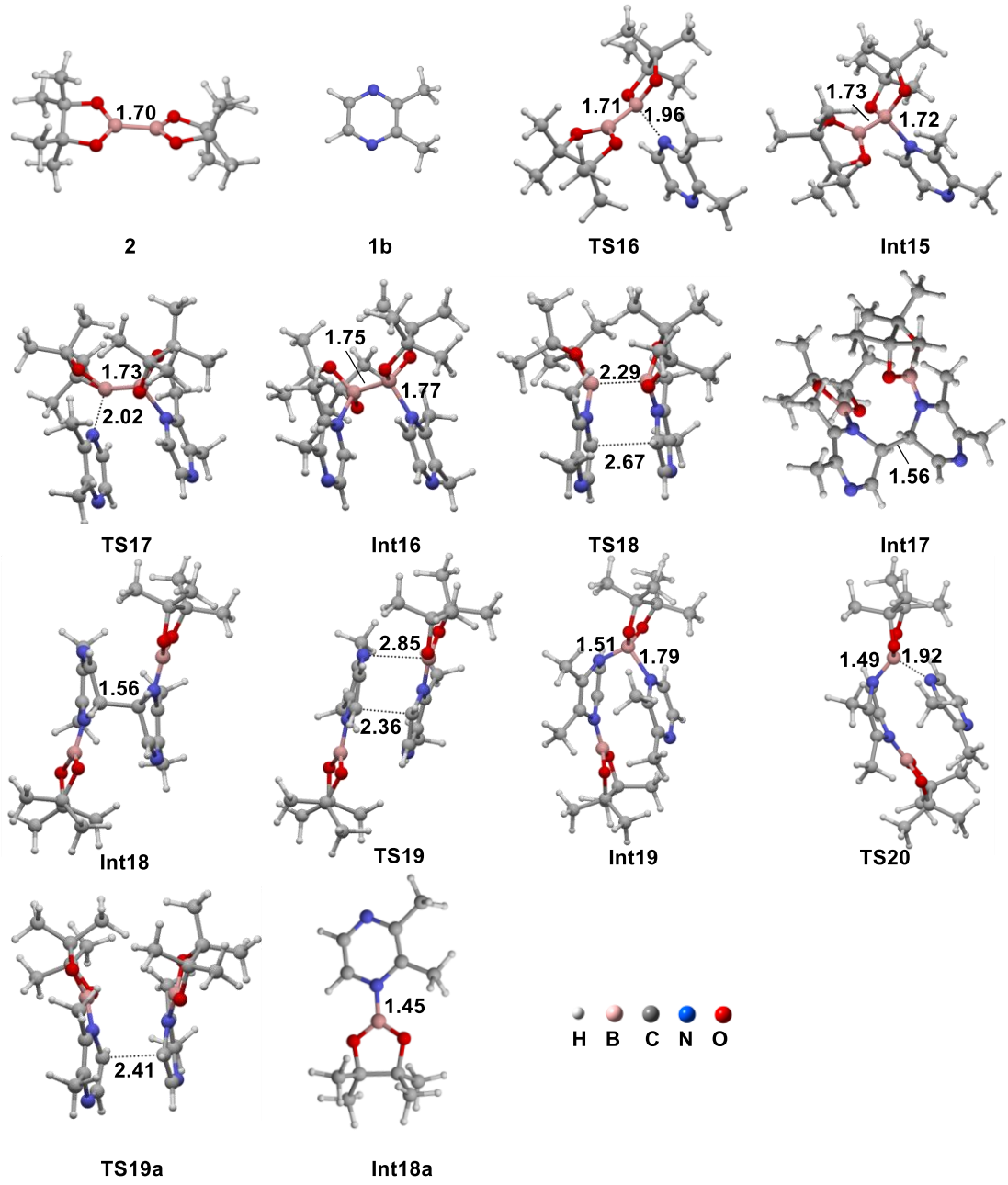


Figure S5. 3D structures of the species involved in the dearomatization reaction of 2,3-dimethylpyrazine without catalyst. Selected distances were shown in Å.

1.5 DFT calculations on the 2,6-dichloro-4,4'-bipyridine-boryl radical react with benzoyl peroxide (BPO)

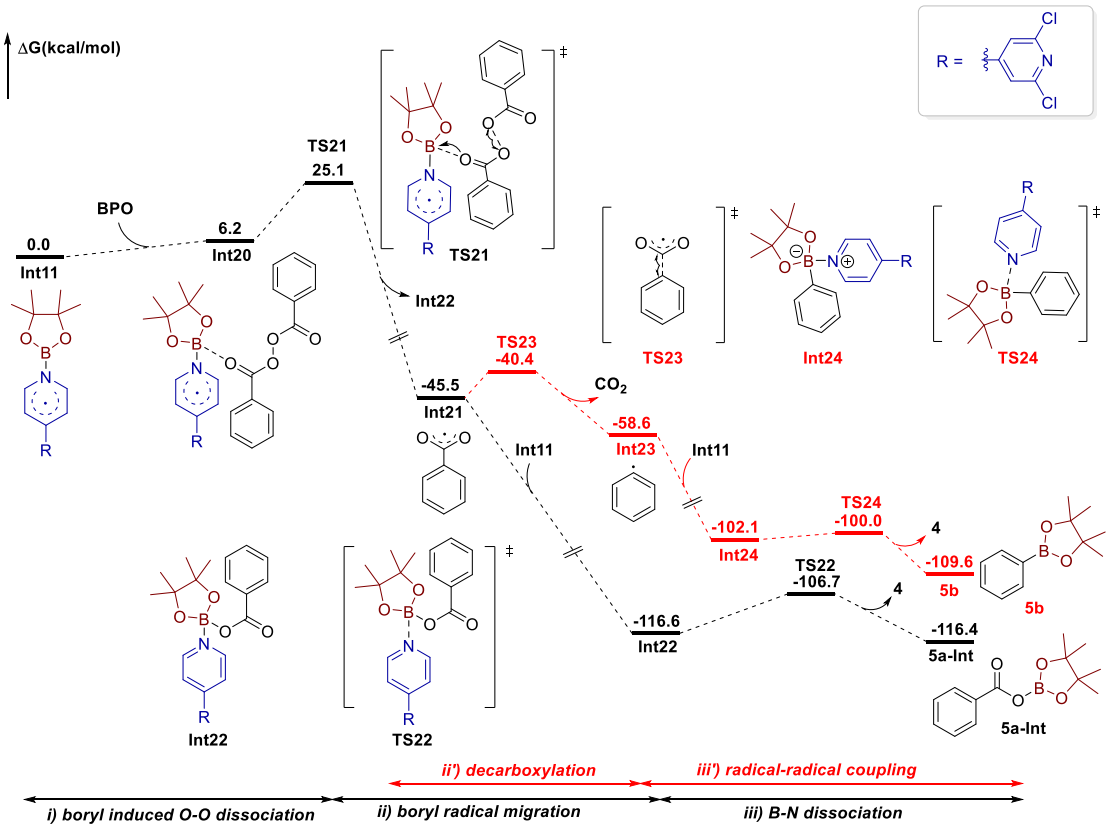


Figure S6. Gibbs free energy profile for the free radical trapping experiment with **BPO** in the solvent (benzene).

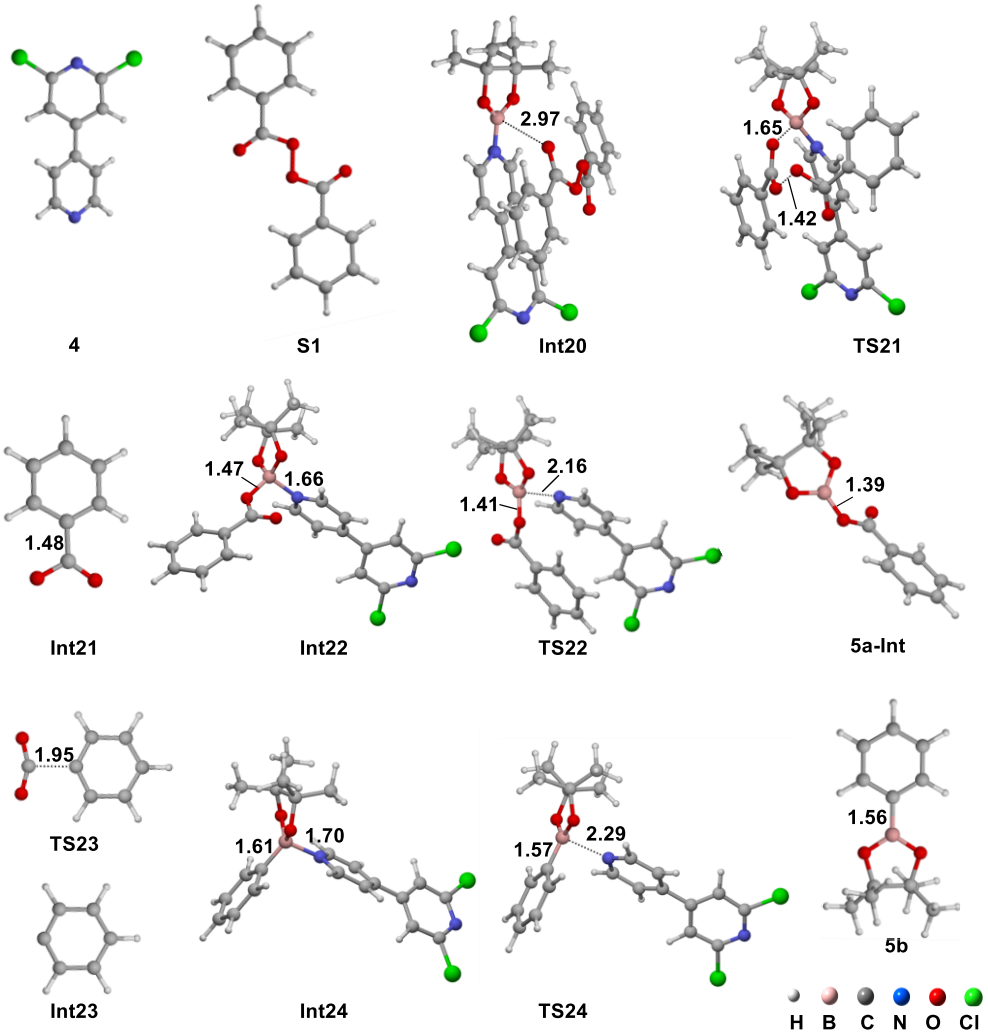


Figure S7. 3D structures of the species involved in the reaction of **S1** and **Int11**. Selected distances were shown in Å.

Free radical trapping experiments with benzoyl peroxide (**BPO**) gave a supportive evidence for the generation of the 2,6-dichloro-4,4'-bipyridine-boron radical intermediate. We also investigated the possible mechanism for this process. The calculated free energy profile is displayed in Figure S6. The boryl induced O-O dissociation of **BPO** involves a barrier of 25.1 kcal/mol. The exclusion of CO_2 from the **Int21** will generate the final product phenylboronate. The whole process is exothermic by 116.4 kcal/mol. The results indicate that the reaction of **BPO** with B_2pin_2 catalyzed by 2,6-dichloro-4,4'-bipyridine is thermodynamically and kinetically favorable.

1.6 DFT calculations on the [3,3]-σ-rearrangement of quinoxaline and 2,3-dichloropyrazine

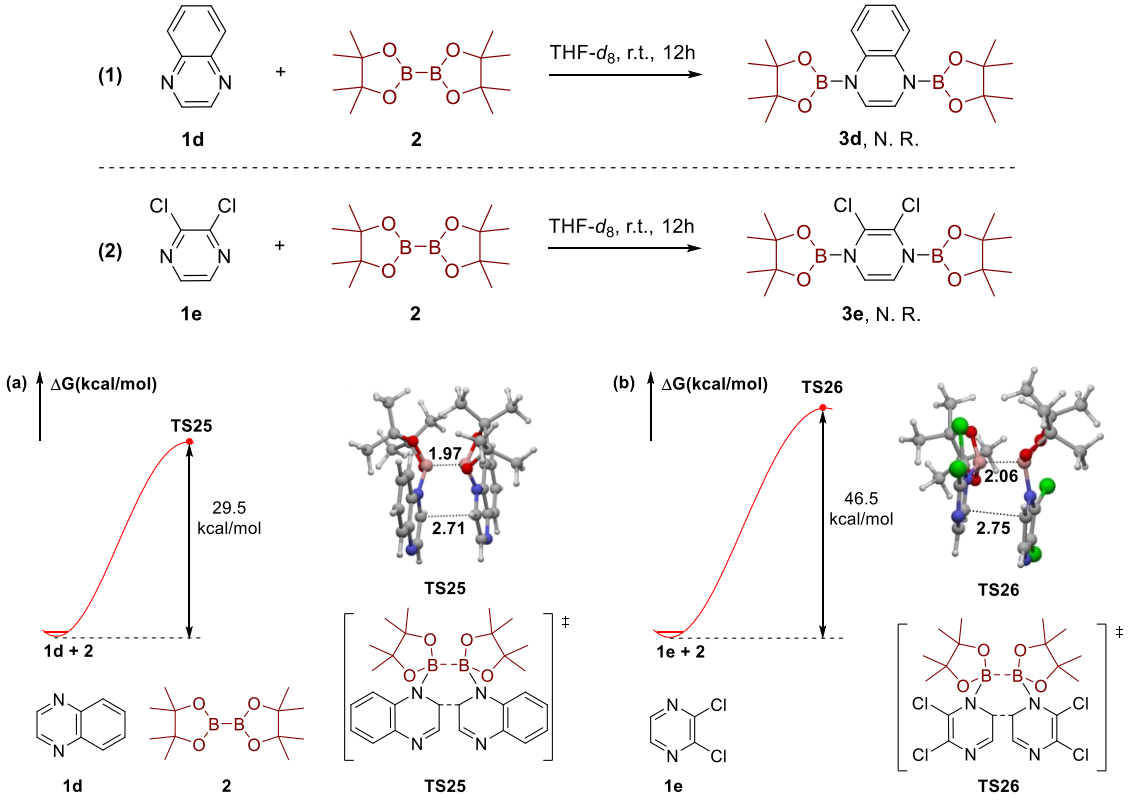


Figure S8. Gibbs free energy profile for the [3,3]-σ-rearrangement of quinoxaline and 2,3-dichloropyrazine

In addition to 2,3-dimethylpyrazine, we also calculated the dearomatization reactions of other large hindered pyrazine substrates. As shown in Figure S8, the [3,3]-σ-rearrangement of quinoxaline(**1ba**) and 2,3-dichloropyrazine(**1bb**) is difficult to occur at the present condition, due to its higher free energy barrier (29.5 kcal/mol and 46.5 kcal/mol).

2. Experimental Studies

2.1 General Information

All air- and moisture-sensitive manipulations were carried out with standard Schlenk techniques under argon or argon-filled glove-box. Anhydrous methyl tert-butyl ether (MTBE), toluene-d_8, benzene-d_6, tetrahydrofuran-d_8 (THF-d_8) were purchased from J&K used as received. 4-Cyanopyridine and $B_2(pin)_2$ was purchased from TCI. Other commercially available reagents were purchased from Acros, J&K and Alfa Aesar Chemical Company. All other commercially available reagents were used without further purification. GC-MS analysis were performed on Shimadzu GC-MS-QP2010 Plus system. NMR spectra were recorded on a Bruker AVANCE III-400 spectrometer.

The 2,6-dichloro-4,4′-bipyridine[1] catalyst and *N*-hydroxyphthalimide (NHPI) ester **S2**[2] were prepared according to the reported procedure. All synthesized substrates matched known ^1H and ^{13}C NMR spectra.

2.2 Experimental Studies on the Reaction Mechanism

a) Electron Paramagnetic Resonance (EPR) Experiments

EPR spectra were obtained using a Bruker EMX-10/12 EPR specteometer at 298.15 K. Experiments were run in anhydrous THF in sealed microcapillaries. The EPR spectrum of the 2,6-dichloro-4,4′-bipyridine-boryl radical intermediate **Int11** was obtained (as shown in Figure S9) through the addition of 2,6-dichloro-4,4′-bipyridine (1.0 equiv.) to a 0.1 M solution of $B_2(pin)_2$ in THF (1.0 ml) (blue line (2)). (For the Microwave frequency = 9.855419 GHz, g = 2.003559), This result provides the evidence for the formation of 2,6-dichloro-4,4′-bipyridine-boryl radical, which is consistent with our DFT calculations.

a) *EPR experiments*

Entry	Sample (in THF)	EPR
(1)	pyrazine + B_2pin_2	inactive
(2)	2,6-dichloro-4,4'-bipyridine + B_2pin_2	active

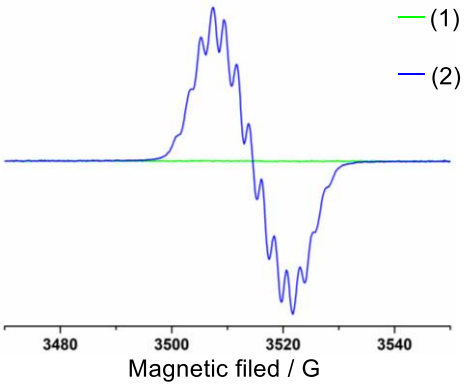
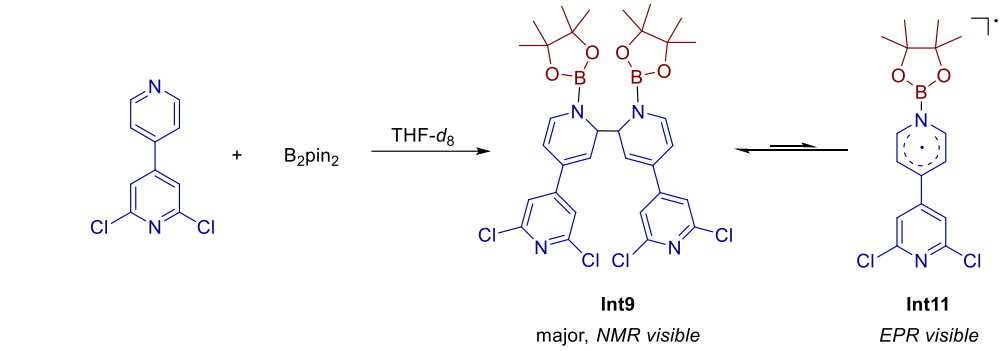
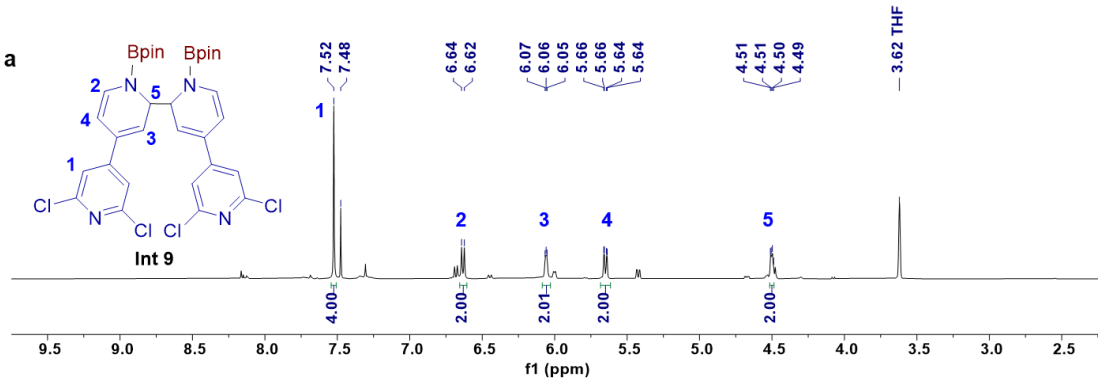


Figure S9. Left: experimental conditions. Right: experimental EPR spectra for 2,6-dichloro-4,4′-bipyridine-B_2pin_2 (blue line) and pyrazine-B_2pin_2 (green line).

b) Detection of the key [3,3]-σ-rearrangement intermediate Int9 by ^{1}H NMR spectroscopy

Experimental procedure: 2,6-dichloro-4,4′-bipyridine (22.4 mg, 0.10 mmol) and B_2pin_2 (12.7 mg, 0.05 mmol) were mixed in 0.5 mL THF-d_8 in a Schlenk tube. The mixture was stirred at room temperature for 2 h. Then the NMR analysis of the crude reaction mixture was carried out immediately. As shown below, the intermediacy of the key [3,3]-σ-intermediate **Int9** could be determined by NMR analysis. Although accompanied by a small amount of other unidentifiable dearomative, the structure of **Int9** could be identified through the comparison of experimental and calculated ^{1}H NMR signals.



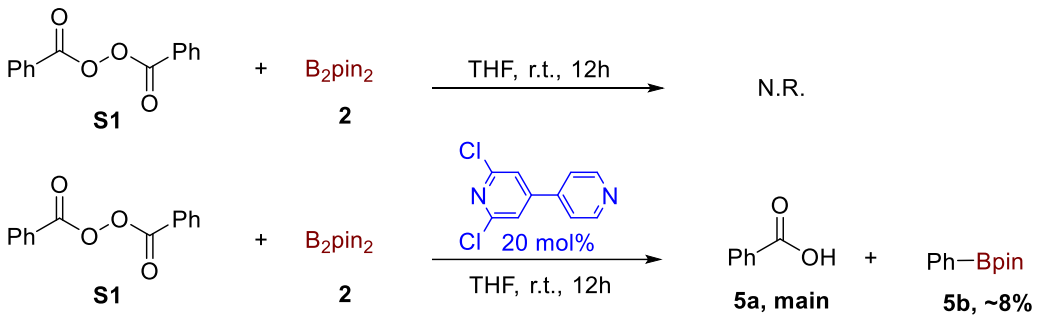


b

Calc.	δ_1 = 7.55	δ_2 = 7.23	δ_3 = 6.02	δ_4 =5.72	δ_5 = 4.70
Exp.	δ_1 = 7.50	δ_2 = 6.63	δ_3 = 6.06	δ_4 =5.65	δ_5 = 4.50

Figure S10. (a) ^{1}H NMR spectrum of 2,6-dichloro-4,4′-bipyridine and B_2pin_2 in THF-d_8 for 2h. **(b)** The calculated ^{1}H NMR chemical shift for the key [3,3]-σ-rearrangement intermediate **Int9** by the Gauge-independent atomic orbital (GIAO) method at B972/pcSseg-2 level[3].

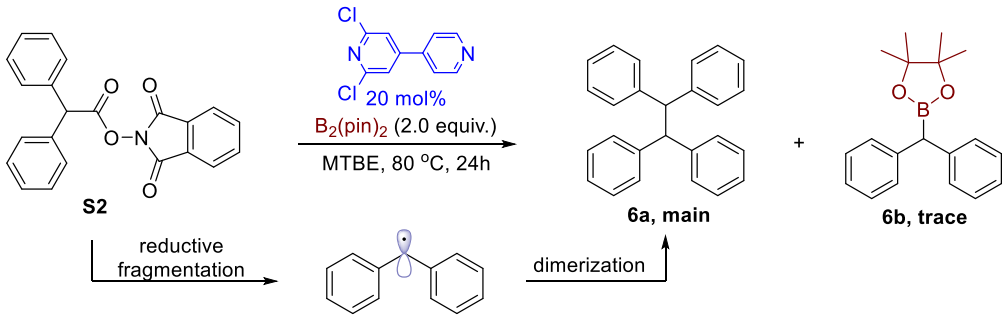
c) Boryl radical mediated decarboxylation reaction of benzoyl peroxide (BPO)



In an oven-dried 10 ml Schlenk tube equipped with a magnetic stir bar, benzoyl peroxide (0.2 mmol, 1.0 equiv), $B_2(pin)_2$ (0.2 mmol, 1.0 equiv), 2,6-dichloro-4,4′-bipyridine (0.04mmol, 20 mol%) and and THF (1.0 mL) was added in turn. After the reaction mixture was stirred at room temperature for 12 h, THF was removed in vaccum, and benzyl ether (0.2 mmol, 1.0 equiv.) was added as the interal stardnad. ^{1}H NMR

analysis of the reaction mixture showed that the phenylboronate **5b** was formed in 8 % yield, with the benzoic acid was detecting as the major product **5a**. However, in the absence of 2,6-dichloro-4,4′-bipyridine catalyst, no reaction occurred.

d) Boryl radical mediated decarboxylation reaction of NHPI ester



Experimental procedure: In an oven-dried 10 ml Schlenk tube equipped with a magnetic stir bar, NHPI ester **S2** (0.2 mmol, 1.0 equiv.), $B_2(pin)_2$ (0.4 mmol, 2.0 equiv.), 2,6-dichloro-4,4′-bipyridine (20 mol%) and MTBE (1.5 mL) was added in turn. Then, the reaction mixture was heated at 80 °C for 24 h. After cooling to room temperature, the GC-MS analysis of the crude reaction mixture was performed. The experimental result indicates that a major dimerization product **6a** of diphenyl methyl radical and a trace amount of decarboxylative borylation product **6b** were generated in the reaction.

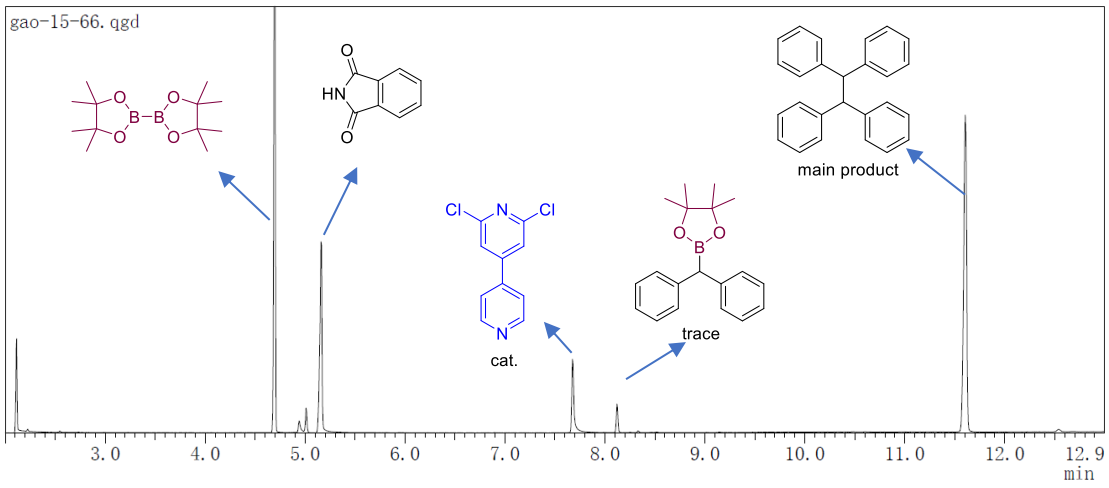


Figure S11. GC-MS analysis of the crude reaction mixture of NHPI ester **S2** (0.2 mmol, 1.0 equiv.), 2,6-dichloro-4,4′-dipyridine (20 mol%), B_2pin_2 (0. 4 mmol, 2.0 equiv.) in MTBE (1.5 mL).

e) Inhibitory tests of pyridine-boryl radical and 1,4-diborylpyrazine by TEMPO

The addition of TEMPO to the noncatalytic and catalytic diborylation reaction of pyrazines. As shown below, the diborylation of 2,3-dimethyl pyrazine was significantly suppressed when TEMPO was added to the standard experimental conditions. In the presence of 1.0 and 2.2 equivalent of TEMPO, the yields of diborylated products decrease to 47% and 0%, respectively (Eq.1). It's probably because the in situ formed 2,6-dichloro-4,4′-bipyridine-boryl radical might be trapped by TEMPO. Besides, we also found that the addition of TEMPO leads to a lower yield of diborylated pyrazine (Eq.2). These results might be attributed to the oxidation of 1,4-diborylpyrazine in the presence of TEMPO (Eq.3).

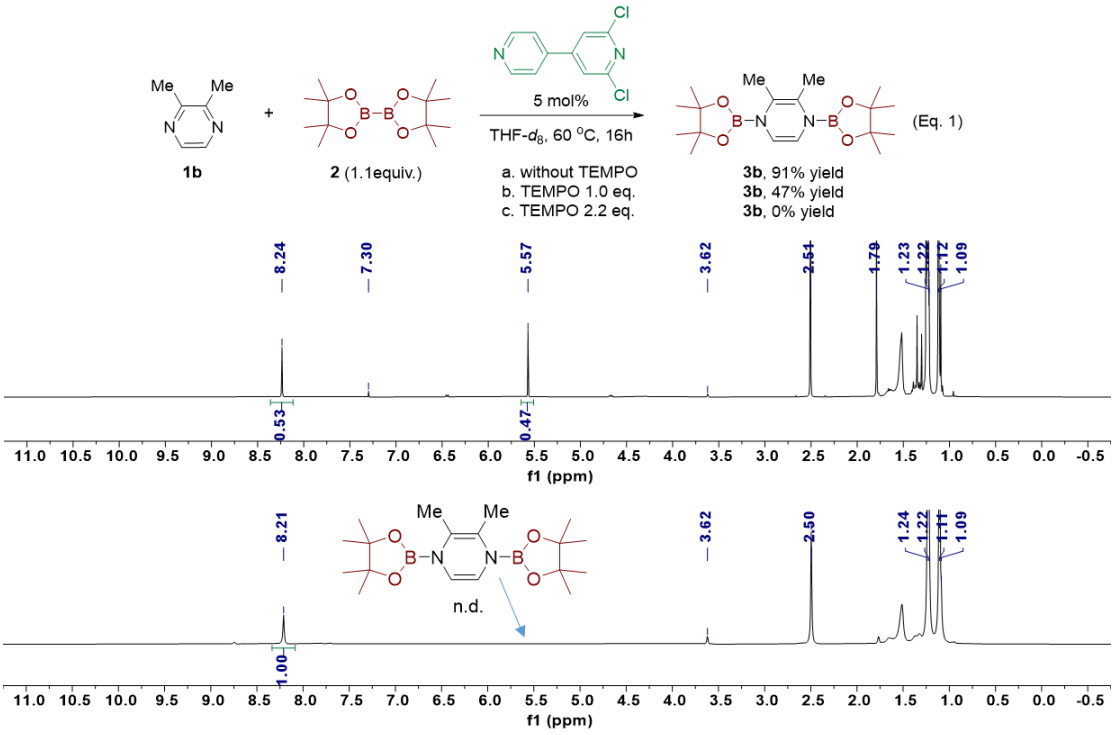


Figure S12. ^{1}H NMR spectrum for the reaction mixture of 2,3-dimethylpyrazine (1.0 equiv), B_2pin_2 (1.1 equiv) and 2,6-dichloro-4,4′-bipyridine (5mol%) in the presence of TEMPO (1.0 or 2.2 equiv.) as the additive in THF-d_8.

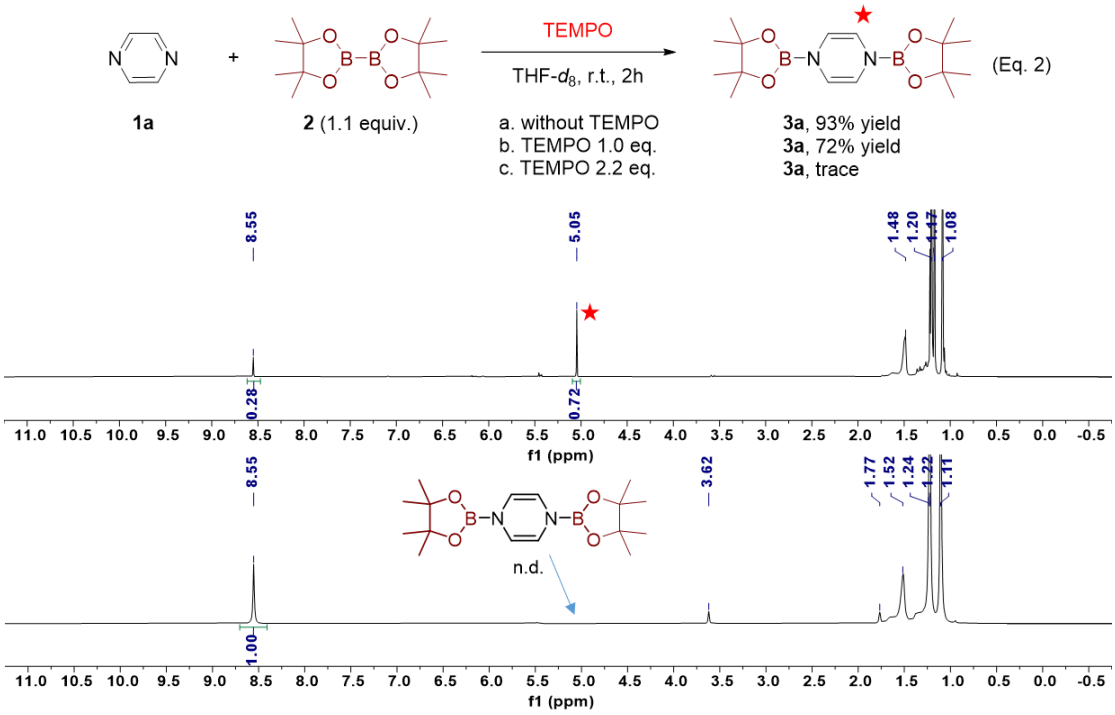


Figure S13. ^{1}H NMR spectrum for the reaction mixture of pyrazine (1.0 equiv) and B_2pin_2 (1.1 equiv) in the presence of TEMPO (1.0 or 2.2 equiv.) as the additive in THF-d_8.

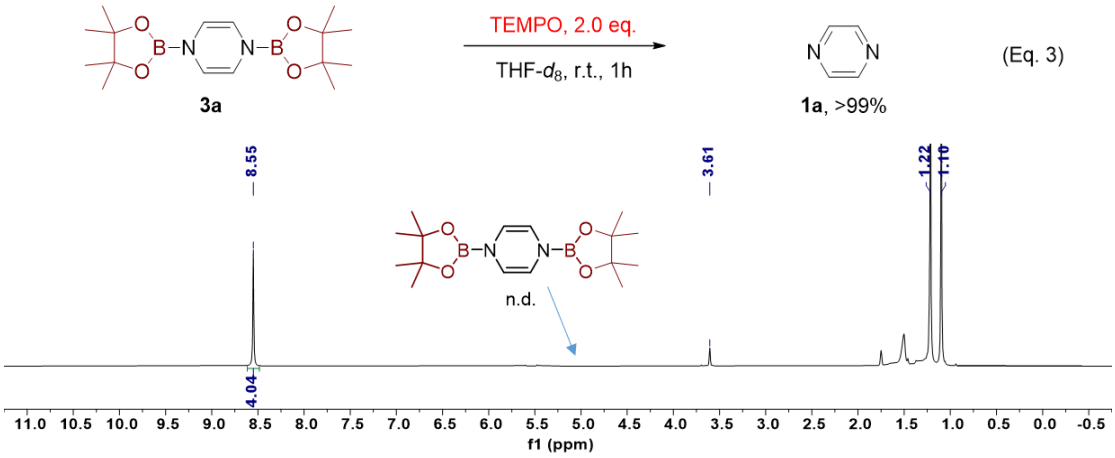
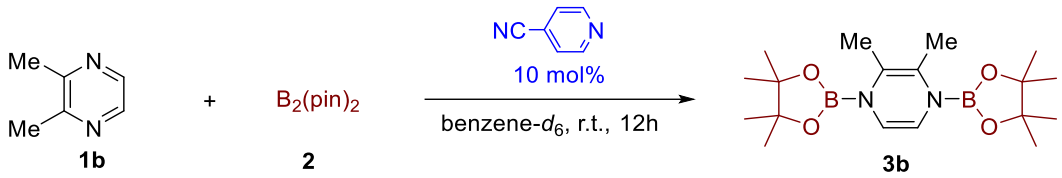


Figure S14. ^{1}H NMR spectrum for the reaction mixture of **3a** (1.0 equiv) and TEMPO (2.0 equiv.) in THF-d_8.

2.3 The diborylation of *N*-heteroarenes with 4-cyanopyridine as the catalyst

(1) Catalytic diborylation of 2,3-dimethylpyrizine with 4-cyanopyridine



1b (0.2 mmol), B_2pin_2 (1.05 equiv.) and 4-cyanopyridine (0.02 mmol, 10 mol%) were mixed in 0.5 mL benzene-d_6 in a Schlenk tube. The mixture was stirred at room temperature for 12h, after which, the ^{1}H NMR analysis of the crude reaction mixture was carried out immediately. The experimental result indicated that in the presence of 10 mol% of 4-cyanopyridine as the catalyst, the diborylation reaction of 2,3-dimethylpyrizine with B_2pin_2 proceeded efficiently at room temperature, affording the dearomative pyrazine in quantitative yield.

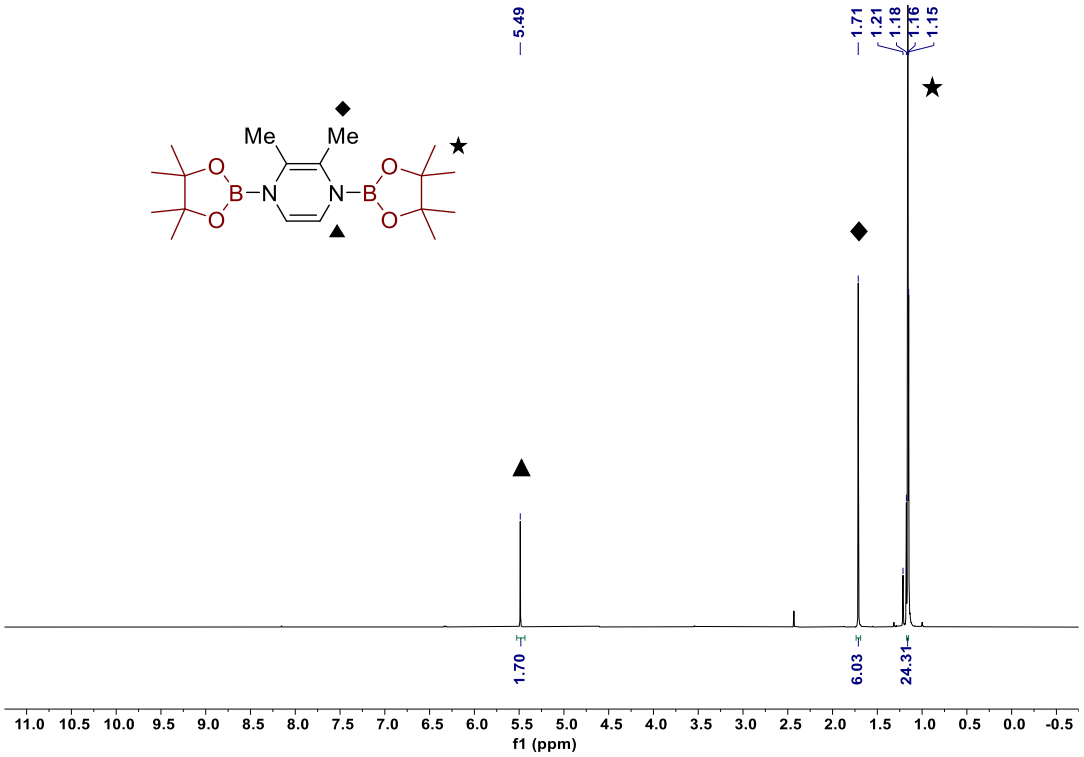
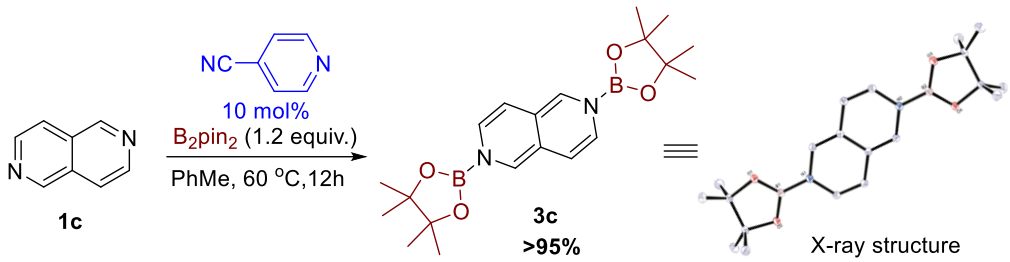


Figure S15. ^{1}H NMR spectrum of compound **3b**.

(2) Catalytic diborylation of 2,6-naphthyridine with 4-cyanopyridine



a) Experimental procedure: In an oven-dried 10 ml Schlenk tube equipped with a magnetic stir bar, 2,6-naphthyridine **1c** (0.2 mmol, 12.8 mg), B_2pin_2 (0.24 mmol, 1.2 equiv), 4-cyanopyridine (0.02 mmol, 10 mol%) and 0.5 mL PhMe-d_8 was added in turn. Then the reaction mixture was stirred at 60 °C for 12h. After which, put this Schlenk tube into a low temperature refrigerator (-30 °C) and the crystals started to precipitate. **3c**: red crystal. **^{1}H NMR** (400 MHz, Toluene-d_8) δ 5.86 (dt, J = 7.8, 1.0 Hz, 2H), 5.23 (t, J = 1.0 Hz, 2H), 4.50 (d, J = 7.9 Hz, 2H), 0.96 (s, 24H). **^{13}C NMR** (100 MHz, Toluene-d_8) δ 137.8, 131.3, 121.7, 113.4, 108.2, 83.7, 24.8. **^{11}B NMR** (128 MHz, Toluene-d_8) δ 23.48.

b) Structural confirmation 3c by single-crystal X-ray diffraction (XRD).

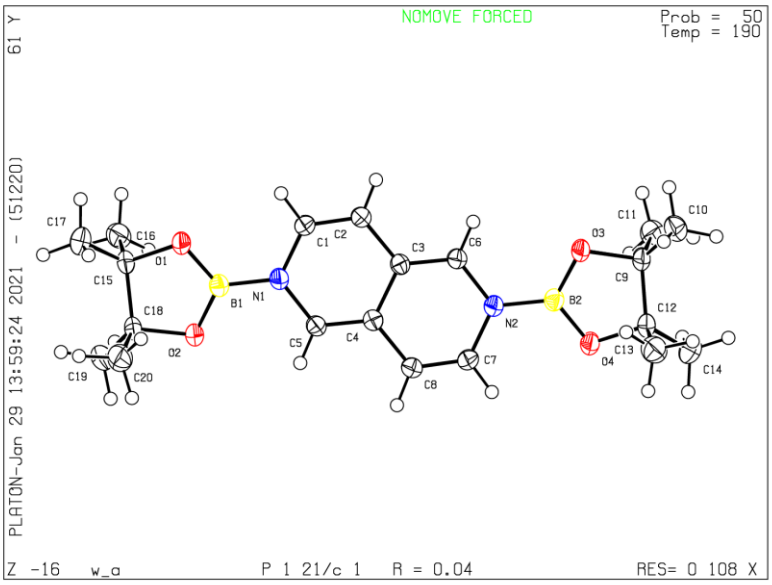


Figure S16. the X-ray structure of **3c** (CCDC No. 2071739).

Table S1. Crystal data and structure refinement for 3c

Molecular Formula	$C_{20}H_{30}B_2N_2O_4$	
Sum formula	$C_{20}H_{30}B_2N_2O_4$	
Formula mass	384.08	
Crystal system	Monoclinic	
Space group	*P*2(1)/c	
Z	4	
Temperature	190 K	
Unit cell dimensions	*a* = 15.7142(11) Å	$\alpha = 90°$.
	b = 11.0458(8) Å	$\beta = 107.916(3)°$.
	c = 12.8792(9) Å	$\gamma = 90°$.
Volume	2127.1(3)Å^3	
Density (calculated)	1.199 *g.cm*$^{-3}$	
Mu (mm-1)	0.415	
F000	824	
F000'	825.83	
h,k,lmax	18,13,15	
Nref	3904	
Tmin, Tmax	0.565,0.751	
Tmin'	0.917	
Correction method = # Reported T Limits: Tmin=0.565 Tmax=0.751 AbsCorr = MULTI-SCAN		
Data completeness	0.984	
Theta(max)	54.003	
R(reflections)	0.0424(3466)	
wR2(reflections)	0.1199(3843)	
S	1.061	
Npar	261	

c) Structural confirmation of 3c by the NMR analysis

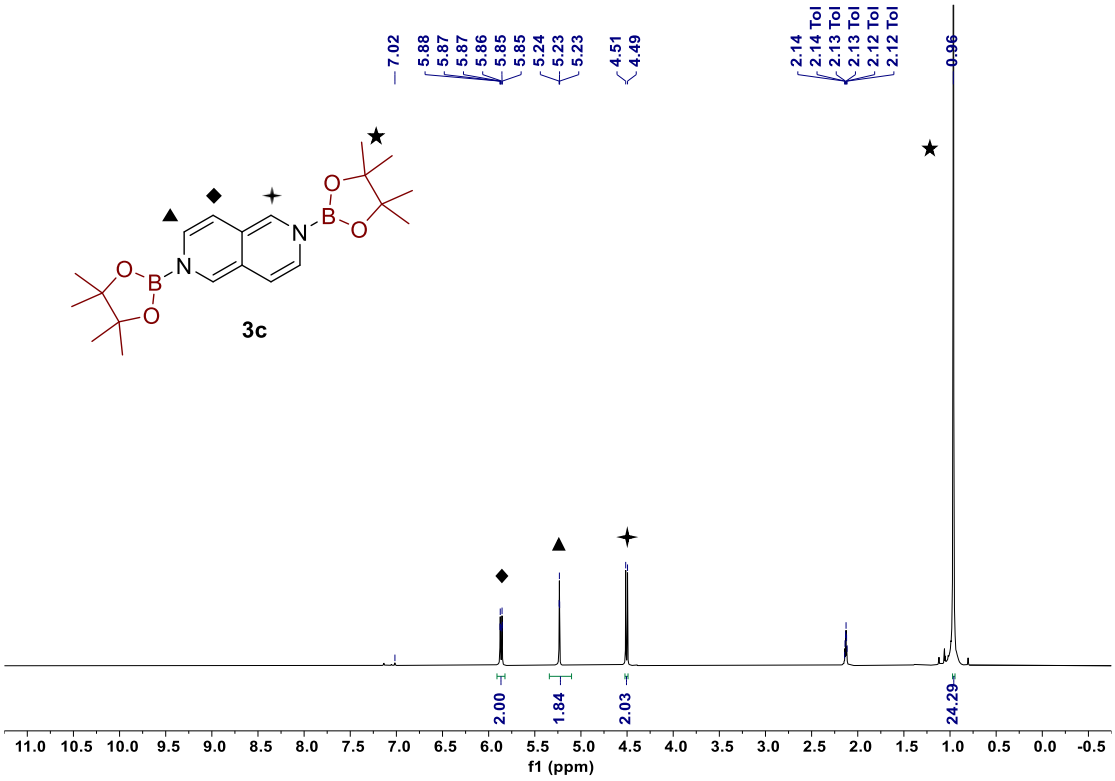


Figure S17. ^{1}H NMR spectrum of compound **3c**

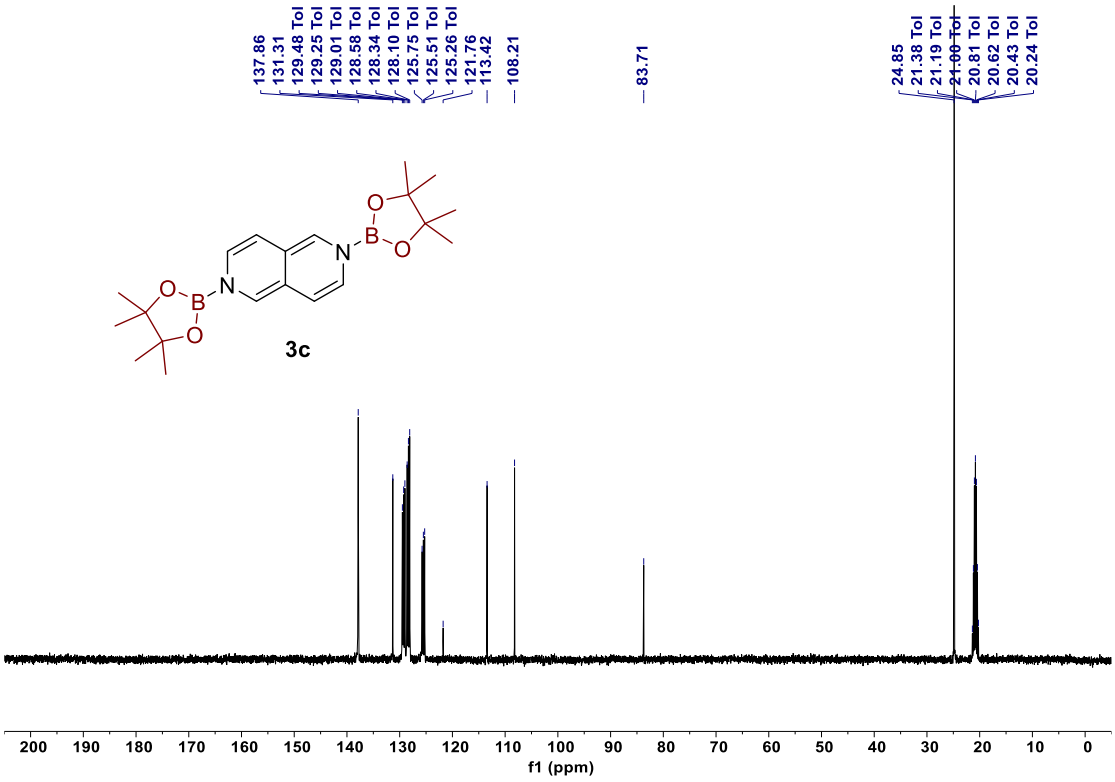


Figure S18. ^{13}C NMR spectrum of compound **3c.**

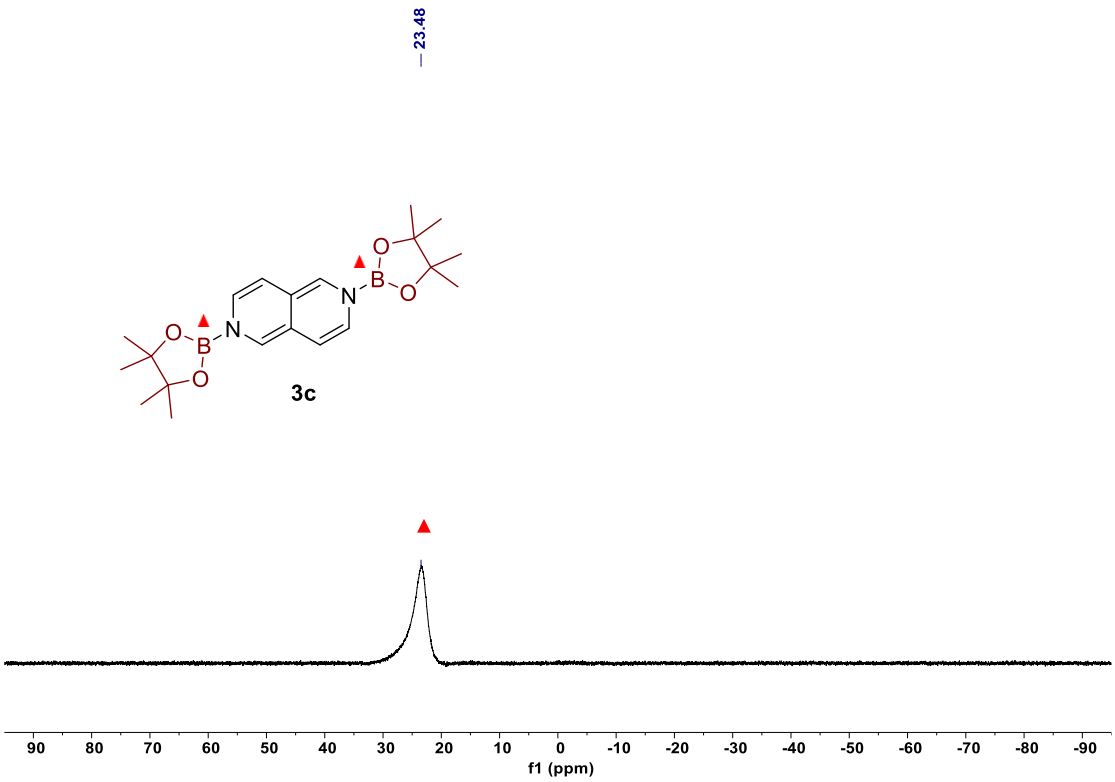


Figure S19. ^{11}B NMR spectrum of compound **3c.**

2.4 Kinetic Studies on the dearomative diborylation of pyrazines

2.4.1 General procedure

A dry NMR tube was charged with indicated concentration of B_2pin_2 (or pyrazine) and THF-d_8 (0.5 mL) in an argon-filled glove box. Then another substrate pyrazine (or B_2pin_2) was added into the NMR tube *via* a micro-syringe and the reaction mixture was monitored by the ^{1}H NMR. At 280, 362, 444, 526, 608, 690 seconds, the molar concentration of **3aa** was determined by the integration of the characteristic peak of which at 4.95 (s, 4H) ppm against the internal standard. These reactions were all performed two times at the same conditions and the average value was taken for each time point. The concentration of **3a** or **3b** (only the data < 30% yield was used) was plotted against the reaction time and the slope of the linear portion of the curve was used to determine the initial rates (k_{in}) of the reaction.

2.4.2 Determination of the reaction orders in pyrazine and B_2pin_2

a. Dependence of the reaction rate on the concentration of pyrazine

The reactions were performed with bis(pinacolato)diboron (B_2pin_2) **2** (50.8 mg, 0.2 mmol, 0.4 M) in the presence of 0.01 M, 0.02 M, 0.04 M, 0.08 M pyrazine. The relationship between k_{in} and **[Pyrazine]^2** was linear, showing the reaction rate exhibits a second-order rate dependence on the concentration of pyrazine.

Table S2. [**3a**] in different concentration of bis(pinacolato)diboron at different time interval

Time (s)	[Pyrazine] = 0.01M	[Pyrazine] = 0.02M	[Pyrazine] = 0.04M	[Pyrazine]= 0.08M
0	0.000000	0.000000	0.000000	0.000000
280	0.000071	0.000254	0.001784	0.008160
362	0.000092	0.00034	0.002372	0.010112
444	0.000118	0.00042	0.002788	0.012512
526	0.00014	0.000494	0.00328	0.014648
608	0.000167	0.000554	0.003768	0.016440

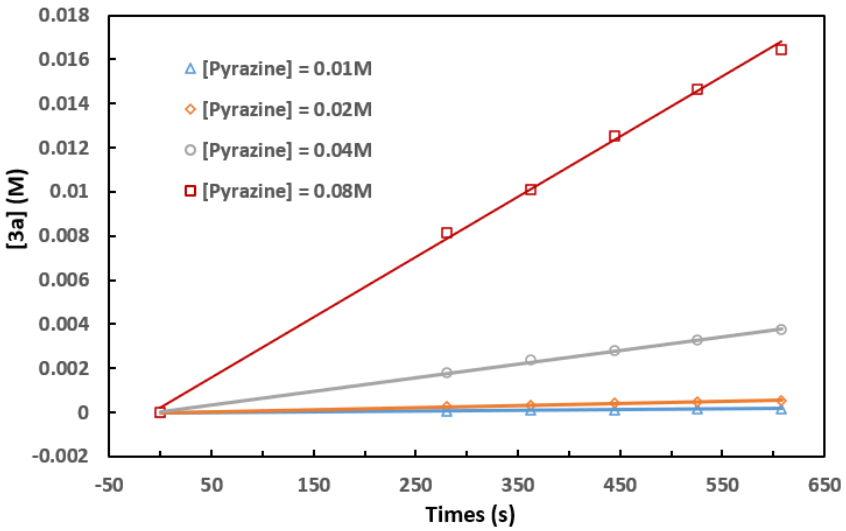


Figure S20. Plot of the change in [**3a**] with time for the reaction of B_2pin_2 (0.4 M) with 0.01 M, 0.02 M, 0.04 M, 0.08 M of pyrazine (**1a)** at room temperature. The curve depicts the results of an unweighted least-square fit to y = a*x + b (0.01 M: a = 2.73 x 10^{-7}, b = 2.99 x 10^{-6}, R^2 = 0.997; 0.02 M: a = 9.26 x 10^{-7}, b = 1.00 x 10^{-6}, R^2 = 0.999; 0.04 M: a = 6.20 x 10^{-6}, b = 3.83 x 10^{-8}, R^2 = 0.999; 0.08 M: a = 2.72 x 10^{-5}, b = 2.3 x 10^{-4}, R^2 = 0.998).

Table S3. The k_{obs} value of [**3a**] in different concentration of pyrazine

[Pyrazine] (M)	[Pyrazine]^2 (M^2)	K_{obs} (mol L^{-1} s^{-1})
0.01	0.0001	2.73E-07
0.02	0.0004	9.26E-07
0.04	0.0016	6.20 E-06
0.08	0.0064	2.72E-05

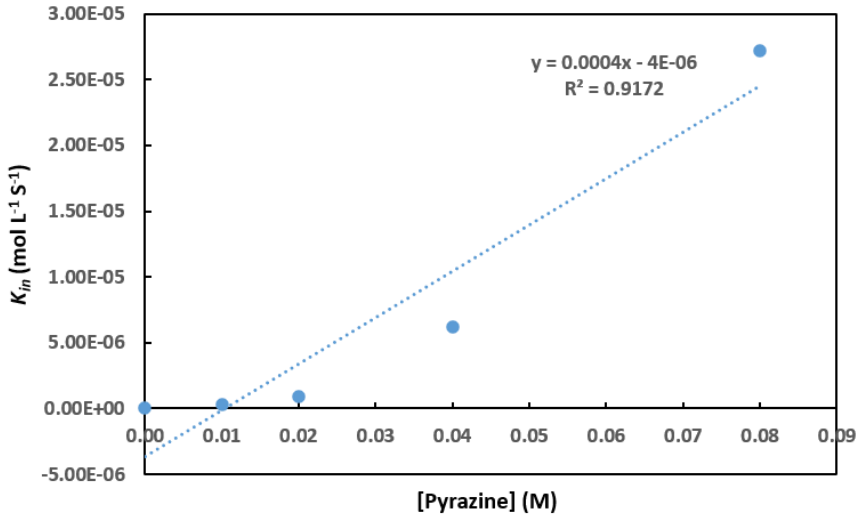


Figure S21. Plot of k_{in} vs. [Pyrazine] with attempted in liner fit.

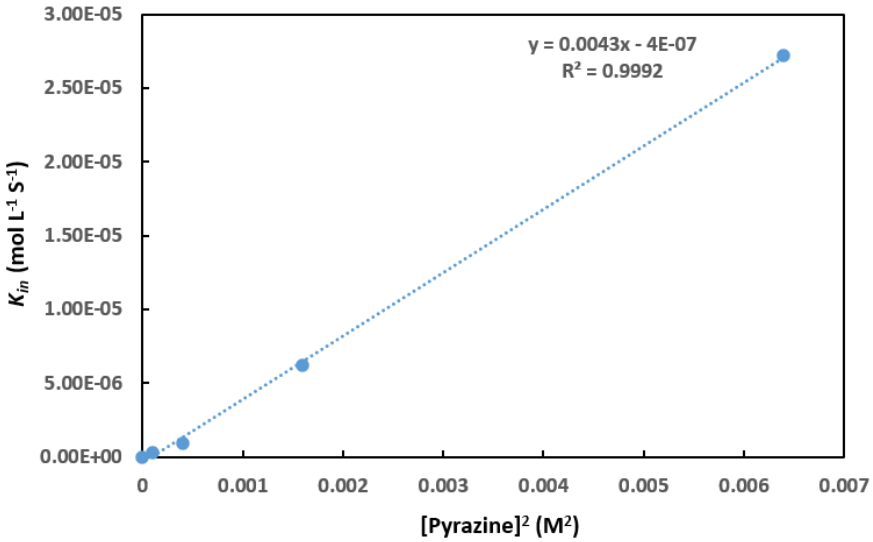


Figure S22. Plot of k_{in} vs. [Pyrazine]^2 with attempted in liner fit. The curve depicts the results of an unweighted least-square fit to y = a*x + b (a = 4. 3 x 10^{-3}, b = 4 x 10^{-7}, R^2 = 0.9992)

b. Dependence of the reaction rate on the concentration of bis(pinacolato)diboron (B_2pin_2)

The reactions were performed with pyrazine (16.0 mg, 0.2 mmol, 0.4 M) in the presence of 0.005 M, 0.01 M, 0.02 M of bis(pinacolato)diboron (B_2pin_2). The relationship between k_{in} and **[B_2pin_2]** was linear, showing the reaction rate exhibits a first-order rate dependence on the concentration of B_2pin_2.

Table S4. [**3a**] in different concentration of B_2pin_2 at different time interval

Time (s)	[B_2pin_2] = 0.005 M	[B_2pin_2] = 0.01 M	[B_2pin_2] = 0.02 M
0	0.00000	0.00000	0.00000
280	0.00212	0.00360	0.00698
362	0.00260	0.00440	0.00844
444	0.00304	0.00516	0.00972

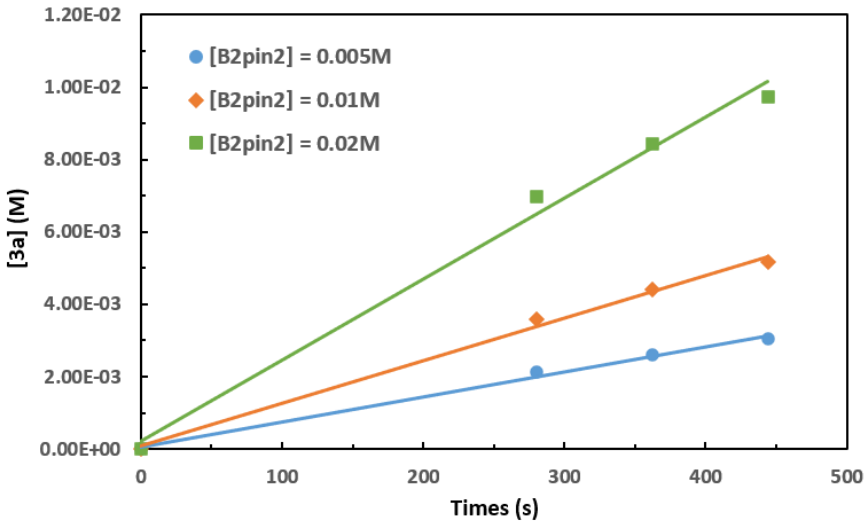


Figure S23. Plot of the change in [**3a**] with time for the reaction of pyrazine (0.4 M) with 0.005 M, 0.01 M, 0.02 M of B_2pin_2 at room temperature. The curve depicts the results of an unweighted least-square fit to $y = a*x + b$ (0.005 M: $a = 6.96 \times 10^{-6}$, $b = 5.02 \times 10^{-5}$, $R^2 = 0.995$; 0.02 M: $a = 1.18 \times 10^{-5}$, $b = 8.51 \times 10^{-5}$, $R^2 = 0.995$; 0.02 M: $a = 2.24 \times 10^{-5}$, $b = 2.11 \times 10^{-4}$, $R^2 = 0.991$).

Table S5. The k_{in} value of [**3a**] in different concentration of B_2pin_2

[B_2pin_2]	k_{in} (mol L^{-1} s^{-1})
0.005 M	6.96E-06
0.01 M	1.18E-05
0.02 M	2.24E-05

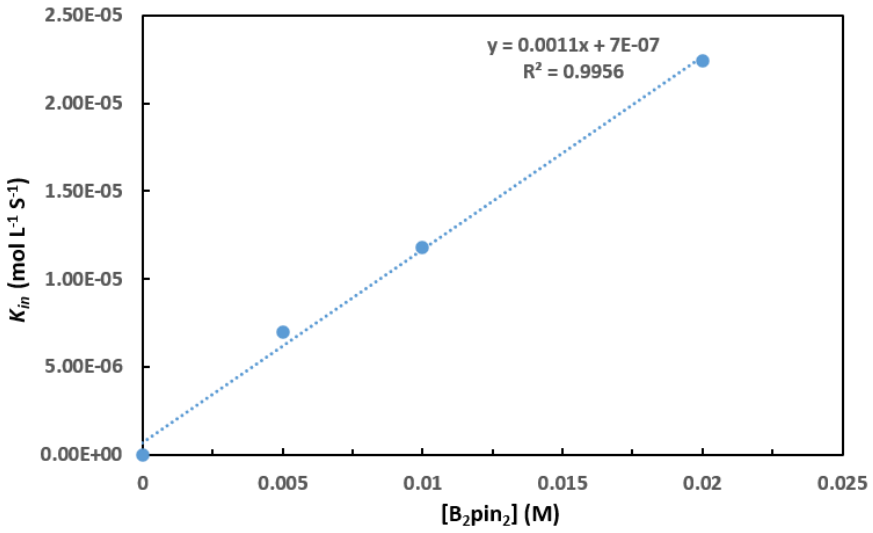


Figure S24. Plot of k_{in} vs. [B_2pin_2] with attempted in liner fit. The curve depicts the results of an unweighted least-square fit to y = a*x + b (a = 1. 1 x 10^{-3}, b = 7 x 10^{-7}, R^2 = 0.9956)

2.4.3 Determination of the reaction orders in 2,6-dichloro-4,4′-bipyridine, 2,3-dimethylpyrazine and B_2pin_2

a. Dependence of the reaction rate on the concentration of 2,6-dichloro-4,4′-bipyridine catalyst

The reactions were performed with 2,3-dimethylpyrazine (43.2 mg, 0.4 mmol, 0.8 M) and bis(pinacolato)diboron (B_2pin_2) (101.6 mg, 0.4 mmol, 0.8 M) in the presence of 0.04 M, 0.08 M, 0.12 M, 0.16 M 2,6-dichloro-4,4′-bipyridine catalyst. The relationship between k_{in} and **[Cat.]**^{2} was linear, showing the reaction rate exhibits a second-order rate dependence on the concentration of 2,6-dichloro-4,4′-bipyridine catalyst.

Table S6. [**3b**] in different concentration of catalyst at different time interval

Time (s)	[Cat.] = 0.04M	[Cat.] = 0.08M	[Cat.] = 0.12M	[Cat.]= 0.16M
0	0.00000	0.00000	0.00000	0.00000
280	0.00000	0.00000	0.00112	0.01064
608	0.00000	0.00008	0.02600	0.08672
1018	0.00000	0.00528	0.08496	0.17056
1428	0.00000	0.02528	0.13968	0.23808
1838	0.00002	0.04888	0.18488	0.30344
2248	0.00008	0.07304	0.23104	0.35408
2658	0.00048	0.09320	0.27120	0.40280
3068	0.00200	-	-	-
3478	0.00512	-	-	-
3888	0.00880	-	-	-

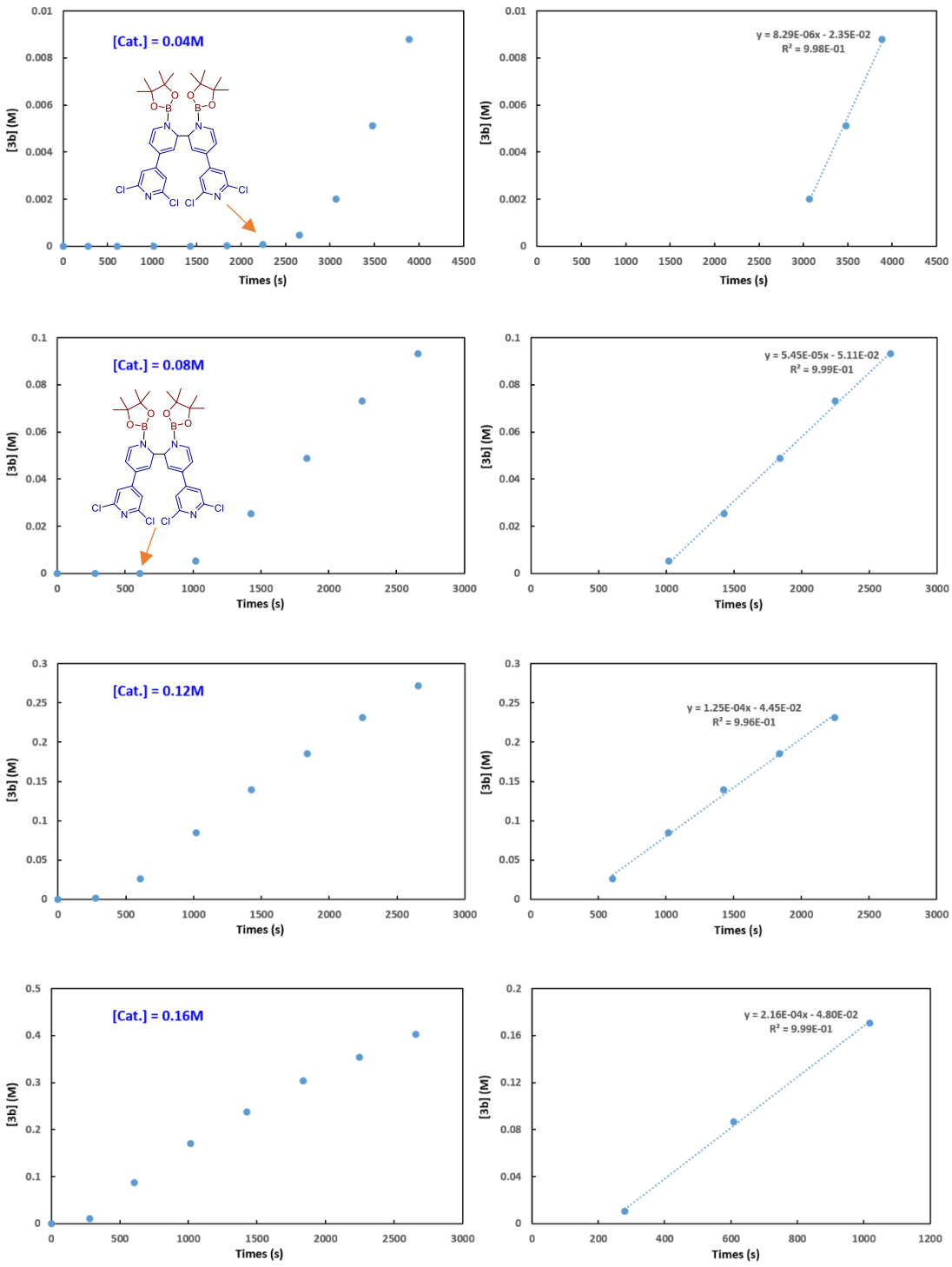


Figure S25. Plot of the change in **[3b]** with time for the reaction of 2,3-dimethylpyrazine (0.8 M), B_2pin_2 (0.8 M) with 0.04 M, 0.08 M, 0.12 M, 0.16 M of 2,6-dichloro-4,4′-bipyridine catalyst at room temperature. The curve depicts the results of an unweighted least-square fit to $y = a*x + b$ (0.04 M: $a = 8.29 \times 10^{-6}$, $b = 2.35 \times 10^{-2}$, $R^2 = 0.998$; 0.08 M: $a = 5.45 \times 10^{-5}$, $b = 5.11 \times 10^{-2}$, $R^2 = 0.999$; 0.12 M: $a = 1.25 \times 10^{-4}$, $b = 4.45 \times 10^{-2}$, $R^2 = 0.996$; 0.16 M: $a = 2.16 \times 10^{-4}$, $b = 4.80 \times 10^{-2}$, $R^2 = 0.999$).

Table S7. The k_{in} value of [**3b**] in different concentration of catalyst

[Pyrazine] (M)	[Pyrazine]^2 (M^2)	K_{obs} (mol L^{-1} s^{-1})
0.00	0.0000	0.0000
0.04	0.0016	8.29E-06
0.08	0.0064	5.45E-05
0.12	0.0144	1.25E-04
0.16	0.0256	2.16E-04

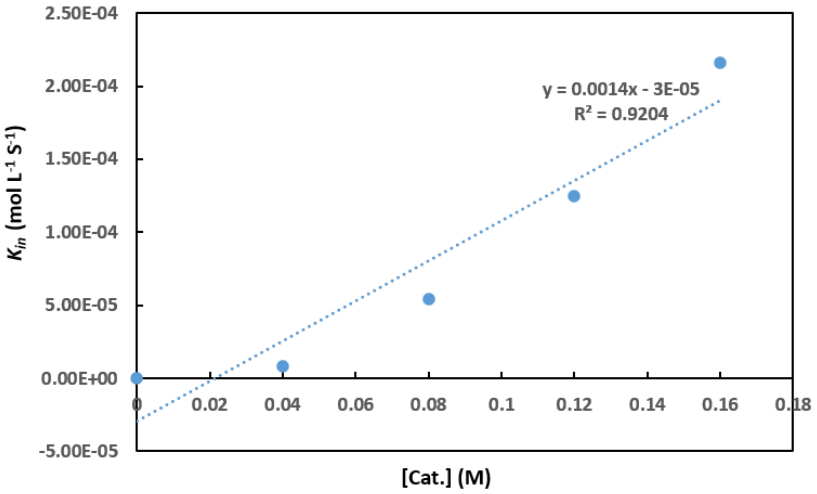


Figure S26. Plot of k_{in} vs. **[Cat.]** with attempted in liner fit.

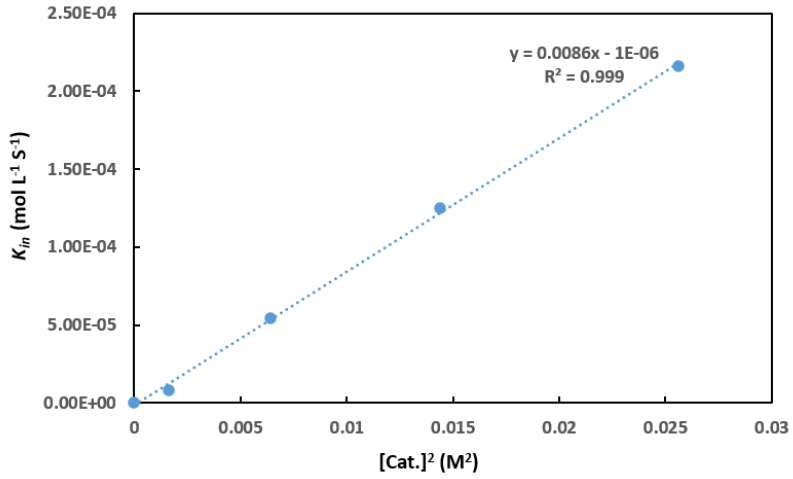


Figure S27. Plot of k_{in} vs. **[Cat.]^2** with attempted in liner fit. The curve depicts the results of an unweighted least-square fit to y = a*x + b (a = 8. 6 x 10^{-3}, b = 1 x 10^{-6}, R^2 = 0.999)

b. Dependence of the reaction rate on the concentration of bis(pinacolato)diboron (B_2pin_2)

The reactions were performed with 2,3-dimethylpyrazine (43.2 mg, 0.4 mmol, 0.8 M) and catalyst (13.38 mg, 0.06 mmol, 0.12 M) in the presence of 0.2 M, 0.4 M, 0.8 M of bis(pinacolato)diboron (B_2pin_2). The relationship between k_{in} and **[B_2pin_2]** was linear, showing the reaction rate exhibits a first-order rate dependence on the concentration of B_2pin_2.

Table S8. [**3b**] in different concentration of B_2pin_2 at different time interval

Time (s)	[B_2pin_2] = 0.2 M	[B_2pin_2] = 0.4 M	[B_2pin_2] = 0.8 M
0	0.00000	0.00000	0.00000
280	0.00000	0.00000	0.00112
608	0.00000	0.00176	0.02600
1018	0.00000	0.01856	0.08496
1428	0.00000	0.05232	0.13968
1838	0.00304	0.08160	0.18488
2248	0.01416	0.10904	0.23104
2658	0.03112	0.13744	0.27120
3068	0.04704	0.16200	-
3478	0.06128	-	-

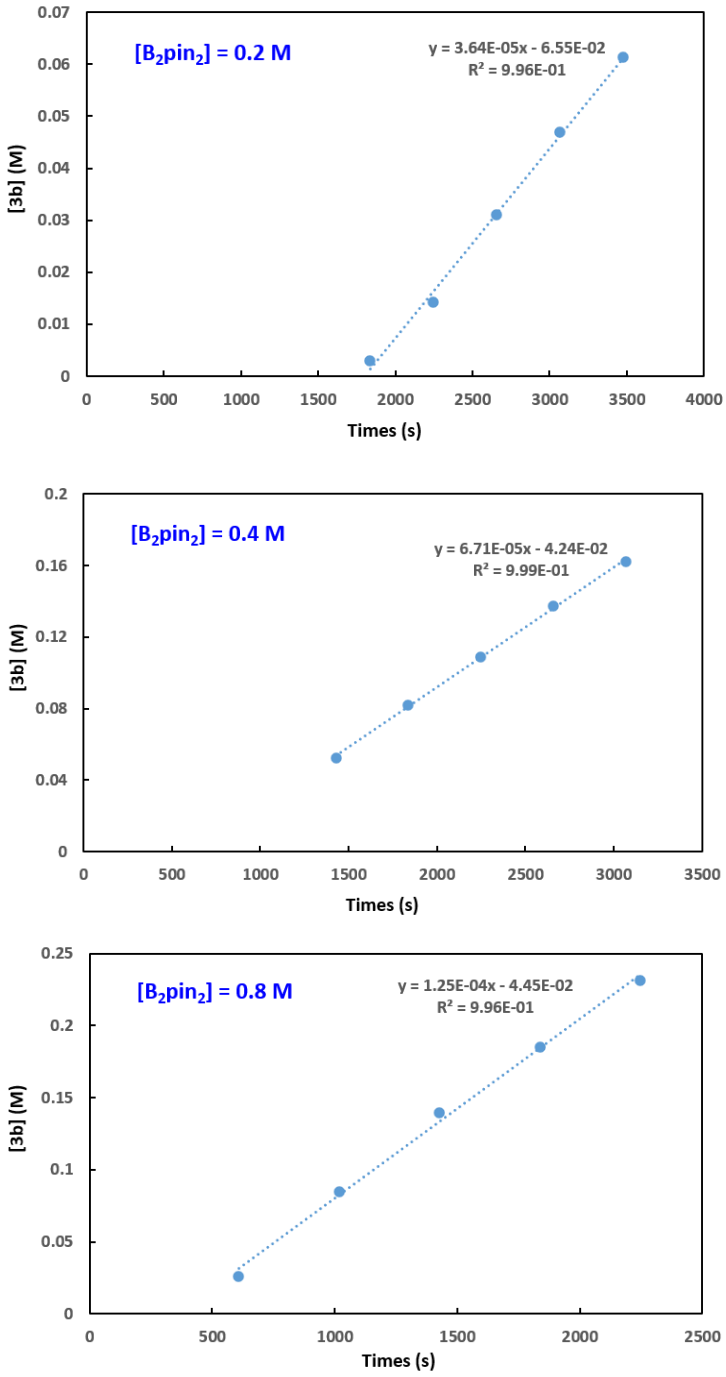


Figure S28. Plot of the change in **[3a]** with time for the reaction of 2,3-dimethylpyrazine (43.2 mg, 0.4 mmol, 0.8 M) and catalyst (13.38 mg, 0.06 mmol, 0.12 M) in the presence of 0.2 M, 0.4 M, 0.8 M of bis(pinacolato)diboron (B_2pin_2) at room temperature. The curve depicts the results of an unweighted least-square fit to $y = a*x + b$ (0.2 M: $a = 3.64 \times 10^{-5}$, $b = 6.55 \times 10^{-2}$, $R^2 = 0.996$; 0.4 M: $a = 6.71 \times 10^{-5}$, $b = 4.42 \times 10^{-2}$, $R^2 = 0.999$; 0.8 M: $a = 1.25 \times 10^{-4}$, $b = 4.45 \times 10^{-2}$, $R^2 = 0.996$).

Table S9. The k_{in} value of [**3b**] in different concentration of B_2pin_2

[B_2pin_2]	**k_{in} (mol L^{-1} s^{-1})**
0.00 M	0.00
0.20 M	3.64E-05
0.40 M	6.71E-05
0.80 M	1.25E-04

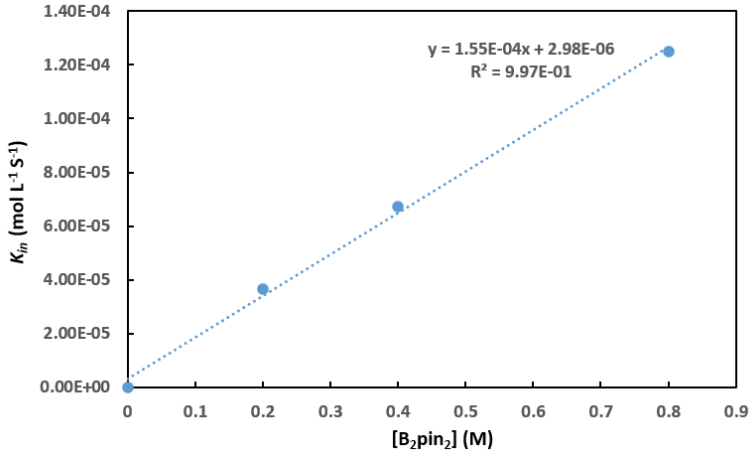


Figure S29. Plot of k_{in} vs. **[B_2pin_2]** with attempted in liner fit. The curve depicts the results of an unweighted least-square fit to y = a*x + b (a = 1. 55 x 10^{-4}, b = 2.98 x 10^{-6}, R^2 = 0.997)

c. Dependence of the reaction rate on the concentration of 2,3-dimethylpyrazine

The reactions were performed with bis(pinacolato)diboron (B_2pin_2) (101.6 mg, 0.4 mmol, 0.8 M) and catalyst (13.38 mg, 0.06 mmol, 0.12 M) in the presence of 0.2 M, 0.4 M, 0.8 M of 2,3-dimethylpyrazine (**1b**). The result suggests that the reaction rate exhibits a zero-order rate dependence on the concentration of 2,3-dimethylpyrazine.

Table S10. [**3b**] in different concentration of B_2pin_2 at different time interval

Time (s)	[1b] = 0.2 M	[1b] = 0.4 M	[1b] = 0.8 M
0	0.00000	0.00000	0.00000
280	0.00536	0.00456	-
362	0.00970	0.00656	-
444	0.02016	0.00896	-
526	0.02962	0.01820	-
608	0.04056	0.02924	0.02600
690	0.05044	0.04032	-
772	0.06076	0.05028	-
854	-	0.06152	-
936	-	0.07160	
1018	-	0.08036	0.08496
1428	-	-	0.13968
1838	-	-	0.18488
2248	-	-	0.23104
2658	-	-	0.27120

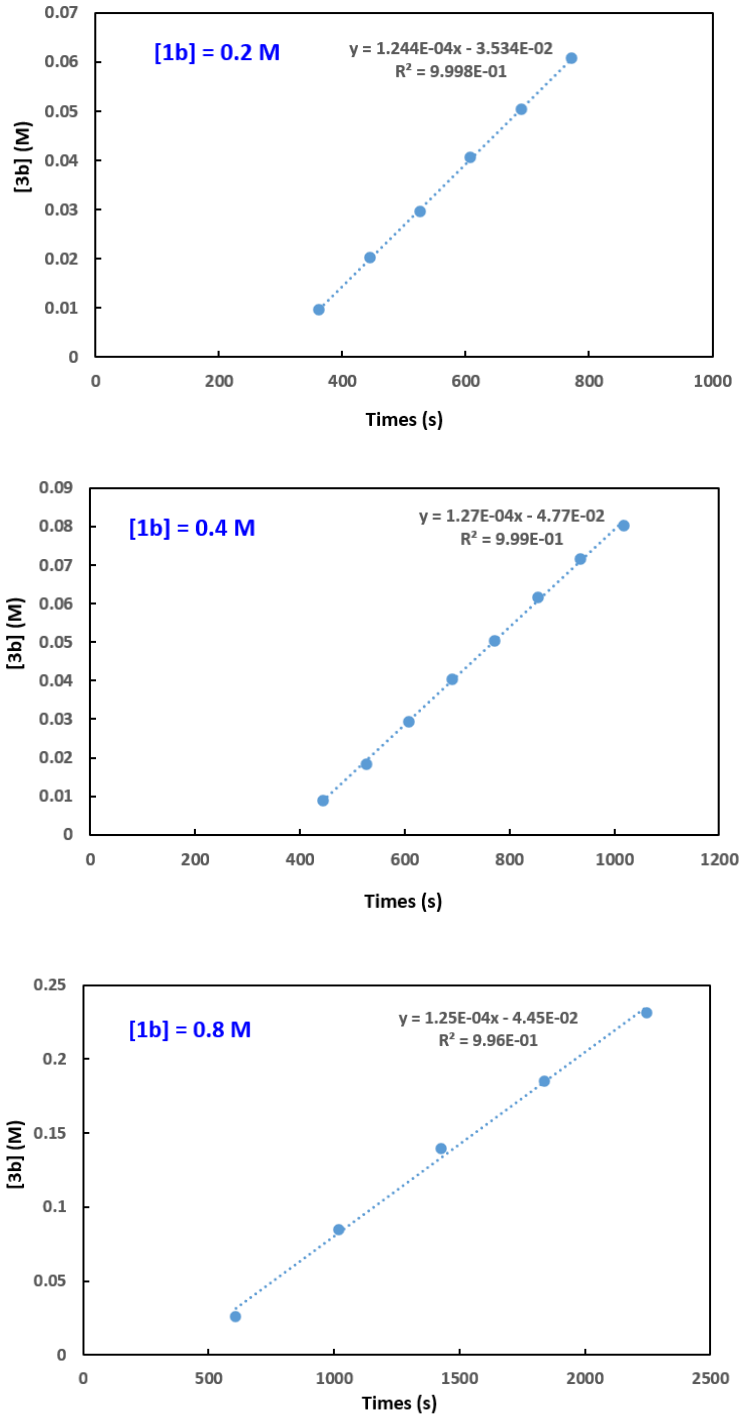


Figure S30. Plot of the change in [**3a**] with time for the reaction of bis(pinacolato)diboron (B_2pin_2) (101.6 mg, 0.4 mmol, 0.8 M) and catalyst (13.38 mg, 0.06 mmol, 0.12 M) in the presence of 0.2 M, 0.4 M, 0.8 M of 2,3-dimethylpyrazine at room temperature. The curve depicts the results of an unweighted least-square fit to $y = a*x + b$ (0.2 M: a = 1.24 x 10^{-4}, b = 3.53 x 10^{-2}, R^2 = 0.999; 0.4 M: a = 1.27 x 10^{-4}, b = 4.77 x 10^{-2}, R^2 = 0.999; 0.8 M: a = 1.25 x 10^{-4}, b = 4.45 x 10^{-2}, R^2 = 0.996).

Table S10. The k_{in} value of [**3b**] in different concentration of 2,3-dimethylpyrazine (**1b**)

[1b]	k_{in} **(mol L^{-1} s^{-1})**
0.00 M	0.00
0.20 M	1.24E-04
0.40 M	1.27E-04
0.80 M	1.25E-04

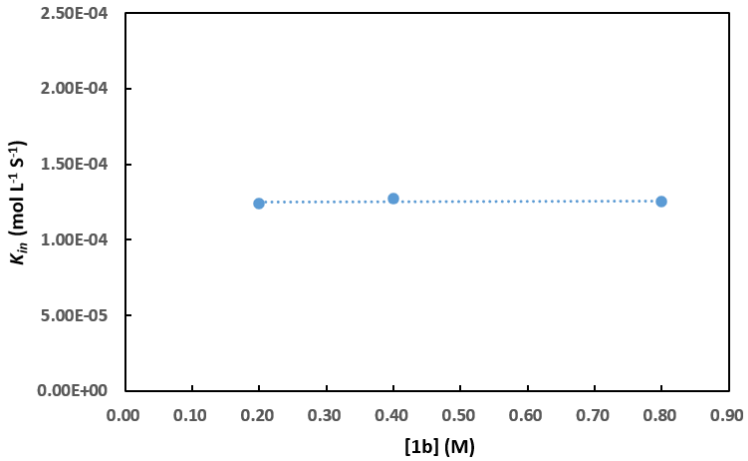


Figure S31. Plot of k_{in} vs. **[1b]** with attempted in liner fit.

3. Cartesian Coordinates and Energies of the Optimized Structures

Geometry optimizations and characters of all the stationary points were calculated by using the M06-2X/6-31G(d, p) method. Single point energies (**Esol**, a.u.) are computed by using the M06-2X/cc-pVTZ method in solvent (benzene). The solvent effect was treated with the solvation model based on density (SMD) with benzene as the solvent.

1a

Thermal correction to Energy=	0.082034
Thermal correction to Enthalpy=	0.082978
Thermal correction to Gibbs Free Energy=	0.050559
Sum of electronic and zero-point Energies=	-264.136273
Sum of electronic and thermal Energies=	-264.132129
Sum of electronic and thermal Enthalpies=	-264.131185
Sum of electronic and thermal Free Energies=	-264.163604

Esol = -264.2544528

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.046996	0.163833	0.000000
2	6	0	1.346765	0.163848	0.000016
3	7	0	2.052090	1.295021	−0.000012
4	6	0	1.346743	2.426179	−0.000054
5	6	0	−0.047020	2.426165	−0.000068
6	7	0	−0.752345	1.294992	−0.000040
7	1	0	−0.602695	−0.769880	0.000022
8	1	0	1.902483	−0.769854	0.000050
9	1	0	1.902441	3.359893	−0.000076
10	1	0	−0.602738	3.359867	−0.000101

1b

Thermal correction to Energy=	0.140690
Thermal correction to Enthalpy=	0.141634
Thermal correction to Gibbs Free Energy=	0.101811
Sum of electronic and zero-point Energies=	-342.687675
Sum of electronic and thermal Energies=	-342.680333
Sum of electronic and thermal Enthalpies=	-342.679389
Sum of electronic and thermal Free Energies=	-342.719211

Esol = -342.8337021

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.040063	0.161565	0.001576
2	6	0	1.346618	0.163703	−0.000411
3	7	0	2.045299	1.302452	−0.001755
4	6	0	1.356197	2.442358	−0.001110
5	6	0	−0.056649	2.440177	0.000949
6	7	0	−0.742241	1.298158	0.002267
7	1	0	−0.601119	−0.768849	0.002641
8	1	0	1.910535	−0.764980	−0.000931
9	6	0	−0.834034	3.724260	0.001707
10	1	0	−0.596553	4.330326	0.882315
11	1	0	−0.599410	4.329638	−0.880128
12	1	0	−1.901321	3.501148	0.003505
13	6	0	2.129603	3.728839	−0.002608
14	1	0	1.890372	4.333581	−0.883651
15	1	0	1.892973	4.334062	0.878808
16	1	0	3.197576	3.509026	−0.004115

2

Thermal correction to Energy=	0.386807
Thermal correction to Enthalpy=	0.387751
Thermal correction to Gibbs Free Energy=	0.319713
Sum of electronic and zero-point Energies=	-821.863685
Sum of electronic and thermal Energies=	-821.844186
Sum of electronic and thermal Enthalpies=	-821.843242
Sum of electronic and thermal Free Energies=	-821.911280

Esol = -822.2015046

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−2.986313	0.686383	0.373177
2	6	0	−2.986406	−0.685440	−0.372735
3	5	0	−0.852480	0.000312	0.000249
4	8	0	−1.615349	1.120932	0.215594
5	8	0	−1.615510	−1.120194	−0.215117
6	6	0	−3.909637	−1.736509	0.220278
7	1	0	−4.949556	−1.395508	0.190549

8	1	0	−3.837185	−2.658499	−0.362751
9	1	0	−3.643906	−1.966111	1.253555
10	6	0	−3.233935	0.547475	1.873599
11	1	0	−3.012597	1.502194	2.357436
12	1	0	−4.273568	0.283122	2.086643
13	1	0	−2.582093	−0.215149	2.310053
14	6	0	−3.909372	1.737590	−0.219859
15	1	0	−4.949344	1.396749	−0.190150
16	1	0	−3.836791	2.659571	0.363169
17	1	0	−3.643584	1.967149	−1.253131
18	6	0	−3.233969	−0.546494	−1.873162
19	1	0	−3.012760	−1.501245	−2.356995
20	1	0	−4.273556	−0.281986	−2.086233
21	1	0	−2.582003	0.216034	−2.309598
22	6	0	2.986440	0.685922	−0.372647
23	6	0	2.986327	−0.685807	0.373437
24	5	0	0.852505	0.000187	0.000309
25	8	0	1.615530	1.120677	−0.215155
26	8	0	1.615377	−1.120395	0.215835
27	6	0	3.909433	−1.737075	−0.219420
28	1	0	4.949397	−1.396209	−0.189709
29	1	0	3.836844	−2.658981	0.363724
30	1	0	3.643695	−1.966773	−1.252673
31	6	0	3.234083	0.546793	−1.873045
32	1	0	3.012884	1.501480	−2.357007
33	1	0	4.273685	0.282274	−2.086030
34	1	0	2.582150	−0.215799	−2.309419
35	6	0	3.909627	1.737077	0.220282
36	1	0	4.949552	1.396086	0.190650
37	1	0	3.837195	2.658993	−0.362867
38	1	0	3.643839	1.966807	1.253516
39	6	0	3.233867	−0.546710	1.873855
40	1	0	3.012514	−1.501371	2.357799
41	1	0	4.273485	−0.282318	2.086922
42	1	0	2.581992	0.215961	2.310179

3a

Thermal correction to Energy=	0.473234
Thermal correction to Enthalpy=	0.474178
Thermal correction to Gibbs Free Energy=	0.395462
Sum of electronic and zero-point Energies=	-1086.082964
Sum of electronic and thermal Energies=	-1086.058487
Sum of electronic and thermal Enthalpies=	-1086.057543

Sum of electronic and thermal Free Energies= -1086.136259

Esol = -1086.518306

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.293170	-6.317886	3.382498
2	5	0	3.009650	-3.656606	-1.337135
3	7	0	1.719172	-5.652897	2.207846
4	8	0	4.134870	-2.861817	-1.388133
5	8	0	2.342092	-3.748891	-2.539786
6	8	0	0.246670	-7.215021	3.403485
7	8	0	1.885896	-6.129797	4.612900
8	6	0	2.837209	-4.784823	2.188177
9	6	0	1.058348	-5.806001	0.965301
10	6	0	4.080317	-2.181377	-2.661612
11	6	0	3.222020	-3.164453	-3.525605
12	6	0	-0.032014	-7.464337	4.799075
13	6	0	1.347948	-7.159699	5.471871
14	6	0	3.239054	-4.160712	1.082438
15	1	0	3.349562	-4.657671	3.132523
16	6	0	1.460329	-5.182086	-0.140475
17	1	0	0.200426	-6.465123	0.967566
18	6	0	5.496960	-1.963323	-3.164122
19	6	0	3.382152	-0.843758	-2.428663
20	6	0	2.382009	-2.498155	-4.601527
21	6	0	4.051422	-4.300382	-4.119339
22	6	0	-0.514204	-8.896120	4.956119
23	6	0	-1.121003	-6.482373	5.224157
24	6	0	1.258969	-6.621379	6.889295
25	6	0	2.306287	-8.346385	5.407778
26	7	0	2.580095	-4.316272	-0.160773
27	1	0	4.095470	-3.499615	1.080688
28	1	0	0.946340	-5.307261	-1.084192
29	1	0	6.016541	-1.263703	-2.503798
30	1	0	5.486344	-1.535810	-4.171837
31	1	0	6.061671	-2.897030	-3.182925
32	1	0	3.365248	-0.235276	-3.337196
33	1	0	2.352939	-0.992757	-2.088161
34	1	0	3.922113	-0.294221	-1.653383
35	1	0	1.823695	-3.258586	-5.154293
36	1	0	3.020201	-1.962042	-5.311197
37	1	0	1.665995	-1.796112	-4.170720

38	1	0	4.697292	−3.946925	−4.927963
39	1	0	4.675125	−4.771967	−3.353798
40	1	0	3.374609	−5.058026	−4.522449
41	1	0	−1.481284	−9.013816	4.459748
42	1	0	−0.642625	−9.145372	6.014292
43	1	0	0.186138	−9.603956	4.509342
44	1	0	−1.439611	−6.656953	6.255641
45	1	0	−0.773087	−5.448672	5.135623
46	1	0	−1.985851	−6.608995	4.567963
47	1	0	2.265209	−6.441102	7.277185
48	1	0	0.766110	−7.345406	7.545936
49	1	0	0.706925	−5.680663	6.924157
50	1	0	2.002960	−9.145767	6.089619
51	1	0	2.359284	−8.753083	4.393283
52	1	0	3.305906	−8.008457	5.692684

3b

Thermal correction to Energy=	0.532336
Thermal correction to Enthalpy=	0.533280
Thermal correction to Gibbs Free Energy=	0.448401
Sum of electronic and zero-point Energies=	-1164.621476
Sum of electronic and thermal Energies=	-1164.593986
Sum of electronic and thermal Enthalpies=	-1164.593042
Sum of electronic and thermal Free Energies=	-1164.677921

Esol = -1165.082003

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.995941	−6.132207	3.230100
2	5	0	2.602241	−3.543550	−1.277206
3	7	0	1.005933	−5.208036	2.151479
4	8	0	3.740177	−2.770003	−1.140222
5	8	0	2.354589	−3.904528	−2.585768
6	8	0	0.359832	−7.356267	3.238937
7	8	0	1.662078	−5.864442	4.411420
8	6	0	1.853279	−4.075245	2.232481
9	6	0	0.205638	−5.286603	0.966163
10	6	0	4.137795	−2.392489	−2.473984
11	6	0	3.538444	−3.551233	−3.333944
12	6	0	0.387321	−7.814669	4.607638
13	6	0	1.653661	−7.091025	5.169902

14	6	0	2.241933	-3.444350	1.130839
15	1	0	2.142801	-3.755466	3.224949
16	6	0	0.601987	-4.650876	-0.150746
17	6	0	5.651848	-2.279059	-2.524410
18	6	0	3.489376	-1.043084	-2.775050
19	6	0	3.128379	-3.155727	-4.742039
20	6	0	4.437451	-4.784847	-3.364424
21	6	0	0.461545	-9.331635	4.616563
22	6	0	-0.904453	-7.336317	5.266809
23	6	0	1.590706	-6.754999	6.650088
24	6	0	2.946503	-7.834582	4.843308
25	7	0	1.817145	-3.892670	-0.144943
26	1	0	2.876701	-2.568227	1.148793
27	1	0	5.978520	-1.444004	-1.898709
28	1	0	5.990151	-2.089554	-3.548161
29	1	0	6.131737	-3.187568	-2.156584
30	1	0	3.802600	-0.653981	-3.747938
31	1	0	2.397853	-1.121973	-2.764927
32	1	0	3.787331	-0.328320	-2.003685
33	1	0	2.723291	-4.026692	-5.264406
34	1	0	3.992759	-2.792259	-5.306898
35	1	0	2.362178	-2.378556	-4.730977
36	1	0	5.328123	-4.617668	-3.976611
37	1	0	4.753502	-5.064299	-2.354809
38	1	0	3.875907	-5.620430	-3.789953
39	1	0	-0.464228	-9.747026	4.209136
40	1	0	0.581246	-9.705375	5.638495
41	1	0	1.293174	-9.692929	4.009146
42	1	0	-0.995095	-7.704958	6.292426
43	1	0	-0.954014	-6.242949	5.282803
44	1	0	-1.754057	-7.708549	4.688149
45	1	0	2.515575	-6.256430	6.952693
46	1	0	1.484230	-7.665964	7.247759
47	1	0	0.756102	-6.087703	6.872416
48	1	0	3.046599	-8.748109	5.436278
49	1	0	2.987990	-8.098923	3.782317
50	1	0	3.794493	-7.181823	5.065579
51	6	0	-0.176465	-4.589057	-1.432189
52	1	0	-0.256693	-3.549865	-1.767831
53	1	0	0.331932	-5.139043	-2.227914
54	1	0	-1.180332	-4.995123	-1.324192
55	6	0	-1.088491	-6.031682	1.123991
56	1	0	-0.921691	-7.109321	1.195461
57	1	0	-1.577814	-5.724892	2.054666

58	1	0	−1.774462	−5.843008	0.300205

4

Thermal correction to Energy=	0.151361
Thermal correction to Enthalpy=	0.152305
Thermal correction to Gibbs Free Energy=	0.101714
Sum of electronic and zero-point Energies=	-1414.192669
Sum of electronic and thermal Energies=	-1414.181684
Sum of electronic and thermal Enthalpies=	-1414.180740
Sum of electronic and thermal Free Energies=	-1414.231331

Esol = -1414.478744

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−1.210561	0.544262	−0.023273
2	6	0	0.184285	0.563755	−0.080155
3	6	0	0.837982	1.791678	−0.078625
4	6	0	−1.125606	2.941432	0.021646
5	6	0	−1.876270	1.770417	0.029414
6	6	0	−1.960512	−0.735746	−0.017691
7	6	0	−1.519556	−1.826467	−0.770625
8	6	0	−2.272341	−2.992380	−0.714920
9	6	0	−3.773289	−2.104847	0.700376
10	6	0	−3.123924	−0.877861	0.742335
11	1	0	0.757200	−0.357495	−0.099666
12	1	0	1.923953	1.828813	−0.114448
13	1	0	−1.624447	3.906789	0.055030
14	1	0	−2.960040	1.819373	0.051455
15	1	0	−0.637358	−1.767845	−1.396262
16	1	0	−3.499506	−0.073133	1.362754
17	7	0	0.207608	2.966799	−0.029861
18	7	0	−3.374333	−3.148318	−0.004046
19	17	0	−5.225221	−2.324499	1.641962
20	17	0	−1.756916	−4.375092	−1.645424

5a-Int

Thermal correction to Energy=	0.307546
Thermal correction to Enthalpy=	0.308490
Thermal correction to Gibbs Free Energy=	0.244663
Sum of electronic and zero-point Energies=	-830.948323

Sum of electronic and thermal Energies=	-830.931419
Sum of electronic and thermal Enthalpies=	-830.930475
Sum of electronic and thermal Free Energies=	-830.994303

Esol = -831.2911279

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.890994	-1.791784	2.476846
2	6	0	0.568326	-0.260268	2.523207
3	5	0	1.611443	-0.781485	0.605524
4	8	0	1.851270	-1.869007	1.393920
5	8	0	0.758076	0.135099	1.141179
6	6	0	-0.851524	0.080273	2.939394
7	1	0	-1.053930	-0.291094	3.948940
8	1	0	-0.981429	1.165614	2.943297
9	1	0	-1.582732	-0.347382	2.251675
10	6	0	-0.310275	-2.635949	2.061515
11	1	0	0.029890	-3.651167	1.842781
12	1	0	-1.058650	-2.684280	2.857130
13	1	0	-0.782717	-2.231763	1.161093
14	6	0	1.526423	-2.348087	3.738546
15	1	0	0.854837	-2.219845	4.593238
16	1	0	1.715737	-3.417315	3.612246
17	1	0	2.475629	-1.856896	3.959195
18	6	0	1.576022	0.531275	3.351725
19	1	0	1.422590	1.597798	3.169563
20	1	0	1.451342	0.340080	4.421066
21	1	0	2.603224	0.280242	3.069805
22	6	0	2.417499	1.164536	-3.758384
23	6	0	2.824902	0.442120	-2.634451
24	6	0	4.166423	0.090710	-2.471234
25	6	0	5.097394	0.464676	-3.434863
26	6	0	4.691005	1.186563	-4.555031
27	6	0	3.351085	1.536858	-4.717120
28	1	0	1.369279	1.424547	-3.861168
29	1	0	4.471229	-0.472427	-1.596496
30	1	0	6.140579	0.192573	-3.312039
31	1	0	5.420396	1.477157	-5.304704
32	1	0	3.036992	2.098946	-5.590448
33	6	0	1.785790	0.071605	-1.634865
34	8	0	0.617030	0.342312	-1.738296
35	8	0	2.286208	-0.644750	-0.598042

5b

Thermal correction to Energy=	0.289623
Thermal correction to Enthalpy=	0.290567
Thermal correction to Gibbs Free Energy=	0.234754
Sum of electronic and zero-point Energies=	-642.417982
Sum of electronic and thermal Energies=	-642.403809
Sum of electronic and thermal Enthalpies=	-642.402864
Sum of electronic and thermal Free Energies=	-642.458678

Esol = -642.679169

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	−6.662502	−1.826166	2.940924
2	8	0	−7.369761	−2.876814	2.413591
3	8	0	−5.840388	−1.218128	2.026298
4	6	0	−4.932741	−1.835329	−0.124197
5	1	0	−5.149120	−2.320847	−1.081172
6	1	0	−4.566045	−0.826190	−0.330253
7	1	0	−4.139714	−2.389571	0.380739
8	6	0	−5.769145	−4.236900	1.277000
9	1	0	−5.344190	−4.541561	0.316590
10	1	0	−4.956462	−3.905673	1.930487
11	1	0	−6.243654	−5.106993	1.737774
12	6	0	−6.815284	−3.138782	1.103339
13	6	0	−6.186853	−1.756477	0.729190
14	6	0	−7.927400	−3.604883	0.179575
15	1	0	−7.552956	−3.725221	−0.842030
16	1	0	−8.304604	−4.573110	0.519445
17	1	0	−8.760161	−2.899619	0.168660
18	6	0	−7.197445	−0.796035	0.107337
19	1	0	−6.757373	0.203662	0.069788
20	1	0	−7.463536	−1.096446	−0.909908
21	1	0	−8.110771	−0.744374	0.707603
22	6	0	−7.686463	−1.671101	6.656749
23	6	0	−7.581029	−2.076899	5.329822
24	6	0	−6.082848	−0.244743	4.882465
25	6	0	−6.182488	0.165300	6.208474
26	1	0	−8.311501	−2.226384	7.349371
27	1	0	−8.124573	−2.952439	4.984676
28	6	0	−6.985738	−0.549051	7.095766

29	1	0	−7.065775	−0.230802	8.130971
30	6	0	−6.779147	−1.370522	4.424078
31	1	0	−5.637569	1.039217	6.552062
32	1	0	−5.458763	0.310765	4.187463

TS1

Thermal correction to Energy=	0.468597
Thermal correction to Enthalpy=	0.469541
Thermal correction to Gibbs Free Energy=	0.392395
Sum of electronic and zero-point Energies=	-1085.927576
Sum of electronic and thermal Energies=	-1085.903296
Sum of electronic and thermal Enthalpies=	-1085.902351
Sum of electronic and thermal Free Energies=	-1085.979498

Esol = -1086.355605

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.818467	−4.135586	3.433908
2	5	0	1.811518	−4.316980	1.532129
3	7	0	1.681276	−2.568501	3.700031
4	8	0	2.841339	−4.965237	0.904016
5	8	0	0.681597	−4.234433	0.761082
6	8	0	2.993856	−4.688167	3.998269
7	8	0	0.671157	−4.914204	3.771656
8	6	0	0.473683	−1.995293	3.936140
9	6	0	2.208047	−2.448414	2.430098
10	6	0	2.429590	−5.206178	−0.466084
11	6	0	0.870186	−5.117930	−0.370304
12	6	0	2.626455	−5.965806	4.533293
13	6	0	1.106703	−5.769512	4.845484
14	6	0	−0.092614	−1.125398	3.048560
15	1	0	0.003190	−2.253645	4.879077
16	6	0	1.589832	−1.488476	1.529684
17	1	0	3.276104	−2.643317	2.334981
18	6	0	2.967669	−6.556512	−0.906941
19	6	0	3.040531	−4.087423	−1.304571
20	6	0	0.189870	−4.509067	−1.584955
21	6	0	0.213930	−6.446297	−0.004437
22	6	0	3.489465	−6.242684	5.755614
23	6	0	2.869399	−7.036261	3.469803

24	6	0	0.278865	−7.043398	4.815139
25	6	0	0.882341	−5.017585	6.158737
26	7	0	0.499969	−0.859145	1.840398
27	1	0	−1.014367	−0.602654	3.269810
28	1	0	2.049136	−1.292898	0.563858
29	1	0	4.060103	−6.524669	−0.934364
30	1	0	2.608294	−6.805845	−1.910493
31	1	0	2.667916	−7.349028	−0.218679
32	1	0	2.829572	−4.220082	−2.369300
33	1	0	2.655994	−3.110669	−0.994395
34	1	0	4.124211	−4.089576	−1.162196
35	1	0	−0.891083	−4.485660	−1.424421
36	1	0	0.389243	−5.108125	−2.479342
37	1	0	0.528447	−3.486687	−1.762627
38	1	0	0.261097	−7.159205	−0.832485
39	1	0	0.690267	−6.894730	0.872646
40	1	0	−0.835112	−6.263509	0.240672
41	1	0	4.528887	−6.382747	5.445438
42	1	0	3.161882	−7.153962	6.267161
43	1	0	3.456202	−5.409648	6.460164
44	1	0	2.715796	−8.043165	3.870084
45	1	0	2.210140	−6.892601	2.609968
46	1	0	3.899842	−6.951405	3.115114
47	1	0	−0.763619	−6.812700	5.052048
48	1	0	0.645512	−7.762507	5.555192
49	1	0	0.306934	−7.508255	3.827685
50	1	0	1.113551	−5.638922	7.029287
51	1	0	1.503193	−4.116442	6.200089
52	1	0	−0.168967	−4.721664	6.219119

Int1

Thermal correction to Energy=	0.472638
Thermal correction to Enthalpy=	0.473582
Thermal correction to Gibbs Free Energy=	0.395295
Sum of electronic and zero-point Energies=	-1086.049316
Sum of electronic and thermal Energies=	-1086.025005
Sum of electronic and thermal Enthalpies=	-1086.024061
Sum of electronic and thermal Free Energies=	-1086.102349

Esol = -1086.481395

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	5	0	1.353985	-4.340137	4.206413
2	5	0	1.448864	-3.537454	1.047656
3	7	0	0.651152	-3.388532	3.417904
4	8	0	1.327844	-4.899632	1.091210
5	8	0	1.665790	-3.043971	-0.207573
6	8	0	2.727838	-4.379254	4.265636
7	8	0	0.735373	-5.308444	4.961251
8	6	0	-0.726845	-3.416327	3.267696
9	6	0	1.351105	-2.642146	2.358938
10	6	0	1.677937	-5.390904	-0.226627
11	6	0	1.414701	-4.138122	-1.125891
12	6	0	3.055730	-5.639741	4.892153
13	6	0	1.778086	-5.925727	5.749956
14	6	0	-1.354437	-2.454048	2.563829
15	1	0	-1.253952	-4.216427	3.776688
16	6	0	0.597394	-1.350802	2.113346
17	1	0	2.364914	-2.414436	2.704304
18	6	0	0.811997	-6.597448	-0.544850
19	6	0	3.150471	-5.787275	-0.176955
20	6	0	2.340635	-4.002448	-2.321652
21	6	0	-0.044568	-4.015329	-1.556211
22	6	0	4.335726	-5.477117	5.692929
23	6	0	3.248941	-6.653066	3.766015
24	6	0	1.450333	-7.397823	5.929516
25	6	0	1.803132	-5.211741	7.098749
26	7	0	-0.675496	-1.287752	2.158142
27	1	0	-2.427713	-2.462554	2.424984
28	1	0	1.158588	-0.446045	1.880087
29	1	0	1.060608	-7.415635	0.136707
30	1	0	0.992249	-6.940352	-1.568680
31	1	0	-0.248880	-6.369127	-0.430557
32	1	0	3.482320	-6.208739	-1.129825
33	1	0	3.782215	-4.927096	0.065014
34	1	0	3.288272	-6.542935	0.600530
35	1	0	2.082431	-3.100982	-2.883465
36	1	0	2.232030	-4.862712	-2.989815
37	1	0	3.384814	-3.925179	-2.013454
38	1	0	-0.308430	-4.771924	-2.300370
39	1	0	-0.715677	-4.115132	-0.697310
40	1	0	-0.200734	-3.026603	-1.994571
41	1	0	5.170245	-5.279995	5.014600
42	1	0	4.559658	-6.392199	6.250399

43	1	0	4.264043	-4.645076	6.395562
44	1	0	3.554292	-7.630410	4.150153
45	1	0	2.328694	-6.768220	3.184427
46	1	0	4.030087	-6.282916	3.096591
47	1	0	0.547909	-7.500973	6.538070
48	1	0	2.267724	-7.914217	6.442861
49	1	0	1.272018	-7.885521	4.969525
50	1	0	2.522503	-5.669892	7.783206
51	1	0	2.058776	-4.154706	6.977975
52	1	0	0.809033	-5.273039	7.548736

TS2

Thermal correction to Energy=	0.470231
Thermal correction to Enthalpy=	0.471175
Thermal correction to Gibbs Free Energy=	0.392903
Sum of electronic and zero-point Energies=	-1086.008932
Sum of electronic and thermal Energies=	-1085.984687
Sum of electronic and thermal Enthalpies=	-1085.983743
Sum of electronic and thermal Free Energies=	-1086.062015

Esol = -1086.438792

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	2.006074	-5.244972	3.111437
2	5	0	1.804313	-5.335338	1.419709
3	7	0	0.980316	-3.460205	3.083338
4	8	0	0.822969	-6.064609	0.785227
5	8	0	2.503167	-4.541714	0.528537
6	8	0	3.234630	-4.905915	3.692777
7	8	0	1.214328	-5.973968	4.017460
8	6	0	-0.334102	-3.443969	3.291682
9	6	0	1.574202	-2.350433	2.650558
10	6	0	1.004130	-5.903602	-0.638245
11	6	0	1.776218	-4.550937	-0.718688
12	6	0	3.125429	-5.147365	5.104661
13	6	0	2.021997	-6.254152	5.170929
14	6	0	-1.067305	-2.282364	3.058869
15	1	0	-0.778588	-4.371373	3.642600
16	6	0	0.827907	-1.195087	2.431985
17	1	0	2.644296	-2.408044	2.473774
18	6	0	-0.357683	-5.905649	-1.313182

19	6	0	1.836933	−7.089816	−1.119433
20	6	0	2.759196	−4.441145	−1.872071
21	6	0	0.845988	−3.338502	−0.694699
22	6	0	2.705075	−3.847741	5.793980
23	6	0	4.488643	−5.578196	5.627177
24	6	0	2.592560	−7.660483	4.983597
25	6	0	1.149018	−6.209125	6.416142
26	7	0	−0.490551	−1.159061	2.629730
27	1	0	−2.140793	−2.260974	3.222144
28	1	0	1.305226	−0.283408	2.084637
29	1	0	−0.820213	−6.890110	−1.201919
30	1	0	−0.259745	−5.694776	−2.383154
31	1	0	−1.025169	−5.165268	−0.868370
32	1	0	1.961433	−7.081095	−2.206154
33	1	0	2.826298	−7.087865	−0.652521
34	1	0	1.328672	−8.015022	−0.835928
35	1	0	3.252494	−3.465661	−1.843415
36	1	0	2.240665	−4.532013	−2.832171
37	1	0	3.529247	−5.212334	−1.813671
38	1	0	0.288738	−3.236107	−1.630350
39	1	0	0.129623	−3.409751	0.131637
40	1	0	1.445890	−2.435554	−0.550567
41	1	0	3.403995	−3.056434	5.507262
42	1	0	2.729481	−3.949554	6.883333
43	1	0	1.699372	−3.539662	5.499919
44	1	0	4.427767	−5.876795	6.679051
45	1	0	4.890719	−6.410556	5.047028
46	1	0	5.190650	−4.742707	5.551792
47	1	0	1.763881	−8.357353	4.832826
48	1	0	3.169562	−7.988707	5.853373
49	1	0	3.234956	−7.701896	4.098999
50	1	0	1.749887	−6.348599	7.321041
51	1	0	0.613612	−5.260502	6.493976
52	1	0	0.409308	−7.013670	6.373326

Int2

Thermal correction to Energy=	0.471319
Thermal correction to Enthalpy=	0.472264
Thermal correction to Gibbs Free Energy=	0.391753
Sum of electronic and zero-point Energies=	-1086.010754
Sum of electronic and thermal Energies=	-1085.986093
Sum of electronic and thermal Enthalpies=	-1085.985149
Sum of electronic and thermal Free Energies=	-1086.065660

Esol = -1086.4426

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.524085	-4.685993	3.149090
2	5	0	1.429377	-4.980692	1.453074
3	7	0	0.829523	-3.140537	3.336885
4	8	0	1.553121	-6.225300	0.869376
5	8	0	1.341724	-3.985179	0.494688
6	8	0	2.872351	-4.529384	3.663012
7	8	0	0.813021	-5.576492	4.024924
8	6	0	-0.465038	-3.012350	3.630259
9	6	0	1.556233	-2.049341	3.093551
10	6	0	1.828090	-6.027774	-0.532762
11	6	0	1.207353	-4.620438	-0.794870
12	6	0	3.056051	-5.547833	4.645391
13	6	0	1.610926	-5.746620	5.199451
14	6	0	-1.037945	-1.746634	3.681586
15	1	0	-1.003430	-3.932633	3.829044
16	6	0	0.956184	-0.796058	3.149562
17	1	0	2.605121	-2.208026	2.870074
18	6	0	1.203197	-7.161589	-1.328771
19	6	0	3.347711	-6.042806	-0.690304
20	6	0	1.930513	-3.786154	-1.839537
21	6	0	-0.286700	-4.681606	-1.106761
22	6	0	4.072206	-5.072273	5.673606
23	6	0	3.570927	-6.800860	3.932131
24	6	0	1.334836	-7.128052	5.774988
25	6	0	1.238685	-4.672192	6.225664
26	7	0	-0.334698	-0.639884	3.441764
27	1	0	-2.089120	-1.628790	3.925237
28	1	0	1.536975	0.099900	2.954585
29	1	0	1.698890	-8.102843	-1.075982
30	1	0	1.323304	-6.991920	-2.403916
31	1	0	0.140088	-7.268013	-1.105687
32	1	0	3.648049	-5.963208	-1.739223
33	1	0	3.805851	-5.223002	-0.128613
34	1	0	3.732917	-6.983732	-0.288714
35	1	0	1.427022	-2.821975	-1.953187
36	1	0	1.921102	-4.290347	-2.811448
37	1	0	2.966454	-3.597171	-1.552389
38	1	0	-0.475583	-5.091630	-2.103156

39	1	0	−0.813805	−5.294700	−0.369662
40	1	0	−0.697685	−3.669308	−1.065748
41	1	0	5.052959	−4.968441	5.200083
42	1	0	4.166994	−5.791530	6.494303
43	1	0	3.792974	−4.101072	6.087704
44	1	0	3.811585	−7.606392	4.633064
45	1	0	2.830567	−7.161939	3.211720
46	1	0	4.479093	−6.538819	3.381349
47	1	0	0.311523	−7.171152	6.160329
48	1	0	2.017971	−7.354660	6.600750
49	1	0	1.439256	−7.897380	5.007718
50	1	0	1.736286	−4.839987	7.186075
51	1	0	1.509187	−3.673213	5.870537
52	1	0	0.157448	−4.700258	6.393105

TS3

Thermal correction to Energy=	0.554695
Thermal correction to Enthalpy=	0.555639
Thermal correction to Gibbs Free Energy=	0.466534
Sum of electronic and zero-point Energies=	-1350.155790
Sum of electronic and thermal Energies=	-1350.126493
Sum of electronic and thermal Enthalpies=	-1350.125548
Sum of electronic and thermal Free Energies=	-1350.214653

Esol = -1350.67713

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.739623	−4.369131	1.639162
2	5	0	1.531098	−4.414824	−0.074827
3	7	0	0.051348	−3.129875	2.020234
4	8	0	0.288175	−4.906422	−0.641631
5	8	0	2.616613	−5.117079	−0.718234
6	8	0	2.755027	−3.606610	2.252864
7	8	0	1.467425	−5.512903	2.412328
8	6	0	−1.159099	−3.557006	1.664707
9	6	0	0.235138	−1.817093	2.158325
10	6	0	0.605655	−6.076028	−1.396707
11	6	0	2.077397	−5.805575	−1.844874
12	6	0	2.996862	−4.164109	3.556614
13	6	0	2.523233	−5.640414	3.373113
14	6	0	−2.194218	−2.649849	1.441266

15	1	0	-1.279746	-4.626528	1.527010
16	6	0	-0.806231	-0.921465	1.930483
17	1	0	1.237505	-1.496654	2.431624
18	6	0	-0.389578	-6.218366	-2.539503
19	6	0	0.506859	-7.278028	-0.455094
20	6	0	2.905564	-7.060012	-2.086731
21	6	0	2.150529	-4.893897	-3.073847
22	6	0	2.150213	-3.404583	4.578089
23	6	0	4.473655	-4.004419	3.885629
24	6	0	3.600666	-6.520737	2.736251
25	6	0	1.982009	-6.298697	4.632927
26	7	0	-2.022236	-1.333358	1.566332
27	1	0	-3.180618	-2.997468	1.147617
28	1	0	-0.651589	0.149004	2.034212
29	1	0	-1.389481	-6.405115	-2.136158
30	1	0	-0.125323	-7.059783	-3.189136
31	1	0	-0.433598	-5.309989	-3.144929
32	1	0	0.684164	-8.225680	-0.973400
33	1	0	1.218757	-7.171663	0.368677
34	1	0	-0.499311	-7.303943	-0.025659
35	1	0	3.908672	-6.780869	-2.423489
36	1	0	2.452480	-7.692607	-2.857925
37	1	0	3.007781	-7.640037	-1.167278
38	1	0	1.877841	-5.424336	-3.991926
39	1	0	1.488608	-4.029179	-2.969400
40	1	0	3.176392	-4.528304	-3.178594
41	1	0	2.391140	-2.338603	4.519765
42	1	0	2.356515	-3.741992	5.598457
43	1	0	1.083376	-3.532885	4.376949
44	1	0	4.724387	-4.515207	4.821384
45	1	0	5.101037	-4.405171	3.087179
46	1	0	4.712150	-2.943261	4.005489
47	1	0	3.154073	-7.483853	2.473039
48	1	0	4.439624	-6.704158	3.414605
49	1	0	3.974206	-6.060784	1.815945
50	1	0	2.749126	-6.342785	5.413566
51	1	0	1.114491	-5.761870	5.021679
52	1	0	1.672011	-7.322437	4.404802
53	6	0	0.581749	-0.778201	-1.278253
54	6	0	0.521969	-2.147579	-1.037212
55	7	0	1.603184	-2.790469	-0.590942
56	6	0	2.735536	-2.107580	-0.401734
57	6	0	2.768694	-0.742754	-0.662598
58	7	0	1.696834	-0.073191	-1.091021

59	1	0	−0.297633	−0.244032	−1.625248
60	1	0	−0.365015	−2.755335	−1.182857
61	1	0	3.579847	−2.670883	−0.020622
62	1	0	3.684283	−0.178702	−0.515251

Int3

Thermal correction to Energy=	0.555676
Thermal correction to Enthalpy=	0.556620
Thermal correction to Gibbs Free Energy=	0.468477
Sum of electronic and zero-point Energies=	-1350.159487
Sum of electronic and thermal Energies=	-1350.130108
Sum of electronic and thermal Enthalpies=	-1350.129163
Sum of electronic and thermal Free Energies=	-1350.217307

Esol = -1350.67861

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.502582	−4.176766	1.604976
2	5	0	1.537228	−4.428118	−0.136035
3	7	0	0.093657	−3.311357	1.818320
4	8	0	0.299386	−4.819965	−0.791901
5	8	0	2.574671	−5.332030	−0.567991
6	8	0	2.591721	−3.403674	2.161001
7	8	0	1.347151	−5.373500	2.411786
8	6	0	−1.078785	−3.950187	1.727101
9	6	0	0.101797	−1.973905	1.861745
10	6	0	0.536605	−6.090082	−1.401070
11	6	0	2.070549	−6.048861	−1.693355
12	6	0	2.902320	−3.966948	3.437928
13	6	0	2.495943	−5.464588	3.249574
14	6	0	−2.258564	−3.218915	1.671660
15	1	0	−1.033632	−5.032155	1.694865
16	6	0	−1.096141	−1.271961	1.803294
17	1	0	1.077671	−1.507453	1.949749
18	6	0	−0.340934	−6.224957	−2.637319
19	6	0	0.180750	−7.169606	−0.376331
20	6	0	2.744286	−7.412879	−1.740622
21	6	0	2.391199	−5.266846	−2.971508
22	6	0	2.051900	−3.274559	4.507102
23	6	0	4.379510	−3.738555	3.723141
24	6	0	3.569297	−6.260661	2.503354

25	6	0	2.116551	-6.181866	4.538207
26	7	0	-2.276117	-1.885093	1.704177
27	1	0	-3.214102	-3.728669	1.599231
28	1	0	-1.096644	-0.186749	1.840446
29	1	0	-1.394213	-6.244691	-2.341412
30	1	0	-0.123725	-7.154564	-3.174546
31	1	0	-0.198050	-5.384405	-3.320046
32	1	0	0.303180	-8.180220	-0.778579
33	1	0	0.797435	-7.054229	0.521123
34	1	0	-0.868699	-7.045788	-0.089461
35	1	0	3.805757	-7.291995	-1.977631
36	1	0	2.295345	-8.051349	-2.509399
37	1	0	2.669858	-7.915594	-0.774305
38	1	0	2.143713	-5.837732	-3.872232
39	1	0	1.844627	-4.319519	-3.005804
40	1	0	3.462643	-5.045600	-2.987956
41	1	0	2.207029	-2.193092	4.440347
42	1	0	2.327303	-3.595888	5.516553
43	1	0	0.987899	-3.483006	4.359262
44	1	0	4.690839	-4.256981	4.636384
45	1	0	4.994900	-4.090280	2.892469
46	1	0	4.570026	-2.669354	3.859318
47	1	0	3.157122	-7.241164	2.246173
48	1	0	4.465982	-6.414352	3.112686
49	1	0	3.837655	-5.761023	1.568484
50	1	0	2.952296	-6.190403	5.246586
51	1	0	1.254693	-5.711639	5.016463
52	1	0	1.853069	-7.219815	4.314377
53	6	0	1.234339	-0.776023	-1.498538
54	6	0	0.937919	-2.102696	-1.204826
55	7	0	1.897295	-2.911970	-0.741002
56	6	0	3.134714	-2.426756	-0.580853
57	6	0	3.398876	-1.099285	-0.890400
58	7	0	2.456455	-0.268229	-1.342211
59	1	0	0.460571	-0.112763	-1.873380
60	1	0	-0.040721	-2.552496	-1.336634
61	1	0	3.873102	-3.118733	-0.194554
62	1	0	4.400449	-0.698994	-0.769055

TS4

Thermal correction to Energy=	0.554988
Thermal correction to Enthalpy=	0.555933
Thermal correction to Gibbs Free Energy=	0.471073

Sum of electronic and zero-point Energies=	-1350.152493
Sum of electronic and thermal Energies=	-1350.123947
Sum of electronic and thermal Enthalpies=	-1350.123003
Sum of electronic and thermal Free Energies=	-1350.207863

Esol = -1350.669004

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.430977	-4.038371	1.770286
2	5	0	1.493619	-4.207156	-0.284281
3	7	0	0.117350	-3.292849	1.802754
4	8	0	0.271632	-4.648229	-0.846703
5	8	0	2.534364	-5.132981	-0.534694
6	8	0	2.569914	-3.334878	2.224251
7	8	0	1.379162	-5.339131	2.331161
8	6	0	-1.068316	-3.957142	1.634339
9	6	0	0.076779	-1.934588	1.803843
10	6	0	0.509233	-5.970852	-1.361722
11	6	0	2.055099	-5.966507	-1.603644
12	6	0	3.022783	-4.043813	3.391320
13	6	0	2.588455	-5.518102	3.086258
14	6	0	-2.231954	-3.252558	1.463967
15	1	0	-1.012855	-5.037189	1.654117
16	6	0	-1.139618	-1.277724	1.643063
17	1	0	1.013588	-1.425989	1.999345
18	6	0	-0.324969	-6.156508	-2.620245
19	6	0	0.090729	-6.978909	-0.293617
20	6	0	2.720010	-7.328240	-1.497375
21	6	0	2.432236	-5.288439	-2.921925
22	6	0	2.283769	-3.458752	4.595956
23	6	0	4.520972	-3.837948	3.537215
24	6	0	3.602089	-6.262034	2.219797
25	6	0	2.261739	-6.341900	4.324346
26	7	0	-2.296507	-1.902992	1.461674
27	1	0	-3.167124	-3.789601	1.340031
28	1	0	-1.153108	-0.190836	1.665004
29	1	0	-1.387323	-6.146945	-2.360252
30	1	0	-0.101576	-7.116709	-3.097072
31	1	0	-0.145334	-5.355679	-3.340022
32	1	0	0.199384	-8.008631	-0.647679
33	1	0	0.680376	-6.841228	0.617958
34	1	0	-0.964785	-6.816001	-0.053969

35	1	0	3.794994	−7.226756	−1.672830
36	1	0	2.316708	−8.019216	−2.245146
37	1	0	2.576041	−7.759034	−0.504982
38	1	0	2.167502	−5.902453	−3.787835
39	1	0	1.934331	−4.318126	−3.019739
40	1	0	3.512711	−5.120667	−2.934046
41	1	0	2.469754	−2.381743	4.634832
42	1	0	2.622836	−3.901487	5.537032
43	1	0	1.204011	−3.617784	4.507564
44	1	0	4.917670	−4.434461	4.365195
45	1	0	5.047022	−4.114826	2.621458
46	1	0	4.728937	−2.784741	3.747018
47	1	0	3.156887	−7.209625	1.901587
48	1	0	4.515349	−6.485533	2.780318
49	1	0	3.846727	−5.692442	1.321315
50	1	0	3.133650	−6.418799	4.982620
51	1	0	1.432782	−5.907723	4.886325
52	1	0	1.974892	−7.353648	4.023777
53	6	0	1.123464	−0.498514	−0.865784
54	6	0	0.824796	−1.857311	−0.800925
55	7	0	1.813143	−2.754367	−0.548075
56	6	0	3.077634	−2.264039	−0.361065
57	6	0	3.304849	−0.913732	−0.421249
58	7	0	2.338200	−0.002356	−0.671778
59	1	0	0.322633	0.202722	−1.086653
60	1	0	−0.155741	−2.267268	−1.012489
61	1	0	3.846937	−2.999338	−0.170423
62	1	0	4.312489	−0.535591	−0.280890

Int4

Thermal correction to Energy=	0.559222
Thermal correction to Enthalpy=	0.560166
Thermal correction to Gibbs Free Energy=	0.474180
Sum of electronic and zero-point Energies=	-1350.223944
Sum of electronic and thermal Energies=	-1350.195264
Sum of electronic and thermal Enthalpies=	-1350.194320
Sum of electronic and thermal Free Energies=	-1350.280306

Esol = -1350.745885

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	1.156685	-3.895644	2.433534
2	5	0	1.581391	-4.008746	-0.984476
3	7	0	0.070275	-3.241436	1.778073
4	8	0	0.405036	-4.547003	-1.442786
5	8	0	2.651306	-4.872683	-1.040672
6	8	0	2.367574	-3.287572	2.650693
7	8	0	1.075078	-5.174597	2.930818
8	6	0	-1.145867	-3.864215	1.535629
9	6	0	0.189262	-1.874122	1.283537
10	6	0	0.660700	-5.955925	-1.649522
11	6	0	2.211403	-5.984101	-1.860508
12	6	0	3.065090	-4.119822	3.606235
13	6	0	2.412539	-5.523768	3.366855
14	6	0	-2.246762	-3.130714	1.283199
15	1	0	-1.158434	-4.945375	1.617746
16	6	0	-1.115164	-1.153134	1.541566
17	1	0	1.019388	-1.388515	1.803939
18	6	0	-0.148673	-6.431764	-2.843451
19	6	0	0.221662	-6.678110	-0.379388
20	6	0	2.896331	-7.253225	-1.387181
21	6	0	2.616813	-5.661428	-3.296427
22	6	0	2.761574	-3.554892	4.991419
23	6	0	4.554253	-4.052280	3.316595
24	6	0	3.070406	-6.292682	2.225852
25	6	0	2.308473	-6.394082	4.607418
26	7	0	-2.248353	-1.739159	1.467031
27	1	0	-3.202236	-3.593451	1.073710
28	1	0	-1.092095	-0.089683	1.779503
29	1	0	-1.214983	-6.370616	-2.610772
30	1	0	0.089714	-7.474195	-3.077513
31	1	0	0.042890	-5.819287	-3.726100
32	1	0	0.364848	-7.759414	-0.460431
33	1	0	0.772612	-6.311546	0.494181
34	1	0	-0.841988	-6.484422	-0.217879
35	1	0	3.974739	-7.169622	-1.547309
36	1	0	2.533711	-8.115986	-1.954996
37	1	0	2.719498	-7.432833	-0.325848
38	1	0	2.377596	-6.484627	-3.975045
39	1	0	2.114790	-4.757103	-3.653696
40	1	0	3.695414	-5.488073	-3.328037
41	1	0	3.065542	-2.505485	5.017972
42	1	0	3.304506	-4.093516	5.772818
43	1	0	1.690703	-3.605648	5.211290
44	1	0	5.105468	-4.730069	3.976049

45	1	0	4.771681	−4.315699	2.279942
46	1	0	4.914828	−3.035771	3.495100
47	1	0	2.467238	−7.180370	2.012153
48	1	0	4.078773	−6.621835	2.492665
49	1	0	3.125141	−5.683412	1.316665
50	1	0	3.303649	−6.606594	5.010715
51	1	0	1.708285	−5.916182	5.383372
52	1	0	1.836353	−7.345485	4.348457
53	6	0	0.778016	−0.440370	−0.694880
54	6	0	0.506571	−1.859124	−0.245047
55	7	0	1.688838	−2.663441	−0.524709
56	6	0	2.901513	−2.060572	−0.221969
57	6	0	2.988746	−0.718173	−0.152689
58	7	0	1.930789	0.099833	−0.579591
59	1	0	−0.036569	0.149750	−1.114431
60	1	0	−0.345671	−2.290079	−0.777137
61	1	0	3.753632	−2.719256	−0.098162
62	1	0	3.917467	−0.220916	0.094539

TS5

Thermal correction to Energy=	0.558119
Thermal correction to Enthalpy=	0.559063
Thermal correction to Gibbs Free Energy=	0.474176
Sum of electronic and zero-point Energies=	-1350.210688
Sum of electronic and thermal Energies=	-1350.182639
Sum of electronic and thermal Enthalpies=	-1350.181695
Sum of electronic and thermal Free Energies=	-1350.266582

Esol = -1350.733089

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.699622	−3.806938	3.010327
2	5	0	1.206274	−4.613829	−1.399677
3	7	0	0.658507	−3.768627	2.032230
4	8	0	0.033393	−4.437513	−2.086666
5	8	0	1.858579	−5.786640	−1.693767
6	8	0	2.395010	−2.693732	3.404921
7	8	0	2.067563	−4.960207	3.658323
8	6	0	−0.087278	−4.889530	1.701553
9	6	0	0.327336	−2.545329	1.316419
10	6	0	−0.216589	−5.680518	−2.785820

11	6	0	1.218157	-6.300800	-2.885837
12	6	0	3.152182	-3.088501	4.572914
13	6	0	3.280031	-4.638066	4.381114
14	6	0	-1.301241	-4.753460	1.133557
15	1	0	0.336546	-5.849217	1.978750
16	6	0	-1.183693	-2.468116	1.196909
17	1	0	0.694147	-1.704329	1.911782
18	6	0	-0.867610	-5.365456	-4.121604
19	6	0	-1.154522	-6.511644	-1.917182
20	6	0	1.261071	-7.818433	-2.853364
21	6	0	2.008196	-5.768695	-4.078907
22	6	0	2.316648	-2.712304	5.793473
23	6	0	4.472003	-2.337339	4.575514
24	6	0	4.449462	-5.025557	3.481013
25	6	0	3.309181	-5.438400	5.671537
26	7	0	-1.922710	-3.497837	1.047717
27	1	0	-1.901195	-5.611372	0.861323
28	1	0	-1.658680	-1.486996	1.231766
29	1	0	-1.861626	-4.942794	-3.952999
30	1	0	-0.981497	-6.276740	-4.717264
31	1	0	-0.281604	-4.642424	-4.691592
32	1	0	-1.449819	-7.435303	-2.423087
33	1	0	-0.680746	-6.765701	-0.964693
34	1	0	-2.052636	-5.925168	-1.706989
35	1	0	2.297731	-8.157233	-2.929840
36	1	0	0.703851	-8.236033	-3.697857
37	1	0	0.841391	-8.210931	-1.925730
38	1	0	1.625289	-6.165465	-5.023150
39	1	0	1.972103	-4.675648	-4.119098
40	1	0	3.053119	-6.071270	-3.973806
41	1	0	2.091893	-1.643618	5.750634
42	1	0	2.851757	-2.916971	6.724886
43	1	0	1.369808	-3.260745	5.806139
44	1	0	5.109296	-2.681515	5.396335
45	1	0	5.006215	-2.468981	3.632918
46	1	0	4.285021	-1.269168	4.713401
47	1	0	4.357082	-6.082335	3.217124
48	1	0	5.410069	-4.874519	3.981134
49	1	0	4.435266	-4.438072	2.557956
50	1	0	4.169791	-5.148884	6.282830
51	1	0	2.397758	-5.291913	6.253646
52	1	0	3.399342	-6.503194	5.440447
53	6	0	1.947933	-1.265270	-0.169922
54	6	0	0.996177	-2.447304	-0.121434

55	7	0	1.743438	-3.636814	-0.504786
56	6	0	3.030783	-3.738031	0.004259
57	6	0	3.685882	-2.635267	0.415764
58	7	0	3.180770	-1.354082	0.147626
59	1	0	1.559069	-0.295382	-0.482348
60	1	0	0.196326	-2.308569	-0.854255
61	1	0	3.478207	-4.726525	-0.007473
62	1	0	4.684166	-2.687009	0.831519

Int5

Thermal correction to Energy=	0.558909
Thermal correction to Enthalpy=	0.559854
Thermal correction to Gibbs Free Energy=	0.472923
Sum of electronic and zero-point Energies=	-1350.224088
Sum of electronic and thermal Energies=	-1350.195315
Sum of electronic and thermal Enthalpies=	-1350.194371
Sum of electronic and thermal Free Energies=	-1350.281302

Esol = -1350.746168

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.020807	-3.797008	2.583089
2	5	0	-1.506156	-1.734337	-1.660841
3	7	0	-0.101615	-3.160152	1.969944
4	8	0	-1.391375	-0.366319	-1.705772
5	8	0	-2.628194	-2.224985	-2.278889
6	8	0	2.242502	-3.182865	2.707188
7	8	0	0.969135	-5.061259	3.113694
8	6	0	-1.336794	-3.784906	1.885769
9	6	0	0.045533	-1.869695	1.298137
10	6	0	-2.652787	0.127031	-2.219504
11	6	0	-3.200320	-1.113289	-3.007384
12	6	0	3.041551	-4.045158	3.552160
13	6	0	2.345023	-5.436993	3.368777
14	6	0	-2.441240	-3.094882	1.552271
15	1	0	-1.352045	-4.837575	2.146675
16	6	0	-1.270017	-1.127137	1.351633
17	1	0	0.824783	-1.300158	1.815801
18	6	0	-2.382862	1.350939	-3.078423
19	6	0	-3.517403	0.498256	-1.018397
20	6	0	-4.712596	-1.251288	-3.000306

21	6	0	-2.660589	-1.193986	-4.433063
22	6	0	2.923395	-3.506750	4.975088
23	6	0	4.481961	-3.991390	3.073753
24	6	0	2.837511	-6.187543	2.134606
25	6	0	2.387609	-6.333024	4.594431
26	7	0	-2.411465	-1.699714	1.402984
27	1	0	-3.410125	-3.570067	1.476896
28	1	0	-1.238972	-0.038936	1.287653
29	1	0	-2.000268	2.160365	-2.450950
30	1	0	-3.306428	1.697275	-3.553095
31	1	0	-1.644427	1.142801	-3.854543
32	1	0	-4.475398	0.920161	-1.335515
33	1	0	-3.698705	-0.365304	-0.372258
34	1	0	-2.991402	1.254024	-0.427954
35	1	0	-5.001979	-2.138823	-3.569463
36	1	0	-5.180099	-0.379149	-3.468368
37	1	0	-5.096716	-1.355488	-1.984221
38	1	0	-3.096591	-0.421738	-5.072744
39	1	0	-1.571571	-1.086989	-4.447999
40	1	0	-2.912066	-2.172358	-4.850295
41	1	0	3.241196	-2.461011	4.984903
42	1	0	3.554964	-4.067264	5.669837
43	1	0	1.888565	-3.552852	5.327642
44	1	0	5.099045	-4.706182	3.627355
45	1	0	4.551955	-4.214682	2.007483
46	1	0	4.887684	-2.990131	3.242714
47	1	0	2.177042	-7.041131	1.958738
48	1	0	3.854992	-6.563259	2.276008
49	1	0	2.813384	-5.548834	1.245481
50	1	0	3.423079	-6.562062	4.865687
51	1	0	1.893388	-5.868466	5.449441
52	1	0	1.878135	-7.275253	4.375669
53	6	0	1.761293	-2.855057	-0.270257
54	6	0	0.515221	-2.003204	-0.191865
55	7	0	-0.514264	-2.571131	-1.061087
56	6	0	-0.542199	-3.952003	-1.191730
57	6	0	0.529119	-4.699308	-0.872772
58	7	0	1.753646	-4.107603	-0.522692
59	1	0	2.715129	-2.377121	-0.047157
60	1	0	0.732725	-0.986422	-0.535634
61	1	0	-1.453475	-4.370122	-1.605090
62	1	0	0.521236	-5.777470	-0.964260

TS6

Thermal correction to Energy=	0.556093
Thermal correction to Enthalpy=	0.557038
Thermal correction to Gibbs Free Energy=	0.471307
Sum of electronic and zero-point Energies=	-1350.189988
Sum of electronic and thermal Energies=	-1350.161431
Sum of electronic and thermal Enthalpies=	-1350.160487
Sum of electronic and thermal Free Energies=	-1350.246217

Esol = -1350.713192

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.094909	-3.804056	2.608592
2	5	0	-1.524842	-1.690002	-1.738816
3	7	0	-0.056306	-3.118562	2.078811
4	8	0	-1.404747	-0.328349	-1.867635
5	8	0	-2.663130	-2.219443	-2.291387
6	8	0	2.288378	-3.165526	2.838824
7	8	0	1.035981	-5.092714	3.073681
8	6	0	-1.244608	-3.791395	1.799888
9	6	0	0.009569	-1.779650	1.671837
10	6	0	-2.689579	0.139204	-2.346527
11	6	0	-3.277515	-1.142669	-3.037318
12	6	0	3.053094	-4.049469	3.692593
13	6	0	2.395729	-5.449748	3.422500
14	6	0	-2.286262	-3.145560	1.229880
15	1	0	-1.274744	-4.834357	2.089690
16	6	0	-1.158318	-1.158918	1.228493
17	1	0	0.861032	-1.217258	2.032474
18	6	0	-2.457902	1.310443	-3.286905
19	6	0	-3.494768	0.583744	-1.128962
20	6	0	-4.786690	-1.278887	-2.934706
21	6	0	-2.822211	-1.295868	-4.486517
22	6	0	2.847088	-3.563379	5.124864
23	6	0	4.517407	-3.954775	3.300523
24	6	0	2.996281	-6.170099	2.218855
25	6	0	2.359054	-6.370862	4.630643
26	7	0	-2.260808	-1.805701	0.892917
27	1	0	-3.200496	-3.684111	1.005543
28	1	0	-1.122287	-0.093144	1.008566
29	1	0	-2.041600	2.151294	-2.725645
30	1	0	-3.402625	1.636033	-3.733935

31	1	0	−1.759597	1.054867	−4.085727
32	1	0	−4.469775	0.983343	−1.422538
33	1	0	−3.630969	−0.243382	−0.426897
34	1	0	−2.942965	1.378268	−0.617780
35	1	0	−5.106868	−2.193924	−3.440486
36	1	0	−5.283842	−0.431463	−3.417469
37	1	0	−5.108262	−1.331957	−1.893251
38	1	0	−3.292741	−0.554460	−5.138199
39	1	0	−1.735669	−1.195427	−4.569604
40	1	0	−3.099550	−2.292605	−4.839101
41	1	0	3.152833	−2.515905	5.189020
42	1	0	3.442063	−4.142215	5.836663
43	1	0	1.793754	−3.629110	5.413893
44	1	0	5.116388	−4.672942	3.869476
45	1	0	4.653236	−4.146954	2.234650
46	1	0	4.891624	−2.950990	3.519840
47	1	0	2.376788	−7.042976	1.993226
48	1	0	4.012502	−6.516059	2.429055
49	1	0	3.000786	−5.522082	1.338189
50	1	0	3.374379	−6.593417	4.974075
51	1	0	1.795890	−5.931819	5.456012
52	1	0	1.880573	−7.314268	4.354449
53	6	0	1.708823	−2.771273	−0.203292
54	6	0	0.673613	−1.932667	−0.617416
55	7	0	−0.445183	−2.503113	−1.236414
56	6	0	−0.532817	−3.893094	−1.195106
57	6	0	0.458637	−4.630770	−0.646177
58	7	0	1.602655	−4.084017	−0.099147
59	1	0	2.614517	−2.314368	0.190375
60	1	0	0.823965	−0.875239	−0.791963
61	1	0	−1.416915	−4.323394	−1.648758
62	1	0	0.374507	−5.711788	−0.611448

Int6

Thermal correction to Energy=	0.557559
Thermal correction to Enthalpy=	0.558503
Thermal correction to Gibbs Free Energy=	0.468711
Sum of electronic and zero-point Energies=	-1350.225309
Sum of electronic and thermal Energies=	-1350.195932
Sum of electronic and thermal Enthalpies=	-1350.194988
Sum of electronic and thermal Free Energies=	-1350.284780

Esol = -1350.753089

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.527354	-4.758800	2.219684
2	5	0	-2.286523	-1.341463	-0.064053
3	7	0	0.438570	-3.948326	1.824336
4	8	0	-2.506558	0.002977	0.365658
5	8	0	-3.433154	-1.831181	-0.754880
6	8	0	1.619253	-6.102200	1.917281
7	8	0	2.599604	-4.283178	2.946977
8	6	0	-0.637607	-4.442518	1.045001
9	6	0	0.310897	-2.593666	2.223190
10	6	0	-3.913174	0.234248	0.220630
11	6	0	-4.283196	-0.699840	-0.977658
12	6	0	2.963702	-6.495891	2.267141
13	6	0	3.339423	-5.449531	3.368650
14	6	0	-1.647025	-3.657554	0.655474
15	1	0	-0.610498	-5.502068	0.826196
16	6	0	-0.709689	-1.831242	1.818919
17	1	0	1.066413	-2.234209	2.909656
18	6	0	-4.147507	1.715137	-0.033538
19	6	0	-4.598757	-0.197919	1.517660
20	6	0	-5.729174	-1.171290	-0.990926
21	6	0	-3.921120	-0.075059	-2.326854
22	6	0	3.817254	-6.354388	1.008988
23	6	0	2.946746	-7.939279	2.740144
24	6	0	2.818303	-5.840044	4.749664
25	6	0	4.815785	-5.098301	3.435325
26	7	0	-1.733893	-2.289953	0.971431
27	1	0	-2.477378	-4.057736	0.084600
28	1	0	-0.809041	-0.805300	2.155060
29	1	0	-3.872561	2.288939	0.856290
30	1	0	-5.202535	1.912543	-0.250886
31	1	0	-3.542817	2.074649	-0.868717
32	1	0	-5.670443	0.023227	1.507706
33	1	0	-4.456318	-1.268833	1.689604
34	1	0	-4.141804	0.343021	2.351070
35	1	0	-5.904020	-1.801491	-1.868028
36	1	0	-6.417949	-0.321367	-1.041230
37	1	0	-5.957749	-1.759448	-0.100264
38	1	0	-4.612617	0.727277	-2.601629
39	1	0	-2.905871	0.333005	-2.311721
40	1	0	-3.970311	-0.849173	-3.098489

41	1	0	3.370707	−6.953095	0.210970
42	1	0	4.839983	−6.704812	1.174181
43	1	0	3.853772	−5.312792	0.675472
44	1	0	3.935330	−8.237238	3.103933
45	1	0	2.217446	−8.088329	3.538248
46	1	0	2.679536	−8.595171	1.907097
47	1	0	2.919478	−4.982804	5.420146
48	1	0	3.381166	−6.677894	5.170611
49	1	0	1.760306	−6.115982	4.705333
50	1	0	5.413779	−5.987370	3.659725
51	1	0	5.165154	−4.666062	2.496049
52	1	0	4.983277	−4.366909	4.230682
53	6	0	1.194764	−0.571459	−1.671757
54	6	0	0.015070	−0.427189	−0.952505
55	7	0	−1.003439	−1.269505	−1.166219
56	6	0	−0.857865	−2.240439	−2.076484
57	6	0	0.334595	−2.357278	−2.779047
58	7	0	1.362734	−1.530434	−2.583270
59	1	0	2.021820	0.111897	−1.506521
60	1	0	−0.149873	0.354297	−0.219625
61	1	0	−1.711758	−2.890610	−2.228352
62	1	0	0.455900	−3.138634	−3.522780

TS7

Thermal correction to Energy=	0.556429
Thermal correction to Enthalpy=	0.557373
Thermal correction to Gibbs Free Energy=	0.465753
Sum of electronic and zero-point Energies=	-1350.223396
Sum of electronic and thermal Energies=	-1350.193925
Sum of electronic and thermal Enthalpies=	-1350.192981
Sum of electronic and thermal Free Energies=	-1350.284602

Esol = -1350.754055

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.107925	−6.151288	4.167806
2	5	0	−2.985521	−2.864780	2.121489
3	7	0	−0.008903	−5.371424	3.788631
4	8	0	−3.140648	−1.521840	2.475125
5	8	0	−4.045515	−3.345345	1.355525
6	8	0	1.240090	−7.487239	3.849634

7	8	0	2.168181	-5.649590	4.894192
8	6	0	-1.068838	-5.888392	3.003243
9	6	0	-0.172138	-4.024179	4.198068
10	6	0	-4.498083	-1.181621	2.135539
11	6	0	-4.833086	-2.197361	0.989765
12	6	0	2.599793	-7.840808	4.184328
13	6	0	2.949803	-6.795806	5.295605
14	6	0	-2.102982	-5.136116	2.621731
15	1	0	-1.001965	-6.940273	2.758391
16	6	0	-1.212261	-3.284662	3.809087
17	1	0	0.584727	-3.643719	4.871234
18	6	0	-4.554522	0.280245	1.723768
19	6	0	-5.345538	-1.414451	3.385821
20	6	0	-6.294018	-2.616439	0.925985
21	6	0	-4.373281	-1.708037	-0.383277
22	6	0	3.437822	-7.656265	2.921445
23	6	0	2.633463	-9.289369	4.640138
24	6	0	2.453233	-7.219778	6.675799
25	6	0	4.414236	-6.396661	5.354834
26	7	0	-2.228003	-3.774182	2.963110
27	1	0	-2.916971	-5.550699	2.039541
28	1	0	-1.335482	-2.262412	4.145213
29	1	0	-4.310534	0.912415	2.582230
30	1	0	-5.558671	0.548590	1.379567
31	1	0	-3.839941	0.496798	0.927302
32	1	0	-6.386982	-1.115920	3.234592
33	1	0	-5.319780	-2.467783	3.681089
34	1	0	-4.930723	-0.822152	4.205712
35	1	0	-6.439131	-3.312863	0.095143
36	1	0	-6.940568	-1.748870	0.758164
37	1	0	-6.604278	-3.115905	1.845442
38	1	0	-5.018609	-0.906572	-0.755414
39	1	0	-3.343725	-1.344799	-0.352641
40	1	0	-4.422810	-2.542898	-1.088461
41	1	0	3.005142	-8.260328	2.119845
42	1	0	4.472959	-7.974124	3.074777
43	1	0	3.436717	-6.610319	2.599827
44	1	0	3.634326	-9.559407	4.991918
45	1	0	1.916445	-9.471153	5.442592
46	1	0	2.380280	-9.943748	3.801548
47	1	0	2.531496	-6.367706	7.355872
48	1	0	3.046915	-8.043441	7.082141
49	1	0	1.404642	-7.530213	6.636341
50	1	0	5.042889	-7.268230	5.563566

51	1	0	4.741312	−5.941876	4.418209
52	1	0	4.564208	−5.669774	6.157785
53	6	0	0.793418	−2.017563	0.364595
54	6	0	−0.456226	−1.838141	0.951451
55	7	0	−1.459274	−2.677020	0.691814
56	6	0	−1.220639	−3.692652	−0.138540
57	6	0	0.033774	−3.860482	−0.717858
58	7	0	1.044022	−3.025455	−0.471790
59	1	0	1.607827	−1.330311	0.574901
60	1	0	−0.670430	−1.020349	1.633792
61	1	0	−2.048148	−4.368022	−0.336067
62	1	0	0.224292	−4.686750	−1.396664

TS8

Thermal correction to Energy=	0.555586
Thermal correction to Enthalpy=	0.556530
Thermal correction to Gibbs Free Energy=	0.468110
Sum of electronic and zero-point Energies=	-1350.176290
Sum of electronic and thermal Energies=	-1350.147156
Sum of electronic and thermal Enthalpies=	-1350.146211
Sum of electronic and thermal Free Energies=	-1350.234631

Esol = -1350.702411

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.335310	2.258331	−3.035215
2	6	0	−0.641903	3.615730	−1.501654
3	6	0	−0.069469	1.142892	−2.388012
4	1	0	0.915153	2.159509	−3.947279
5	6	0	−0.997712	2.522675	−0.706228
6	1	0	−0.894420	4.607968	−1.130505
7	1	0	0.121711	0.142332	−2.749856
8	1	0	−1.637442	2.614470	0.162659
9	7	0	−0.823134	1.234647	−1.212062
10	6	0	2.813392	−1.171576	−0.676686
11	6	0	2.411261	−1.949485	0.626175
12	5	0	1.454173	0.084174	0.621084
13	8	0	2.375555	0.180279	−0.385246
14	8	0	1.277060	−1.187467	1.111311
15	6	0	1.975014	−3.385396	0.398684
16	1	0	2.801754	−3.977542	−0.006161

17	1	0	1.673246	-3.830179	1.351302
18	1	0	1.132108	-3.440455	-0.292103
19	6	0	2.053272	-1.649275	-1.908314
20	1	0	2.235727	-0.946422	-2.725801
21	1	0	2.400224	-2.637752	-2.223516
22	1	0	0.977331	-1.697617	-1.714471
23	6	0	4.306882	-1.140097	-0.956497
24	1	0	4.692772	-2.155172	-1.093491
25	1	0	4.492972	-0.578700	-1.875816
26	1	0	4.857709	-0.659318	-0.146439
27	6	0	3.479534	-1.879089	1.714364
28	1	0	3.061335	-2.268940	2.645793
29	1	0	4.358813	-2.473761	1.452967
30	1	0	3.796761	-0.846428	1.889819
31	6	0	-2.410611	-1.949500	-0.626421
32	6	0	-2.815564	-1.170727	0.675057
33	5	0	-1.456280	0.085633	-0.621953
34	8	0	-1.277261	-1.186060	-1.111235
35	8	0	-2.379635	0.181509	0.382585
36	6	0	-4.309395	-1.141479	0.953219
37	1	0	-4.693682	-2.157056	1.090991
38	1	0	-4.497445	-0.579324	1.871676
39	1	0	-4.860179	-0.662621	0.141997
40	6	0	-3.477816	-1.882491	-1.715840
41	1	0	-3.057884	-2.272744	-2.646321
42	1	0	-4.356242	-2.478508	-1.454621
43	1	0	-3.796792	-0.850653	-1.892942
44	6	0	-1.971733	-3.384253	-0.396606
45	1	0	-2.797441	-3.977441	0.008817
46	1	0	-1.668685	-3.829889	-1.348426
47	1	0	-1.128947	-3.436473	0.294560
48	6	0	-2.055924	-1.645618	1.908066
49	1	0	-2.239793	-0.941607	2.724229
50	1	0	-2.401924	-2.634028	2.224530
51	1	0	-0.979788	-1.693097	1.715109
52	6	0	0.996204	2.521325	0.706640
53	6	0	0.641946	3.614246	1.502930
54	6	0	-0.331959	2.256745	3.038470
55	6	0	0.071063	1.141368	2.390079
56	1	0	1.634733	2.613187	-0.163132
57	1	0	0.893832	4.606507	1.131408
58	1	0	-0.909534	2.157820	3.951964
59	7	0	0.821909	1.233168	1.212281
60	1	0	-0.119236	0.140800	2.752376

61	7	0	−0. 028864	3. 543799	2. 638968
62	7	0	0. 031280	3. 545356	−2. 636287

Int7

Thermal correction to Energy=	0.276739
Thermal correction to Enthalpy=	0.277684
Thermal correction to Gibbs Free Energy=	0.221709
Sum of electronic and zero-point Energies=	-675.086092
Sum of electronic and thermal Energies=	-675.071915
Sum of electronic and thermal Enthalpies=	-675.070971
Sum of electronic and thermal Free Energies=	-675.126945

Esol = -675.3635296

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	−6. 658806	−1. 810559	2. 961064
2	8	0	−7. 381623	−2. 856849	2. 457421
3	8	0	−5. 827690	−1. 201421	2. 061667
4	6	0	−4. 945449	−1. 824307	−0. 097841
5	1	0	−5. 171465	−2. 314344	−1. 050039
6	1	0	−4. 582085	−0. 815838	−0. 312180
7	1	0	−4. 147868	−2. 376006	0. 402510
8	6	0	−5. 765803	−4. 217483	1. 335732
9	1	0	−5. 336462	−4. 526340	0. 378894
10	1	0	−4. 956073	−3. 877424	1. 988594
11	1	0	−6. 237391	−5. 086855	1. 800549
12	6	0	−6. 816298	−3. 127130	1. 148368
13	6	0	−6. 191513	−1. 742872	0. 765383
14	6	0	−7. 924052	−3. 601480	0. 225135
15	1	0	−7. 545240	−3. 724765	−0. 794288
16	1	0	−8. 297884	−4. 569672	0. 568326
17	1	0	−8. 759022	−2. 899059	0. 208590
18	6	0	−7. 209631	−0. 784531	0. 155032
19	1	0	−6. 771732	0. 215740	0. 111751
20	1	0	−7. 484618	−1. 086856	−0. 859012
21	1	0	−8. 118020	−0. 734622	0. 763096
22	6	0	−7. 640783	−1. 612517	6. 543113
23	6	0	−7. 569617	−2. 050834	5. 254917
24	7	0	−6. 764041	−1. 383097	4. 332444
25	6	0	−6. 065904	−0. 276525	4. 816295
26	6	0	−6. 193395	0. 094598	6. 121147

27	7	0	−6.971466	−0.537923	7.039732
28	1	0	−8.276642	−2.152639	7.239415
29	1	0	−8.111733	−2.910139	4.882840
30	1	0	−5.637327	0.960808	6.469719
31	1	0	−5.440230	0.243509	4.102883

TS9

Thermal correction to Energy=	0.539425
Thermal correction to Enthalpy=	0.540369
Thermal correction to Gibbs Free Energy=	0.443993
Sum of electronic and zero-point Energies=	-2236.067316
Sum of electronic and thermal Energies=	-2236.035962
Sum of electronic and thermal Enthalpies=	-2236.035018
Sum of electronic and thermal Free Energies=	-2236.131395

Esol = -2236.664635

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.801487	−5.693480	3.124082
2	5	0	1.727094	−5.645396	1.423809
3	8	0	1.938472	−4.544361	3.921879
4	8	0	2.214434	−6.833001	3.824043
5	8	0	1.491276	−4.496479	0.695268
6	8	0	1.683872	−6.769698	0.624552
7	6	0	2.055208	−4.123797	6.292905
8	1	0	2.297922	−3.066755	6.151270
9	1	0	0.969159	−4.216041	6.360257
10	1	0	2.495321	−4.448791	7.241600
11	6	0	1.008534	−6.795286	5.911302
12	1	0	1.085184	−6.644666	6.992571
13	1	0	0.189186	−6.180296	5.532840
14	1	0	0.763078	−7.845531	5.727613
15	6	0	0.730370	−7.310685	−1.522533
16	1	0	0.564995	−6.957996	−2.545792
17	1	0	1.227108	−8.283388	−1.574674
18	1	0	−0.237967	−7.449701	−1.037025
19	6	0	−0.517976	−4.895501	−0.523551
20	1	0	−0.975065	−5.125281	−1.490525
21	1	0	−0.871588	−5.626600	0.212025
22	1	0	−0.851886	−3.903004	−0.208172
23	6	0	1.008658	−4.897944	−0.603655

24	6	0	1.601686	−6.334070	−0.749039
25	6	0	2.328309	−6.470020	5.209180
26	6	0	2.609615	−4.933312	5.130185
27	6	0	4.093589	−4.620257	4.935553
28	1	0	4.198089	−3.562119	4.681555
29	1	0	4.677460	−4.820526	5.838957
30	1	0	4.507271	−5.209331	4.111681
31	6	0	3.449090	−7.289658	5.832802
32	1	0	3.641505	−6.969877	6.862373
33	1	0	3.162722	−8.345181	5.853448
34	1	0	4.372572	−7.201793	5.257861
35	6	0	1.484238	−3.898533	−1.644765
36	1	0	1.200822	−4.223314	−2.651326
37	1	0	1.020998	−2.925704	−1.458320
38	1	0	2.567457	−3.770521	−1.608471
39	6	0	3.023983	−6.335053	−1.304514
40	1	0	3.451038	−7.333112	−1.177262
41	1	0	3.042490	−6.082449	−2.368695
42	1	0	3.654978	−5.623792	−0.763492
43	6	0	−2.972356	−6.013007	2.474094
44	6	0	−2.174132	−7.161223	2.444048
45	6	0	−0.823885	−7.046146	2.746021
46	6	0	−1.015950	−4.776390	3.106560
47	6	0	−2.374283	−4.796634	2.814100
48	6	0	−4.417054	−6.085901	2.143560
49	6	0	−5.189672	−7.171051	2.562722
50	6	0	−6.534695	−7.172586	2.214985
51	6	0	−6.385554	−5.210392	1.129522
52	6	0	−5.030621	−5.072669	1.403809
53	1	0	−2.588813	−8.123472	2.163513
54	1	0	−2.956335	−3.882792	2.868352
55	1	0	−4.770628	−7.973709	3.157429
56	1	0	−4.473584	−4.220772	1.032502
57	7	0	−0.268427	−5.878807	3.073908
58	7	0	−7.135303	−6.226250	1.516864
59	1	0	−0.489430	−3.863988	3.375498
60	1	0	−0.147804	−7.896739	2.716117
61	17	0	−7.190568	−3.972536	0.202124
62	17	0	−7.537604	−8.504156	2.726657

Int8

Thermal correction to Energy=	0.540798
Thermal correction to Enthalpy=	0.541742

Thermal correction to Gibbs Free Energy=	0.444285
Sum of electronic and zero-point Energies=	-2236.069528
Sum of electronic and thermal Energies=	-2236.037825
Sum of electronic and thermal Enthalpies=	-2236.036881
Sum of electronic and thermal Free Energies=	-2236.134338

Esol = -2236.667861

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.978119	-5.957508	2.918319
2	5	0	1.320439	-5.876715	1.229516
3	8	0	1.442810	-4.825681	3.702297
4	8	0	1.376475	-7.161676	3.601742
5	8	0	0.444423	-5.391876	0.271919
6	8	0	2.539238	-6.202792	0.667512
7	6	0	2.349385	-4.444452	5.895059
8	1	0	2.751751	-3.460665	5.635694
9	1	0	1.335374	-4.304491	6.275936
10	1	0	2.970824	-4.864293	6.693464
11	6	0	0.625957	-6.796353	5.869336
12	1	0	0.940016	-6.638540	6.906076
13	1	0	-0.100537	-6.020748	5.609025
14	1	0	0.130172	-7.770138	5.807539
15	6	0	3.382292	-6.592836	-1.560870
16	1	0	3.349215	-6.257023	-2.602655
17	1	0	4.425900	-6.585810	-1.234709
18	1	0	3.018699	-7.620731	-1.510533
19	6	0	0.498529	-6.907270	-1.571584
20	1	0	0.854651	-7.103875	-2.586992
21	1	0	0.786665	-7.745624	-0.930298
22	1	0	-0.593290	-6.852587	-1.592555
23	6	0	1.047353	-5.590892	-1.024108
24	6	0	2.565380	-5.669554	-0.671789
25	6	0	1.818025	-6.785080	4.907166
26	6	0	2.359161	-5.341567	4.665659
27	6	0	3.751946	-5.353652	4.030180
28	1	0	3.984689	-4.342262	3.684192
29	1	0	4.527181	-5.664444	4.737761
30	1	0	3.769495	-6.019805	3.162301
31	6	0	2.865144	-7.787299	5.371542
32	1	0	3.328411	-7.467353	6.311237
33	1	0	2.396426	-8.761815	5.539617

34	1	0	3.644425	−7.913286	4.617615
35	6	0	0.660748	−4.438496	−1.936894
36	1	0	1.175205	−4.518449	−2.900180
37	1	0	−0.416374	−4.463573	−2.124870
38	1	0	0.905033	−3.474232	−1.487587
39	6	0	3.224913	−4.293960	−0.587460
40	1	0	4.212009	−4.405454	−0.131181
41	1	0	3.347396	−3.840734	−1.575567
42	1	0	2.636747	−3.617934	0.040493
43	6	0	−3.474119	−5.712183	2.953823
44	6	0	−2.823671	−6.949124	2.925549
45	6	0	−1.439765	−6.984084	2.956689
46	6	0	−1.313576	−4.670917	3.039683
47	6	0	−2.694052	−4.554638	3.014571
48	6	0	−4.954950	−5.630415	2.917258
49	6	0	−5.696842	−6.512157	2.128617
50	6	0	−7.079252	−6.372553	2.139270
51	6	0	−7.020132	−4.649490	3.581724
52	6	0	−5.633529	−4.668693	3.668346
53	1	0	−3.384378	−7.876747	2.905991
54	1	0	−3.150024	−3.570866	3.018468
55	1	0	−5.221831	−7.262414	1.508132
56	1	0	−5.110140	−3.975263	4.315300
57	7	0	−0.713309	−5.864068	3.012370
58	7	0	−7.741523	−5.471207	2.841278
59	17	0	−7.907609	−3.468581	4.506644
60	17	0	−8.043634	−7.443951	1.159560
61	1	0	−0.647007	−3.816966	3.090826
62	1	0	−0.867699	−7.906033	2.955870

TS10

Thermal correction to Energy=	0.693297
Thermal correction to Enthalpy=	0.694241
Thermal correction to Gibbs Free Energy=	0.568098
Sum of electronic and zero-point Energies=	-3650.271403
Sum of electronic and thermal Energies=	-3650.227786
Sum of electronic and thermal Enthalpies=	-3650.226841
Sum of electronic and thermal Free Energies=	-3650.352985

Esol = -3651.129036

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	5	0	0.766106	-6.813142	1.100275
2	5	0	0.781088	-5.745096	-0.248619
3	8	0	1.914337	-7.027988	1.880769
4	8	0	-0.073839	-7.938736	1.161543
5	8	0	1.464935	-6.278965	-1.421904
6	8	0	1.277292	-4.401059	-0.034123
7	6	0	2.627820	-8.606342	3.558679
8	1	0	3.672557	-8.289033	3.494735
9	1	0	2.138886	-8.006516	4.328810
10	1	0	2.610885	-9.657486	3.866183
11	6	0	-0.266603	-8.571364	3.479103
12	1	0	0.040987	-9.285307	4.249462
13	1	0	-0.067403	-7.559268	3.839622
14	1	0	-1.344650	-8.681474	3.326105
15	6	0	3.139122	-3.068995	-0.739250
16	1	0	3.833686	-2.855354	-1.558926
17	1	0	2.690368	-2.122490	-0.421348
18	1	0	3.702302	-3.476715	0.102606
19	6	0	3.766447	-5.912617	-0.876083
20	1	0	4.669665	-5.325860	-1.073092
21	1	0	3.539842	-5.886410	0.194264
22	1	0	3.965487	-6.952264	-1.152691
23	6	0	2.565987	-5.417799	-1.688557
24	6	0	2.048102	-4.035183	-1.179397
25	6	0	0.452482	-8.833764	2.156089
26	6	0	1.958847	-8.423539	2.204933
27	6	0	2.783793	-9.106587	1.112405
28	1	0	3.773862	-8.643295	1.081275
29	1	0	2.908241	-10.178089	1.297049
30	1	0	2.313991	-8.963128	0.134006
31	6	0	0.196932	-10.264692	1.705341
32	1	0	0.675811	-10.980515	2.381902
33	1	0	-0.878818	-10.464917	1.708300
34	1	0	0.570490	-10.433433	0.693535
35	6	0	2.888969	-5.463931	-3.176033
36	1	0	3.672387	-4.742475	-3.433105
37	1	0	3.249159	-6.462305	-3.441444
38	1	0	2.004729	-5.253732	-3.781527
39	6	0	1.137706	-3.355099	-2.207014
40	1	0	0.617105	-2.520801	-1.725905
41	1	0	1.706985	-2.956630	-3.052859
42	1	0	0.391155	-4.054877	-2.594654
43	6	0	-1.776465	-3.324941	3.570782

44	6	0	−2.421910	−4.495872	3.162305
45	6	0	−1.662653	−5.512350	2.595121
46	6	0	0.278736	−4.302631	2.802463
47	6	0	−0.394791	−3.232881	3.382356
48	6	0	−2.538928	−2.208547	4.182744
49	6	0	−3.826513	−1.896327	3.740199
50	6	0	−4.479585	−0.836136	4.355650
51	6	0	−2.757687	−0.414175	5.734765
52	6	0	−1.985771	−1.444728	5.213216
53	1	0	−3.489480	−4.626472	3.305413
54	1	0	0.148133	−2.335187	3.658659
55	1	0	−4.299658	−2.440192	2.931799
56	1	0	−1.001734	−1.655056	5.614374
57	7	0	−0.344683	−5.418053	2.422325
58	7	0	−3.975302	−0.101103	5.329627
59	6	0	−4.969948	−5.476911	−1.700313
60	6	0	−5.567475	−4.284778	−2.115214
61	6	0	−6.924894	−4.316177	−2.409910
62	6	0	−7.105407	−6.505116	−1.933261
63	6	0	−5.760241	−6.624378	−1.605641
64	6	0	−3.525472	−5.521550	−1.364854
65	6	0	−2.904371	−4.444471	−0.727612
66	6	0	−1.553140	−4.524047	−0.428423
67	6	0	−1.404854	−6.647428	−1.348010
68	6	0	−2.749538	−6.642138	−1.677973
69	1	0	−4.999435	−3.369571	−2.230060
70	1	0	−5.356900	−7.571441	−1.268324
71	1	0	−3.463546	−3.558355	−0.446891
72	1	0	−3.176854	−7.493238	−2.196037
73	7	0	−0.830622	−5.605430	−0.735985
74	7	0	−7.690895	−5.388751	−2.326643
75	1	0	1.345833	−4.269376	2.604832
76	1	0	−2.114094	−6.443446	2.257862
77	1	0	−0.745934	−7.480964	−1.564007
78	1	0	−1.001295	−3.729387	0.064436
79	17	0	−2.105664	0.558019	7.026881
80	17	0	−6.084739	−0.410015	3.822426
81	17	0	−8.128322	−7.911565	−1.822975
82	17	0	−7.708427	−2.850601	−2.933940

Int9

Thermal correction to Energy= 0.694552

Thermal correction to Enthalpy= 0.695496

Thermal correction to Gibbs Free Energy=	0.571850
Sum of electronic and zero-point Energies=	-3650.274940
Sum of electronic and thermal Energies=	-3650.231399
Sum of electronic and thermal Enthalpies=	-3650.230455
Sum of electronic and thermal Free Energies=	-3650.354101

Esol = -3651.128686

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.535324	−6.537035	1.270444
2	5	0	0.730040	−5.658353	−0.231990
3	8	0	1.748156	−6.902354	1.986050
4	8	0	−0.304891	−7.717107	1.204213
5	8	0	1.529619	−6.290568	−1.270015
6	8	0	1.183551	−4.286687	−0.105813
7	6	0	2.505279	−8.714333	3.369129
8	1	0	3.556311	−8.423172	3.283043
9	1	0	2.088227	−8.212376	4.244719
10	1	0	2.466533	−9.797242	3.531483
11	6	0	−0.386910	−8.507019	3.482807
12	1	0	−0.078526	−9.297166	4.174792
13	1	0	−0.111846	−7.542120	3.919167
14	1	0	−1.476640	−8.547111	3.386095
15	6	0	3.055134	−2.967637	−0.810001
16	1	0	3.801531	−2.811993	−1.596464
17	1	0	2.559916	−2.010175	−0.619485
18	1	0	3.567152	−3.272873	0.104977
19	6	0	3.782597	−5.783550	−0.643656
20	1	0	4.663349	−5.158330	−0.822933
21	1	0	3.481067	−5.707453	0.405742
22	1	0	4.057450	−6.824651	−0.835750
23	6	0	2.614133	−5.415981	−1.561711
24	6	0	2.024194	−4.007723	−1.225571
25	6	0	0.243615	−8.686212	2.097744
26	6	0	1.763809	−8.321235	2.097840
27	6	0	2.491020	−8.888182	0.875833
28	1	0	3.507930	−8.485571	0.862094
29	1	0	2.555928	−9.980838	0.902176
30	1	0	1.994292	−8.568452	−0.045468
31	6	0	−0.078124	−10.074759	1.563010
32	1	0	0.427520	−10.852042	2.146078
33	1	0	−1.156245	−10.254684	1.623225

34	1	0	0.223413	-10.167520	0.517554
35	6	0	3.023663	-5.595906	-3.017864
36	1	0	3.803674	-4.880495	-3.301229
37	1	0	3.421754	-6.604569	-3.162711
38	1	0	2.171636	-5.471294	-3.689532
39	6	0	1.168590	-3.458715	-2.371990
40	1	0	0.596408	-2.598888	-2.009034
41	1	0	1.783412	-3.126117	-3.214399
42	1	0	0.466697	-4.214617	-2.736724
43	6	0	-1.502484	-3.355129	3.607593
44	6	0	-2.236326	-4.415877	3.068962
45	6	0	-1.567167	-5.433805	2.408768
46	6	0	0.486560	-4.420216	2.781578
47	6	0	-0.112130	-3.370928	3.457720
48	6	0	-2.180273	-2.244081	4.317789
49	6	0	-3.427589	-1.782396	3.891499
50	6	0	-4.003615	-0.738139	4.603909
51	6	0	-2.280527	-0.602066	6.040174
52	6	0	-1.585707	-1.636678	5.425979
53	1	0	-3.312927	-4.470738	3.186936
54	1	0	0.501199	-2.563504	3.841571
55	1	0	-3.924939	-2.200218	3.024515
56	1	0	-0.630900	-1.969001	5.814765
57	7	0	-0.235426	-5.426734	2.270221
58	7	0	-3.460109	-0.150223	5.653809
59	6	0	-4.942996	-5.823368	-1.925249
60	6	0	-5.623806	-4.700343	-2.401324
61	6	0	-6.967717	-4.852444	-2.719344
62	6	0	-6.984946	-7.028271	-2.156182
63	6	0	-5.642414	-7.025738	-1.799223
64	6	0	-3.508454	-5.745933	-1.557824
65	6	0	-2.976193	-4.596681	-0.966393
66	6	0	-1.632068	-4.570113	-0.630718
67	6	0	-1.318519	-6.726770	-1.426882
68	6	0	-2.650573	-6.825881	-1.790044
69	1	0	-5.125946	-3.749073	-2.545412
70	1	0	-5.169724	-7.922002	-1.416343
71	1	0	-3.598938	-3.735590	-0.749413
72	1	0	-3.006909	-7.728931	-2.272889
73	7	0	-0.828940	-5.617017	-0.857485
74	7	0	-7.648323	-5.978615	-2.605675
75	1	0	1.555204	-4.485215	2.614468
76	1	0	-2.066894	-6.296093	1.977919
77	1	0	-0.601284	-7.525213	-1.576313

78	1	0	−1.147590	−3.713472	−0.172060
79	17	0	−1.577481	0.178209	7.430977
80	17	0	−5.557070	−0.128367	4.099437
81	17	0	−7.895209	−8.507168	−2.005287
82	17	0	−7.854613	−3.477219	−3.319697

TS11

Thermal correction to Energy=	0.693645
Thermal correction to Enthalpy=	0.694590
Thermal correction to Gibbs Free Energy=	0.572833
Sum of electronic and zero-point Energies=	-3650.264216
Sum of electronic and thermal Energies=	-3650.221158
Sum of electronic and thermal Enthalpies=	-3650.220214
Sum of electronic and thermal Free Energies=	-3650.341970

Esol = -3651.116452

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.040469	−6.819770	1.385762
2	5	0	1.122784	−6.011614	−0.558565
3	8	0	2.221337	−6.465343	2.080153
4	8	0	0.896417	−8.222761	1.309968
5	8	0	2.417066	−6.220767	−1.090534
6	8	0	0.808172	−4.635430	−0.512243
7	6	0	3.587141	−7.552873	3.728276
8	1	0	4.366024	−6.787053	3.675249
9	1	0	2.872151	−7.255798	4.497621
10	1	0	4.058223	−8.495081	4.027902
11	6	0	0.981235	−8.819100	3.626222
12	1	0	1.561556	−9.279913	4.430830
13	1	0	0.676398	−7.817993	3.948253
14	1	0	0.080067	−9.417511	3.465648
15	6	0	1.952384	−2.565121	−0.933666
16	1	0	2.728894	−2.071016	−1.526497
17	1	0	1.023695	−1.999066	−1.050632
18	1	0	2.240872	−2.533772	0.118882
19	6	0	3.871678	−4.579324	−0.088948
20	1	0	4.338008	−3.595869	−0.201001
21	1	0	3.292117	−4.611702	0.837336
22	1	0	4.667234	−5.324227	−0.010822
23	6	0	2.998754	−4.920720	−1.293531

24	6	0	1.739863	-3.995104	-1.400941
25	6	0	1.771996	-8.756221	2.318451
26	6	0	2.918428	-7.690345	2.367770
27	6	0	3.974354	-7.919725	1.289737
28	1	0	4.680538	-7.086197	1.308733
29	1	0	4.534178	-8.842352	1.470254
30	1	0	3.520652	-7.949609	0.295630
31	6	0	2.207698	-10.149022	1.896118
32	1	0	2.950429	-10.553992	2.591075
33	1	0	1.343031	-10.818997	1.894296
34	1	0	2.634963	-10.140287	0.891408
35	6	0	3.850064	-4.968104	-2.554521
36	1	0	4.243347	-3.974897	-2.796036
37	1	0	4.699056	-5.638846	-2.395629
38	1	0	3.280806	-5.339017	-3.408776
39	6	0	1.124359	-4.011841	-2.801057
40	1	0	0.147015	-3.522571	-2.763184
41	1	0	1.747459	-3.479773	-3.525752
42	1	0	0.981746	-5.038325	-3.154413
43	6	0	-2.489836	-4.474608	2.159384
44	6	0	-2.574783	-5.826218	1.813946
45	6	0	-1.431192	-6.580808	1.632378
46	6	0	-0.085960	-4.720515	2.139014
47	6	0	-1.192152	-3.940677	2.332502
48	6	0	-3.693508	-3.651676	2.354982
49	6	0	-4.889538	-3.944456	1.685440
50	6	0	-5.985575	-3.128804	1.923403
51	6	0	-4.859968	-1.819682	3.351762
52	6	0	-3.687171	-2.547322	3.218194
53	1	0	-3.534846	-6.323700	1.723939
54	1	0	-1.447503	-7.644970	1.431298
55	1	0	0.925105	-4.354016	2.256475
56	1	0	-1.047498	-2.901043	2.603231
57	1	0	-4.963001	-4.760916	0.978372
58	1	0	-2.811133	-2.275386	3.792635
59	7	0	-0.189028	-6.037499	1.776225
60	7	0	-5.996816	-2.083236	2.730987
61	6	0	-3.061094	-9.670125	-2.143110
62	6	0	-4.362308	-9.512322	-1.646204
63	6	0	-5.324226	-10.431662	-2.036999
64	6	0	-3.881134	-11.595778	-3.295749
65	6	0	-2.820020	-10.753853	-2.998751
66	6	0	-1.989944	-8.727715	-1.783683
67	6	0	-2.267833	-7.396462	-1.462905

68	6	0	−1.249695	−6.522726	−1.131729
69	6	0	0.346825	−8.221649	−1.434071
70	6	0	−0.630725	−9.116719	−1.770383
71	1	0	−4.617684	−8.718501	−0.955653
72	1	0	−1.848952	−10.924769	−3.445508
73	1	0	−3.280124	−7.008964	−1.509274
74	1	0	−1.409653	−5.468226	−0.943295
75	1	0	1.398134	−8.475352	−1.407971
76	1	0	−0.337452	−10.132776	−2.008978
77	7	0	0.052241	−6.925770	−1.101676
78	7	0	−5.114352	−11.459530	−2.840137
79	17	0	−7.485642	−3.473945	1.097275
80	17	0	−4.876856	−0.441858	4.425298
81	17	0	−6.952430	−10.255135	−1.429692
82	17	0	−3.606044	−12.951478	−4.362072

Int10

Thermal correction to Energy=	0.697484
Thermal correction to Enthalpy=	0.698428
Thermal correction to Gibbs Free Energy=	0.573131
Sum of electronic and zero-point Energies=	-3650.327686
Sum of electronic and thermal Energies=	-3650.284158
Sum of electronic and thermal Enthalpies=	-3650.283213
Sum of electronic and thermal Free Energies=	-3650.408510

Esol = -3651.187378

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	−0.904756	−8.278608	2.368845
2	5	0	1.369721	−4.839753	−0.194419
3	8	0	0.422099	−8.428784	2.054952
4	8	0	−1.569827	−9.460672	2.580238
5	8	0	1.941432	−6.079955	−0.066113
6	8	0	2.267464	−3.827565	−0.425771
7	6	0	2.003584	−10.247661	2.222793
8	1	0	2.743860	−9.768489	1.576769
9	1	0	2.204730	−9.950574	3.253490
10	1	0	2.130478	−11.331366	2.136196
11	6	0	−0.176850	−10.684228	4.091576
12	1	0	0.545631	−11.495331	4.216452
13	1	0	0.247468	−9.769147	4.515863

14	1	0	-1.079462	-10.935044	4.654339
15	6	0	4.656768	-3.602673	-0.162834
16	1	0	5.620573	-4.110180	-0.270026
17	1	0	4.698433	-2.671065	-0.733363
18	1	0	4.505260	-3.352675	0.888561
19	6	0	3.684368	-5.763412	1.532191
20	1	0	4.759376	-5.673359	1.711029
21	1	0	3.181690	-4.907059	1.993307
22	1	0	3.321845	-6.673393	2.017672
23	6	0	3.366256	-5.847209	0.041920
24	6	0	3.534671	-4.476191	-0.694835
25	6	0	-0.548722	-10.487473	2.624728
26	6	0	0.606668	-9.839815	1.789958
27	6	0	0.430293	-10.030120	0.285931
28	1	0	1.122897	-9.362705	-0.233728
29	1	0	0.639194	-11.059694	-0.017483
30	1	0	-0.587983	-9.775598	-0.025378
31	6	0	-1.114695	-11.768429	2.038113
32	1	0	-0.337348	-12.536173	1.972894
33	1	0	-1.911952	-12.146584	2.683476
34	1	0	-1.530855	-11.602725	1.042954
35	6	0	4.108722	-7.004305	-0.602096
36	1	0	5.183651	-6.800101	-0.632277
37	1	0	3.954313	-7.913474	-0.015153
38	1	0	3.756223	-7.188589	-1.618405
39	6	0	3.643900	-4.630786	-2.209094
40	1	0	3.541674	-3.646457	-2.672768
41	1	0	4.609778	-5.052119	-2.500609
42	1	0	2.849478	-5.275647	-2.597039
43	6	0	-2.580399	-4.484364	3.117167
44	6	0	-3.409416	-5.689409	3.168950
45	6	0	-2.847723	-6.876072	2.876993
46	6	0	-0.814509	-5.806067	1.974011
47	6	0	-1.329182	-4.557852	2.628671
48	6	0	-3.102817	-3.211607	3.664176
49	6	0	-3.966691	-3.192284	4.763297
50	6	0	-4.400927	-1.955016	5.219707
51	6	0	-3.261860	-0.832813	3.647188
52	6	0	-2.747323	-1.990291	3.082111
53	1	0	-4.442841	-5.638911	3.488870
54	1	0	-0.664276	-3.699970	2.658915
55	1	0	-4.273176	-4.103139	5.262814
56	1	0	-2.116100	-1.952415	2.201925
57	7	0	-1.534458	-6.997248	2.447060

58	7	0	−4.070660	−0.790563	4.691218
59	6	0	−4.235554	−4.191057	−0.758498
60	6	0	−4.637024	−3.255727	−1.717048
61	6	0	−5.990440	−3.180485	−2.017160
62	6	0	−6.534074	−4.789925	−0.553197
63	6	0	−5.220374	−4.975660	−0.149015
64	6	0	−2.810933	−4.346905	−0.387511
65	6	0	−1.920028	−3.187017	−0.438246
66	6	0	−0.594028	−3.381506	−0.324940
67	6	0	−0.898303	−5.718444	0.407288
68	6	0	−2.312501	−5.554734	−0.067157
69	1	0	−3.922466	−2.623054	−2.228992
70	1	0	−4.969392	−5.683141	0.632487
71	1	0	−2.311903	−2.193567	−0.616758
72	1	0	−2.931307	−6.445982	−0.106673
73	7	0	−0.039548	−4.628475	−0.077507
74	7	0	−6.934443	−3.919563	−1.463333
75	17	0	−2.840933	0.710099	2.941474
76	17	0	−5.466153	−1.893318	6.603644
77	17	0	−7.789382	−5.756697	0.185291
78	17	0	−6.524364	−2.031559	−3.220637
79	1	0	0.251236	−5.942287	2.193353
80	1	0	−3.376221	−7.816874	2.993697
81	1	0	−0.480930	−6.666252	0.047063
82	1	0	0.127190	−2.580923	−0.455399

TS12

Thermal correction to Energy=	0.694254
Thermal correction to Enthalpy=	0.695199
Thermal correction to Gibbs Free Energy=	0.576755
Sum of electronic and zero-point Energies=	-3650.301676
Sum of electronic and thermal Energies=	-3650.258736
Sum of electronic and thermal Enthalpies=	-3650.257792
Sum of electronic and thermal Free Energies=	-3650.376235

Esol = -3651.156534

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	−0.716216	−8.243112	2.547994
2	5	0	1.368882	−5.011061	−0.401652
3	8	0	0.620723	−8.302336	2.254845

4	8	0	-1.329408	-9.459272	2.668629
5	8	0	1.854799	-6.286404	-0.282343
6	8	0	2.325985	-4.046690	-0.555105
7	6	0	2.284032	-10.054661	2.312878
8	1	0	3.010194	-9.501338	1.710230
9	1	0	2.460080	-9.818426	3.363804
10	1	0	2.460497	-11.123382	2.156049
11	6	0	0.101722	-10.722525	4.112138
12	1	0	0.857757	-11.508331	4.190899
13	1	0	0.480014	-9.822398	4.606204
14	1	0	-0.795984	-11.051780	4.641139
15	6	0	4.704735	-3.967052	-0.139457
16	1	0	5.643306	-4.526451	-0.201669
17	1	0	4.833879	-3.025810	-0.680021
18	1	0	4.501865	-3.734995	0.907334
19	6	0	3.500824	-6.109346	1.433592
20	1	0	4.564443	-6.111489	1.687505
21	1	0	3.039893	-5.222373	1.880966
22	1	0	3.026541	-6.993280	1.869707
23	6	0	3.282591	-6.138296	-0.076253
24	6	0	3.572854	-4.762043	-0.764427
25	6	0	-0.258563	-10.440794	2.656896
26	6	0	0.875270	-9.682131	1.888287
27	6	0	0.725699	-9.761328	0.371892
28	1	0	1.369928	-9.001814	-0.080419
29	1	0	1.009502	-10.745688	-0.010538
30	1	0	-0.305787	-9.555635	0.066853
31	6	0	-0.755877	-11.700359	1.971383
32	1	0	0.058251	-12.424163	1.866424
33	1	0	-1.543116	-12.159800	2.574700
34	1	0	-1.164741	-11.484525	0.982938
35	6	0	3.997976	-7.320892	-0.703439
36	1	0	5.082079	-7.174967	-0.666985
37	1	0	3.761977	-8.232937	-0.147435
38	1	0	3.696075	-7.465161	-1.742326
39	6	0	3.766240	-4.885703	-2.272478
40	1	0	3.748658	-3.886352	-2.714195
41	1	0	4.723784	-5.354458	-2.514680
42	1	0	2.963589	-5.475157	-2.726054
43	6	0	-2.711720	-4.472681	2.856687
44	6	0	-3.414496	-5.735689	3.047768
45	6	0	-2.760832	-6.912871	2.970159
46	6	0	-0.755502	-5.795442	2.312029
47	6	0	-1.352539	-4.567072	2.601619

48	6	0	−3.410622	−3.195914	2.921236
49	6	0	−4.775581	−3.116522	3.258142
50	6	0	−5.400722	−1.879871	3.208549
51	6	0	−3.549020	−0.832263	2.538229
52	6	0	−2.786300	−1.985703	2.554180
53	1	0	−4.470310	−5.762810	3.283016
54	1	0	−0.738067	−3.683006	2.475545
55	1	0	−5.351312	−3.981034	3.558694
56	1	0	−1.747209	−1.939829	2.258507
57	7	0	−1.406639	−6.988820	2.667428
58	7	0	−4.828520	−0.739291	2.859853
59	6	0	−4.253553	−3.969231	0.018074
60	6	0	−4.772222	−2.669557	−0.139249
61	6	0	−6.122099	−2.460238	0.098626
62	6	0	−6.487018	−4.596372	0.627187
63	6	0	−5.171343	−4.964588	0.413096
64	6	0	−2.829858	−4.246481	−0.119733
65	6	0	−1.863417	−3.176509	−0.335935
66	6	0	−0.545805	−3.442559	−0.446264
67	6	0	−0.933163	−5.744557	0.057599
68	6	0	−2.308772	−5.528693	−0.043926
69	1	0	−4.159532	−1.832101	−0.443316
70	1	0	−4.872411	−5.990072	0.581200
71	1	0	−2.177587	−2.146377	−0.440558
72	1	0	−2.950117	−6.393085	0.084711
73	7	0	−0.037784	−4.729998	−0.321087
74	7	0	−6.991512	−3.383224	0.475645
75	17	0	−2.785353	0.662520	2.026866
76	17	0	−7.094070	−1.786908	3.627089
77	17	0	−7.615660	−5.823950	1.173335
78	17	0	−6.760383	−0.846136	−0.097622
79	1	0	0.319940	−5.886594	2.200753
80	1	0	−3.243583	−7.865609	3.156329
81	1	0	−0.516422	−6.745874	0.026619
82	1	0	0.191984	−2.676539	−0.656739

Int11

Thermal correction to Energy=	0.346402
Thermal correction to Enthalpy=	0.347346
Thermal correction to Gibbs Free Energy=	0.273474
Sum of electronic and zero-point Energies=	-1825.147855
Sum of electronic and thermal Energies=	-1825.126566
Sum of electronic and thermal Enthalpies=	-1825.125622

Sum of electronic and thermal Free Energies= -1825.199494

Esol = -1825.592568

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	3.474797	-7.968450	7.295907
2	8	0	4.273943	-8.809954	6.578265
3	8	0	3.692923	-7.971074	8.642679
4	6	0	6.341506	-9.967234	7.050753
5	1	0	6.264212	-10.604629	6.166151
6	1	0	6.892084	-9.065927	6.776419
7	1	0	6.908836	-10.510217	7.813063
8	6	0	6.060459	-7.712323	8.866959
9	1	0	7.017865	-8.196609	9.076564
10	1	0	6.140735	-7.177833	7.915393
11	1	0	5.862419	-6.981444	9.654808
12	6	0	4.920714	-8.725652	8.836306
13	6	0	4.951609	-9.636962	7.563089
14	6	0	4.118426	-10.904602	7.723433
15	1	0	4.008198	-11.382147	6.746773
16	1	0	4.599277	-11.613070	8.403065
17	1	0	3.119702	-10.675396	8.107640
18	6	0	4.831631	-9.475766	10.152656
19	1	0	5.702324	-10.126461	10.279773
20	1	0	4.816604	-8.762616	10.980875
21	1	0	3.926801	-10.083137	10.207149
22	6	0	0.490583	-5.510270	5.438895
23	6	0	1.303204	-6.427271	4.697841
24	6	0	2.238301	-7.200009	5.302367
25	6	0	1.702361	-6.249511	7.417431
26	6	0	0.750322	-5.471392	6.846683
27	6	0	-0.514577	-4.688189	4.813615
28	6	0	-0.615684	-4.563452	3.407274
29	6	0	-1.606032	-3.755605	2.885578
30	6	0	-2.393747	-3.191152	4.895568
31	6	0	-1.462012	-3.955911	5.568199
32	1	0	1.173676	-6.550828	3.629669
33	1	0	0.208863	-4.794475	7.496237
34	1	0	0.070784	-5.058918	2.734617
35	1	0	-1.492210	-3.997426	6.648156
36	7	0	2.468766	-7.135657	6.670875
37	7	0	-2.498424	-3.065794	3.580719

38	1	0	1.925354	-6.225134	8.476775
39	1	0	2.852624	-7.910968	4.764341
40	17	0	-3.572286	-2.292548	5.833504
41	17	0	-1.721466	-3.594851	1.142756

TS13

Thermal correction to Energy=	0.489063
Thermal correction to Enthalpy=	0.490007
Thermal correction to Gibbs Free Energy=	0.397213
Sum of electronic and zero-point Energies=	-2167.845372
Sum of electronic and thermal Energies=	-2167.815982
Sum of electronic and thermal Enthalpies=	-2167.815037
Sum of electronic and thermal Free Energies=	-2167.907831

Esol = -2168.410819

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	-4.907587	-2.458134	2.102913
2	8	0	-5.891504	-3.086402	1.369507
3	8	0	-4.926532	-1.082220	1.993993
4	6	0	-4.986653	-0.675805	-0.358843
5	1	0	-5.590325	-0.392067	-1.225270
6	1	0	-4.220890	0.088753	-0.205172
7	1	0	-4.483937	-1.623101	-0.576911
8	6	0	-7.286138	-2.433844	-0.478843
9	1	0	-7.871116	-1.620518	-0.919737
10	1	0	-6.465968	-2.685063	-1.153344
11	1	0	-7.935491	-3.308998	-0.389787
12	6	0	-6.774333	-2.038785	0.896293
13	6	0	-5.834723	-0.784739	0.905944
14	6	0	-7.938627	-1.908236	1.874268
15	1	0	-8.674749	-1.186225	1.509648
16	1	0	-8.434630	-2.878097	1.971192
17	1	0	-7.596936	-1.592798	2.862922
18	6	0	-6.532784	0.532517	1.194830
19	1	0	-5.800419	1.344250	1.183085
20	1	0	-7.286139	0.744408	0.429572
21	1	0	-7.016697	0.522565	2.173073
22	6	0	-0.110777	-5.228701	3.660725
23	6	0	0.029968	-6.633884	3.532535
24	6	0	1.201845	-7.223695	3.957580

25	6	0	2.102692	-5.289134	4.602969
26	6	0	0.998659	-4.552216	4.228572
27	6	0	-1.298908	-4.535523	3.242225
28	6	0	-2.483360	-5.220403	2.817049
29	6	0	-3.597212	-4.545661	2.434973
30	6	0	-2.521867	-2.472259	2.810652
31	6	0	-1.388044	-3.105770	3.207492
32	1	0	-0.741874	-7.252192	3.095558
33	1	0	0.998345	-3.483765	4.393774
34	1	0	-2.530076	-6.302193	2.803197
35	1	0	-0.538663	-2.485873	3.466510
36	7	0	2.245712	-6.602222	4.489014
37	7	0	-3.653479	-3.164710	2.426539
38	6	0	-6.857059	-4.532454	5.416472
39	6	0	-6.498411	-3.966884	4.204525
40	7	0	-5.755213	-2.855556	4.157145
41	6	0	-5.363760	-2.304618	5.306149
42	6	0	-5.731832	-2.894630	6.537694
43	7	0	-6.473818	-3.998838	6.579478
44	1	0	-7.462180	-5.433349	5.457373
45	1	0	-6.801251	-4.388245	3.250564
46	6	0	-5.295889	-2.295588	7.842568
47	1	0	-5.609734	-2.946042	8.659037
48	1	0	-4.208932	-2.173809	7.879326
49	1	0	-5.740478	-1.305615	7.990284
50	6	0	-4.521785	-1.064413	5.254435
51	1	0	-4.876695	-0.319796	5.972621
52	1	0	-3.482040	-1.296254	5.512156
53	1	0	-4.552162	-0.635033	4.252379
54	17	0	3.470982	-4.442800	5.307107
55	17	0	1.368619	-8.963424	3.789239
56	1	0	-2.600469	-1.393304	2.754857
57	1	0	-4.500436	-5.048147	2.110319

Int12

Thermal correction to Energy=	0.490386
Thermal correction to Enthalpy=	0.491330
Thermal correction to Gibbs Free Energy=	0.400302
Sum of electronic and zero-point Energies=	-2167.851220
Sum of electronic and thermal Energies=	-2167.822002
Sum of electronic and thermal Enthalpies=	-2167.821058
Sum of electronic and thermal Free Energies=	-2167.912086

Esol = -2168.413672

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	−5.187092	−2.554743	2.578109
2	8	0	−5.932912	−3.160174	1.526862
3	8	0	−5.139087	−1.148321	2.370242
4	6	0	−4.333429	−0.993284	0.110087
5	1	0	−4.582552	−0.752859	−0.927524
6	1	0	−3.589958	−0.270151	0.457535
7	1	0	−3.885219	−1.991346	0.139773
8	6	0	−6.665561	−2.545145	−0.675412
9	1	0	−7.022716	−1.724079	−1.305530
10	1	0	−5.706029	−2.895122	−1.059701
11	1	0	−7.382429	−3.367674	−0.752126
12	6	0	−6.547584	−2.102202	0.774204
13	6	0	−5.562177	−0.915370	1.016034
14	6	0	−7.935959	−1.821089	1.351403
15	1	0	−8.471530	−1.074667	0.757732
16	1	0	−8.524120	−2.743753	1.341140
17	1	0	−7.872185	−1.458808	2.382396
18	6	0	−6.191721	0.465542	0.931973
19	1	0	−5.427609	1.229132	1.102556
20	1	0	−6.623778	0.634863	−0.059600
21	1	0	−6.973052	0.593061	1.683532
22	6	0	−0.040579	−5.137926	3.484184
23	6	0	0.077993	−6.542353	3.670381
24	6	0	1.324495	−7.076454	3.911188
25	6	0	2.344680	−5.098364	3.820335
26	6	0	1.177598	−4.410540	3.571851
27	6	0	−1.298551	−4.499236	3.233287
28	6	0	−2.533047	−5.223329	3.146543
29	6	0	−3.715360	−4.586416	2.936909
30	6	0	−2.642042	−2.501928	2.835460
31	6	0	−1.429211	−3.083990	3.041364
32	1	0	−0.776853	−7.203171	3.631069
33	1	0	1.216551	−3.336892	3.452457
34	1	0	−2.557759	−6.302245	3.234364
35	1	0	−0.562324	−2.434845	3.045083
36	7	0	2.468338	−6.408358	3.993772
37	7	0	−3.811511	−3.221031	2.804559
38	6	0	−7.706649	−4.102972	5.125926
39	6	0	−7.032469	−3.747592	3.973402

40	7	0	−6.012093	−2.874821	4.031614
41	6	0	−5.651273	−2.354604	5.216315
42	6	0	−6.358424	−2.748364	6.376246
43	7	0	−7.371860	−3.608683	6.317923
44	1	0	−8.532258	−4.806107	5.087359
45	1	0	−7.271468	−4.134702	2.991374
46	6	0	−5.983910	−2.217206	7.728937
47	1	0	−4.925412	−2.390153	7.943864
48	1	0	−6.163670	−1.139289	7.795124
49	1	0	−6.588630	−2.719665	8.483361
50	6	0	−4.495766	−1.407083	5.298211
51	1	0	−4.628057	−0.721947	6.136105
52	1	0	−3.567377	−1.966354	5.464082
53	1	0	−4.398500	−0.828335	4.381156
54	17	0	3.843537	−4.185614	3.929917
55	17	0	1.456803	−8.814686	4.140440
56	1	0	−2.755852	−1.435447	2.681759
57	1	0	−4.648981	−5.132651	2.852669

TS14

Thermal correction to Energy=	0.488070
Thermal correction to Enthalpy=	0.489014
Thermal correction to Gibbs Free Energy=	0.398011
Sum of electronic and zero-point Energies=	-2167.830166
Sum of electronic and thermal Energies=	-2167.801040
Sum of electronic and thermal Enthalpies=	-2167.800095
Sum of electronic and thermal Free Energies=	-2167.891099

Esol = -2168.39231

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	−1.785073	−5.808640	6.622501
2	8	0	−1.427230	−4.714573	7.409667
3	8	0	−3.095022	−6.219945	6.847661
4	6	0	−4.772324	−5.783078	8.512154
5	1	0	−5.196840	−5.027695	9.181310
6	1	0	−5.585523	−6.197087	7.909416
7	1	0	−4.349584	−6.589969	9.113358
8	6	0	−2.136809	−5.281058	9.618210
9	1	0	−2.878920	−5.137337	10.408718
10	1	0	−2.039304	−6.352400	9.417293

11	1	0	-1.172658	-4.912436	9.978716
12	6	0	-2.508623	-4.522637	8.345250
13	6	0	-3.725211	-5.165297	7.599124
14	6	0	-2.653051	-3.038085	8.634376
15	1	0	-3.518549	-2.851620	9.278324
16	1	0	-1.760818	-2.676124	9.152869
17	1	0	-2.769975	-2.463051	7.713710
18	6	0	-4.389174	-4.204166	6.614102
19	1	0	-5.064170	-4.775051	5.970049
20	1	0	-4.974398	-3.441618	7.136456
21	1	0	-3.649408	-3.711062	5.979419
22	6	0	-0.660107	-8.688812	4.670433
23	6	0	-1.346040	-8.017665	5.638028
24	6	0	0.537305	-6.620331	5.934668
25	6	0	1.148622	-7.306861	4.902869
26	1	0	-1.107847	-9.569515	4.217007
27	7	0	-0.810192	-6.881097	6.228377
28	6	0	0.650322	-5.281303	1.283427
29	6	0	1.122072	-6.564504	0.993506
30	6	0	1.997767	-6.688264	-0.078366
31	6	0	1.951427	-4.487314	-0.539570
32	6	0	1.078223	-4.206236	0.503632
33	6	0	-0.263513	-5.091494	2.433582
34	6	0	-1.356777	-5.941083	2.616837
35	6	0	-2.095000	-5.838794	3.784826
36	6	0	-0.783311	-4.109755	4.553883
37	6	0	-0.015315	-4.111106	3.398155
38	1	0	0.851937	-7.416921	1.611106
39	1	0	0.732378	-3.195824	0.685854
40	1	0	-1.608955	-6.691185	1.874988
41	1	0	0.809021	-3.413910	3.288588
42	7	0	-1.770879	-4.986586	4.767591
43	7	0	2.409876	-5.688673	-0.838657
44	1	0	-0.581072	-3.428003	5.375637
45	1	0	-2.935288	-6.495740	3.985751
46	17	0	2.502470	-3.179079	-1.555367
47	17	0	2.630303	-8.263734	-0.475800
48	1	0	-2.342182	-8.295092	5.959061
49	6	0	1.247442	-5.612883	6.789112
50	1	0	2.328114	-5.727242	6.695464
51	1	0	0.990491	-4.578897	6.538307
52	1	0	0.969603	-5.755168	7.836845
53	6	0	2.553163	-6.962861	4.473936
54	1	0	2.793073	-7.531602	3.574116

55	1	0	2.664644	−5.894416	4.260984
56	1	0	3.288141	−7.223713	5.243038
57	7	0	0.557877	−8.312680	4.203762

Int13

Thermal correction to Energy=	0.335799
Thermal correction to Enthalpy=	0.336744
Thermal correction to Gibbs Free Energy=	0.273664
Sum of electronic and zero-point Energies=	-753.629426
Sum of electronic and thermal Energies=	-753.612119
Sum of electronic and thermal Enthalpies=	-753.611175
Sum of electronic and thermal Free Energies=	-753.674254

Esol = -753.9335337

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	−6.587001	−1.707178	2.936284
2	8	0	−7.344200	−2.758119	2.477362
3	8	0	−5.765121	−1.166490	1.981852
4	6	0	−4.955218	−1.889172	−0.172661
5	1	0	−5.216508	−2.412168	−1.097946
6	1	0	−4.577762	−0.897962	−0.437356
7	1	0	−4.155235	−2.437001	0.328194
8	6	0	−5.783917	−4.202402	1.384565
9	1	0	−5.385084	−4.564046	0.432964
10	1	0	−4.951512	−3.849848	2.001232
11	1	0	−6.260947	−5.039352	1.900596
12	6	0	−6.817076	−3.099262	1.173990
13	6	0	−6.175551	−1.748676	0.719434
14	6	0	−7.954347	−3.590534	0.296196
15	1	0	−7.601946	−3.761655	−0.725814
16	1	0	−8.336873	−4.537255	0.686640
17	1	0	−8.777494	−2.874550	0.270263
18	6	0	−7.190615	−0.792610	0.099436
19	1	0	−6.734187	0.196166	0.006393
20	1	0	−7.498945	−1.126752	−0.894963
21	1	0	−8.081045	−0.701570	0.729060
22	6	0	−7.633246	−1.718265	6.470928
23	6	0	−7.500993	−2.047540	5.161167
24	7	0	−6.694054	−1.279813	4.314449
25	6	0	−6.058625	−0.163272	4.896095

26	6	0	−6.248759	0.093553	6.238661
27	7	0	−7.024110	−0.659346	7.062413
28	1	0	−8.265143	−2.334849	7.104504
29	1	0	−7.991448	−2.897460	4.707950
30	6	0	−5.583833	1.275065	6.904042
31	1	0	−4.493600	1.232159	6.822380
32	1	0	−5.912950	2.225743	6.472979
33	1	0	−5.852291	1.265098	7.960661
34	6	0	−5.214630	0.693633	4.005353
35	1	0	−5.796094	1.079788	3.162140
36	1	0	−4.810328	1.538624	4.560037
37	1	0	−4.381548	0.128187	3.576797

Int14

Thermal correction to Energy=	0.686102
Thermal correction to Enthalpy=	0.687047
Thermal correction to Gibbs Free Energy=	0.578253
Sum of electronic and zero-point Energies=	-2578.828341
Sum of electronic and thermal Energies=	-2578.789312
Sum of electronic and thermal Enthalpies=	-2578.788368
Sum of electronic and thermal Free Energies=	-2578.897161

Esol = -2579.541948

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.583856	−0.758387	0.872370
2	5	0	−2.340451	0.821734	3.635802
3	8	0	2.096062	0.046258	−0.129318
4	8	0	1.719910	−2.106722	0.592110
5	8	0	−2.829549	2.091328	4.089842
6	8	0	−3.285164	−0.195705	3.971828
7	6	0	4.324249	−0.780070	−0.381210
8	1	0	4.667397	0.257844	−0.362457
9	1	0	4.343255	−1.165416	0.643334
10	1	0	5.022325	−1.365074	−0.986087
11	6	0	3.149601	−3.404269	−0.848823
12	1	0	3.620356	−3.448902	−1.836011
13	1	0	3.929964	−3.360998	−0.086967
14	1	0	2.580530	−4.326235	−0.701517
15	6	0	−5.177000	−0.411617	5.431725
16	1	0	−6.026072	0.112372	5.883342

17	1	0	-5.557050	-1.312114	4.940041
18	1	0	-4.491611	-0.721704	6.222830
19	6	0	-3.310300	1.623045	6.389785
20	1	0	-4.085580	1.472257	7.147410
21	1	0	-2.622545	0.772471	6.406947
22	1	0	-2.743806	2.521911	6.650012
23	6	0	-3.902593	1.806533	4.991202
24	6	0	-4.470712	0.470671	4.413601
25	6	0	2.217194	-2.208386	-0.754523
26	6	0	2.909468	-0.821060	-0.954559
27	6	0	2.900126	-0.313191	-2.384548
28	1	0	3.328387	0.692883	-2.422908
29	1	0	3.505690	-0.964118	-3.023172
30	1	0	1.888208	-0.276023	-2.791788
31	6	0	1.007426	-2.396249	-1.666073
32	1	0	1.298784	-2.561527	-2.707478
33	1	0	0.436843	-3.262870	-1.321285
34	1	0	0.362079	-1.513490	-1.621360
35	6	0	-4.881201	2.970729	4.980738
36	1	0	-5.767932	2.742039	5.581373
37	1	0	-4.403164	3.857340	5.407661
38	1	0	-5.197777	3.212916	3.964095
39	6	0	-5.376915	0.708645	3.203476
40	1	0	-5.547328	-0.246633	2.697968
41	1	0	-6.348036	1.119844	3.495751
42	1	0	-4.907538	1.395970	2.493073
43	6	0	0.287120	-1.311135	2.853293
44	6	0	-0.615990	-0.931395	3.757103
45	6	0	0.163318	1.309073	3.629384
46	6	0	1.067427	0.961539	2.691558
47	1	0	0.563839	-2.343404	2.680364
48	7	0	-0.904948	0.429937	3.981944
49	6	0	-0.719301	1.072582	-2.013402
50	6	0	-1.207588	0.230227	-3.015820
51	6	0	-0.648810	0.345779	-4.282425
52	6	0	0.739018	1.997037	-3.656119
53	6	0	0.293367	1.978081	-2.341065
54	6	0	-1.259338	1.016017	-0.633987
55	6	0	-1.783270	-0.164725	-0.093224
56	6	0	-2.264550	-0.162274	1.205009
57	6	0	-1.766987	2.093358	1.448693
58	6	0	-1.283175	2.168636	0.156588
59	1	0	-2.004982	-0.479405	-2.831014
60	1	0	0.748602	2.620271	-1.597883

61	1	0	−1.791839	−1.090346	−0.657922
62	1	0	−2.674239	−1.042376	1.686681
63	1	0	−1.804718	2.950069	2.113201
64	1	0	−0.941559	3.122630	−0.227069
65	7	0	−2.233178	0.946119	1.962551
66	7	0	0.298361	1.204078	−4.616366
67	17	0	1.999708	3.114500	−4.104109
68	17	0	−1.219582	−0.702742	−5.553856
69	1	0	−1.171877	−1.649672	4.349498
70	6	0	0.189656	2.575680	4.437525
71	1	0	−0.763244	3.104148	4.345273
72	1	0	0.297103	2.321590	5.498117
73	1	0	0.996658	3.251615	4.155732
74	6	0	2.262641	1.766832	2.275757
75	1	0	3.171428	1.158537	2.352718
76	1	0	2.182011	2.077811	1.229705
77	1	0	2.392377	2.654406	2.892582
78	7	0	0.976712	−0.334594	2.085648

TS15

Thermal correction to Energy=	0.684859
Thermal correction to Enthalpy=	0.685803
Thermal correction to Gibbs Free Energy=	0.576602
Sum of electronic and zero-point Energies=	-2578.825933
Sum of electronic and thermal Energies=	-2578.786984
Sum of electronic and thermal Enthalpies=	-2578.786040
Sum of electronic and thermal Free Energies=	-2578.895241

Esol = -2579.541201

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.585941	−0.802127	0.712081
2	5	0	−2.305264	0.756746	3.835520
3	8	0	2.107151	0.010428	−0.277369
4	8	0	1.725806	−2.148116	0.423094
5	8	0	−2.742871	2.046263	4.167092
6	8	0	−3.253780	−0.214707	4.161725
7	6	0	4.341422	−0.806225	−0.506258
8	1	0	4.680996	0.232540	−0.475236
9	1	0	4.348991	−1.199732	0.515386
10	1	0	5.048933	−1.384175	−1.107022

11	6	0	3.182488	-3.430471	-1.004556
12	1	0	3.669745	-3.465989	-1.984077
13	1	0	3.949993	-3.390337	-0.229563
14	1	0	2.614291	-4.355497	-0.873831
15	6	0	-5.199600	-0.306224	5.566474
16	1	0	-6.071872	0.247314	5.929388
17	1	0	-5.550252	-1.252922	5.145557
18	1	0	-4.547730	-0.532077	6.412317
19	6	0	-3.467405	1.853658	6.432184
20	1	0	-4.312761	1.790955	7.123708
21	1	0	-2.797331	1.008162	6.616282
22	1	0	-2.916650	2.775021	6.640815
23	6	0	-3.921698	1.874385	4.972801
24	6	0	-4.462807	0.485212	4.496354
25	6	0	2.244339	-2.238567	-0.917260
26	6	0	2.934203	-0.847253	-1.097945
27	6	0	2.939636	-0.325343	-2.522845
28	1	0	3.380356	0.675708	-2.548974
29	1	0	3.539613	-0.977045	-3.165967
30	1	0	1.929779	-0.270147	-2.932867
31	6	0	1.051351	-2.423490	-1.850647
32	1	0	1.362734	-2.584994	-2.886906
33	1	0	0.473883	-3.291071	-1.519986
34	1	0	0.407112	-1.539897	-1.816145
35	6	0	-4.863571	3.042031	4.728850
36	1	0	-5.808227	2.898474	5.263505
37	1	0	-4.405174	3.965840	5.093203
38	1	0	-5.076755	3.164236	3.665061
39	6	0	-5.326742	0.590811	3.239654
40	1	0	-5.475570	-0.413435	2.832087
41	1	0	-6.308060	1.019272	3.465191
42	1	0	-4.840508	1.201486	2.475641
43	6	0	0.290091	-1.362579	2.692479
44	6	0	-0.612881	-0.994158	3.598118
45	6	0	0.151096	1.267076	3.463537
46	6	0	1.048254	0.916661	2.522654
47	1	0	0.565163	-2.394219	2.514663
48	7	0	-0.895429	0.367779	3.830675
49	6	0	-0.649943	1.116449	-2.124621
50	6	0	-1.064905	0.274637	-3.160069
51	6	0	-0.448160	0.420556	-4.396394
52	6	0	0.860401	2.099745	-3.684541
53	6	0	0.352045	2.052600	-2.393624
54	6	0	-1.262606	1.029254	-0.776711

55	6	0	−1.740370	−0.181256	−0.262838
56	6	0	−2.309137	−0.197978	1.004046
57	6	0	−1.975724	2.061004	1.267964
58	6	0	−1.401924	2.175251	0.010566
59	1	0	−1.851044	−0.457886	−3.022168
60	1	0	0.747057	2.702856	−1.623641
61	1	0	−1.649894	−1.107413	−0.820733
62	1	0	−2.681243	−1.116384	1.447748
63	1	0	−2.093566	2.919671	1.924183
64	1	0	−1.085099	3.147524	−0.350324
65	7	0	−2.415072	0.900187	1.759474
66	7	0	0.489537	1.308068	−4.675262
67	17	0	2.111714	3.256730	−4.057187
68	17	0	−0.923492	−0.633428	−5.703356
69	1	0	−1.157483	−1.712551	4.199693
70	6	0	0.172155	2.547946	4.249488
71	1	0	−0.639452	3.216476	3.948079
72	1	0	0.006390	2.317838	5.306619
73	1	0	1.116555	3.083024	4.155139
74	6	0	2.223437	1.741738	2.090254
75	1	0	3.146503	1.155949	2.171191
76	1	0	2.129968	2.034463	1.040707
77	1	0	2.332377	2.644119	2.689223
78	7	0	0.974403	−0.384401	1.925273

TS16

Thermal correction to Energy=	0.529184
Thermal correction to Enthalpy=	0.530128
Thermal correction to Gibbs Free Energy=	0.446162
Sum of electronic and zero-point Energies=	-1164.560320
Sum of electronic and thermal Energies=	-1164.533081
Sum of electronic and thermal Enthalpies=	-1164.532137
Sum of electronic and thermal Free Energies=	-1164.616104

Esol = -1165.015432

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.983719	−5.019135	3.173833
2	5	0	1.876289	−5.115665	1.465167
3	7	0	0.957151	−3.356682	3.268084
4	8	0	1.196355	−6.089706	0.767349

5	8	0	2.396544	-4.157510	0.610983
6	8	0	3.217536	-4.758197	3.830966
7	8	0	1.218375	-5.904214	3.970492
8	6	0	-0.353832	-3.548857	3.471194
9	6	0	1.391278	-2.140353	2.929407
10	6	0	1.450159	-5.889607	-0.639439
11	6	0	1.822812	-4.375791	-0.694567
12	6	0	3.319425	-5.656585	4.941097
13	6	0	1.825111	-5.958183	5.269518
14	6	0	-1.245482	-2.500017	3.343750
15	6	0	0.457727	-1.083633	2.798047
16	6	0	0.207245	-6.272985	-1.425889
17	6	0	2.617481	-6.800095	-1.015119
18	6	0	2.844158	-4.004742	-1.756917
19	6	0	0.598067	-3.467554	-0.795233
20	6	0	4.097950	-4.982343	6.060961
21	6	0	4.067765	-6.899686	4.456288
22	6	0	1.567925	-7.334555	5.864843
23	6	0	1.201925	-4.883947	6.163718
24	7	0	-0.842178	-1.271039	3.006279
25	1	0	-2.307947	-2.647773	3.511631
26	1	0	0.025707	-7.346274	-1.323016
27	1	0	0.338245	-6.050477	-2.489988
28	1	0	-0.675160	-5.743763	-1.061600
29	1	0	2.832952	-6.759291	-2.086815
30	1	0	3.521353	-6.523942	-0.463964
31	1	0	2.360038	-7.829259	-0.751904
32	1	0	3.046730	-2.930828	-1.712302
33	1	0	2.464417	-4.237194	-2.757237
34	1	0	3.786661	-4.533920	-1.606532
35	1	0	0.122756	-3.533720	-1.778127
36	1	0	-0.142811	-3.723778	-0.030832
37	1	0	0.910292	-2.431460	-0.635215
38	1	0	5.130587	-4.816194	5.740679
39	1	0	4.118257	-5.611291	6.957389
40	1	0	3.664511	-4.014360	6.320084
41	1	0	4.258328	-7.607614	5.268701
42	1	0	3.499936	-7.408806	3.671475
43	1	0	5.027717	-6.588477	4.035497
44	1	0	0.500308	-7.451829	6.072879
45	1	0	2.113089	-7.462209	6.806146
46	1	0	1.865744	-8.125091	5.173806
47	1	0	1.571004	-4.958998	7.191228
48	1	0	1.419695	-3.879266	5.791416

49	1	0	0.116236	−5.018982	6.182905
50	6	0	2.849039	−1.910943	2.672788
51	1	0	3.202699	−1.053344	3.253806
52	1	0	3.432418	−2.790577	2.936575
53	1	0	3.008547	−1.687623	1.613471
54	1	0	−0.649738	−4.560220	3.729336
55	6	0	0.911236	0.291935	2.406428
56	1	0	0.043141	0.945440	2.320123
57	1	0	1.597711	0.709346	3.150286
58	1	0	1.443549	0.274003	1.449902

Int15

Thermal correction to Energy=	0.530501
Thermal correction to Enthalpy=	0.531445
Thermal correction to Gibbs Free Energy=	0.446431
Sum of electronic and zero-point Energies=	-1164.561468
Sum of electronic and thermal Energies=	-1164.533890
Sum of electronic and thermal Enthalpies=	-1164.532946
Sum of electronic and thermal Free Energies=	-1164.617960

Esol = -1165.017112

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.617146	−4.611751	3.152236
2	5	0	1.533711	−4.936552	1.457022
3	7	0	0.949067	−3.038609	3.343197
4	8	0	1.637392	−6.207917	0.927256
5	8	0	1.440675	−3.987472	0.451057
6	8	0	2.942874	−4.545301	3.742209
7	8	0	0.828335	−5.497538	3.973491
8	6	0	−0.317699	−2.971875	3.777178
9	6	0	1.601458	−1.914613	3.016853
10	6	0	1.888968	−6.080555	−0.486862
11	6	0	1.276295	−4.681593	−0.804554
12	6	0	3.041037	−5.624703	4.666848
13	6	0	1.570931	−5.772817	5.163038
14	6	0	−0.941665	−1.746208	3.905699
15	6	0	0.940214	−0.674660	3.178682
16	6	0	1.239244	−7.244728	−1.216468
17	6	0	3.405279	−6.118883	−0.670528
18	6	0	1.987913	−3.903747	−1.899440

19	6	0	−0.223624	−4.742424	−1.085919
20	6	0	4.046007	−5.260236	5.750354
21	6	0	3.514322	−6.864935	3.903439
22	6	0	1.200392	−7.165240	5.652982
23	6	0	1.223140	−4.734464	6.233907
24	7	0	−0.314207	−0.604233	3.617441
25	1	0	−1.966725	−1.680078	4.256196
26	1	0	1.730906	−8.177694	−0.927644
27	1	0	1.341067	−7.127944	−2.300483
28	1	0	0.179571	−7.329562	−0.969314
29	1	0	3.687296	−6.093204	−1.727185
30	1	0	3.882109	−5.277427	−0.158163
31	1	0	3.789081	−7.042852	−0.230148
32	1	0	1.491348	−2.940791	−2.048269
33	1	0	1.955938	−4.451986	−2.846712
34	1	0	3.030851	−3.712244	−1.640081
35	1	0	−0.434174	−5.197913	−2.057909
36	1	0	−0.742701	−5.313753	−0.310665
37	1	0	−0.624551	−3.725343	−1.086159
38	1	0	5.046765	−5.188116	5.314075
39	1	0	4.073462	−6.024186	6.534911
40	1	0	3.806233	−4.297033	6.205965
41	1	0	3.691751	−7.716009	4.568688
42	1	0	2.781529	−7.150074	3.142515
43	1	0	4.452533	−6.622531	3.395375
44	1	0	0.162348	−7.172659	5.999386
45	1	0	1.838837	−7.471420	6.488847
46	1	0	1.293286	−7.898312	4.849563
47	1	0	1.691670	−4.971919	7.194281
48	1	0	1.545804	−3.733316	5.931959
49	1	0	0.138618	−4.720298	6.381093
50	6	0	3.007354	−1.999952	2.508465
51	1	0	3.702882	−2.126236	3.342172
52	1	0	3.123291	−2.865158	1.855934
53	1	0	3.267940	−1.098793	1.953844
54	1	0	−0.783068	−3.919804	4.018694
55	6	0	1.629896	0.623296	2.868757
56	1	0	0.976201	1.445980	3.158116
57	1	0	2.576968	0.711137	3.408859
58	1	0	1.849234	0.709391	1.799753

TS17

Thermal correction to Energy= 0.672339

Thermal correction to Enthalpy=	0.673283
Thermal correction to Gibbs Free Energy=	0.573014
Sum of electronic and zero-point Energies=	-1507.259823
Sum of electronic and thermal Energies=	-1507.224398
Sum of electronic and thermal Enthalpies=	-1507.223454
Sum of electronic and thermal Free Energies=	-1507.323723

Esol = -1507.82974

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.780623	-4.512608	1.637207
2	5	0	1.678931	-4.679019	-0.086201
3	7	0	0.229828	-3.258267	1.927329
4	8	0	0.447555	-5.193048	-0.657567
5	8	0	2.755312	-5.462338	-0.639862
6	8	0	2.830537	-3.791973	2.266693
7	8	0	1.488946	-5.661199	2.427010
8	6	0	-1.050349	-3.543953	1.679060
9	6	0	0.600957	-1.972374	1.997994
10	6	0	0.752817	-6.409565	-1.337477
11	6	0	2.245328	-6.205261	-1.743874
12	6	0	3.043122	-4.354561	3.569088
13	6	0	2.550838	-5.820711	3.370655
14	6	0	-1.970640	-2.489822	1.457701
15	6	0	-0.314636	-0.956944	1.790092
16	6	0	-0.205130	-6.583293	-2.507995
17	6	0	0.580920	-7.556392	-0.339401
18	6	0	3.050977	-7.490105	-1.875047
19	6	0	2.391117	-5.367597	-3.017827
20	6	0	2.192733	-3.592076	4.586392
21	6	0	4.518369	-4.217659	3.915715
22	6	0	3.613145	-6.705460	2.714041
23	6	0	2.011739	-6.489152	4.626489
24	7	0	-1.596205	-1.214173	1.506070
25	1	0	-1.224799	-6.716470	-2.133142
26	1	0	0.053530	-7.467873	-3.100095
27	1	0	-0.197006	-5.709522	-3.163749
28	1	0	0.768031	-8.533461	-0.796092
29	1	0	1.249510	-7.414607	0.515082
30	1	0	-0.447466	-7.545348	0.034886
31	1	0	4.072789	-7.254472	-2.187994
32	1	0	2.612699	-8.159215	-2.623527

33	1	0	3.103149	-8.013827	-0.918275
34	1	0	2.136024	-5.940835	-3.914977
35	1	0	1.753486	-4.479403	-2.984045
36	1	0	3.431180	-5.038228	-3.103680
37	1	0	2.440832	-2.527312	4.536072
38	1	0	2.385328	-3.936013	5.607361
39	1	0	1.126629	-3.710154	4.373617
40	1	0	4.755428	-4.744034	4.846471
41	1	0	5.146628	-4.615149	3.115882
42	1	0	4.769376	-3.161071	4.052391
43	1	0	3.153857	-7.661644	2.446119
44	1	0	4.456550	-6.905316	3.382421
45	1	0	3.980314	-6.241019	1.793473
46	1	0	2.784197	-6.553236	5.400521
47	1	0	1.154034	-5.946574	5.029065
48	1	0	1.686886	-7.505990	4.387789
49	6	0	0.473370	-1.175814	-1.449536
50	6	0	0.587921	-2.524893	-1.173242
51	7	0	1.753596	-3.038039	-0.745274
52	6	0	2.817059	-2.230138	-0.631000
53	6	0	2.665862	-0.852109	-0.917735
54	7	0	1.503345	-0.337076	-1.309102
55	1	0	-0.473586	-0.756675	-1.775739
56	6	0	4.145773	-2.772774	-0.201725
57	1	0	4.919528	-2.425897	-0.893930
58	1	0	4.393383	-2.408494	0.799358
59	1	0	4.135119	-3.859739	-0.182640
60	1	0	-0.229269	-3.230388	-1.265012
61	6	0	3.829543	0.085627	-0.781835
62	1	0	4.612575	-0.151385	-1.509781
63	1	0	3.487764	1.106173	-0.954117
64	1	0	4.281284	0.018533	0.212586
65	6	0	-1.492549	-4.975044	1.640074
66	1	0	-2.320883	-5.128582	2.340369
67	1	0	-1.841649	-5.234556	0.636637
68	1	0	-0.663955	-5.631794	1.900506
69	6	0	-3.410375	-2.784487	1.153876
70	1	0	-3.505646	-3.441320	0.283408
71	1	0	-3.893858	-3.292514	1.994965
72	1	0	-3.935997	-1.849755	0.957872
73	1	0	-0.013112	0.085595	1.834379
74	1	0	1.652052	-1.794208	2.202493

Int16

Thermal correction to Energy=	0.673353
Thermal correction to Enthalpy=	0.674297
Thermal correction to Gibbs Free Energy=	0.573298
Sum of electronic and zero-point Energies=	-1507.259703
Sum of electronic and thermal Energies=	-1507.223901
Sum of electronic and thermal Enthalpies=	-1507.222957
Sum of electronic and thermal Free Energies=	-1507.323956

Esol = -1507.829543

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.600497	-4.410982	1.651496
2	5	0	1.612796	-4.689086	-0.072768
3	7	0	0.242770	-3.292486	1.880282
4	8	0	0.413258	-5.178673	-0.724688
5	8	0	2.704984	-5.494309	-0.543378
6	8	0	2.743650	-3.727084	2.210383
7	8	0	1.349097	-5.562745	2.495544
8	6	0	-1.045304	-3.609640	1.688546
9	6	0	0.584229	-1.996346	1.985364
10	6	0	0.740554	-6.403709	-1.380046
11	6	0	2.261441	-6.230621	-1.680535
12	6	0	3.024078	-4.292370	3.491767
13	6	0	2.488502	-5.748263	3.329664
14	6	0	-1.998007	-2.568996	1.563799
15	6	0	-0.368989	-1.004356	1.865149
16	6	0	-0.137154	-6.563679	-2.613295
17	6	0	0.477795	-7.541864	-0.391580
18	6	0	3.049578	-7.530711	-1.752086
19	6	0	2.513535	-5.398564	-2.941280
20	6	0	2.256565	-3.516097	4.565728
21	6	0	4.521087	-4.187653	3.746148
22	6	0	3.480062	-6.647891	2.587184
23	6	0	2.052522	-6.412579	4.628540
24	7	0	-1.656162	-1.286066	1.642259
25	1	0	-1.183018	-6.671481	-2.309092
26	1	0	0.141864	-7.457311	-3.182061
27	1	0	-0.063905	-5.693967	-3.270177
28	1	0	0.687006	-8.524409	-0.826113
29	1	0	1.083783	-7.402917	0.509640
30	1	0	-0.575928	-7.517528	-0.096912

31	1	0	4.095880	-7.314627	-1.988835
32	1	0	2.654900	-8.191993	-2.531188
33	1	0	3.021590	-8.054850	-0.794535
34	1	0	2.309262	-5.968614	-3.853345
35	1	0	1.894043	-4.497221	-2.951720
36	1	0	3.564067	-5.092153	-2.955063
37	1	0	2.515168	-2.454692	4.495952
38	1	0	2.510761	-3.859822	5.573370
39	1	0	1.176071	-3.619732	4.427657
40	1	0	4.805847	-4.718707	4.660909
41	1	0	5.087437	-4.599995	2.908436
42	1	0	4.804335	-3.136679	3.864356
43	1	0	2.984258	-7.596706	2.359158
44	1	0	4.370199	-6.864421	3.186817
45	1	0	3.776202	-6.189431	1.638896
46	1	0	2.888424	-6.489162	5.332619
47	1	0	1.240376	-5.859800	5.105242
48	1	0	1.693965	-7.424666	4.418903
49	6	0	0.516705	-1.128689	-1.427533
50	6	0	0.610180	-2.486094	-1.186665
51	7	0	1.764234	-3.030078	-0.763717
52	6	0	2.838022	-2.240248	-0.622864
53	6	0	2.709784	-0.852594	-0.874212
54	7	0	1.557748	-0.308608	-1.257888
55	1	0	-0.420830	-0.687224	-1.751962
56	6	0	4.160005	-2.815098	-0.215269
57	1	0	4.917511	-2.539007	-0.957069
58	1	0	4.465367	-2.405891	0.751534
59	1	0	4.104292	-3.897591	-0.134509
60	1	0	-0.217422	-3.175758	-1.305537
61	6	0	3.888826	0.061228	-0.711166
62	1	0	4.685249	-0.194666	-1.417776
63	1	0	3.573441	1.088666	-0.892728
64	1	0	4.314057	-0.013436	0.294562
65	6	0	-1.476073	-5.041214	1.597944
66	1	0	-2.291403	-5.221329	2.306482
67	1	0	-1.846540	-5.250666	0.590519
68	1	0	-0.649913	-5.713624	1.815565
69	6	0	-3.445413	-2.888748	1.330740
70	1	0	-3.575234	-3.522781	0.448174
71	1	0	-3.870716	-3.429720	2.182537
72	1	0	-3.998737	-1.960064	1.191542
73	1	0	-0.089827	0.042605	1.935251
74	1	0	1.638031	-1.801794	2.146649

TS18

Thermal correction to Energy=	0.673337
Thermal correction to Enthalpy=	0.674281
Thermal correction to Gibbs Free Energy=	0.575713
Sum of electronic and zero-point Energies=	-1507.236065
Sum of electronic and thermal Energies=	-1507.201163
Sum of electronic and thermal Enthalpies=	-1507.200219
Sum of electronic and thermal Free Energies=	-1507.298787

Esol = -1507.806372

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.395386	-4.131739	1.933058
2	5	0	1.565412	-4.343654	-0.338112
3	7	0	0.134902	-3.318840	1.872310
4	8	0	0.350791	-4.861026	-0.839050
5	8	0	2.617548	-5.253708	-0.555557
6	8	0	2.553923	-3.447041	2.354742
7	8	0	1.373649	-5.440262	2.448569
8	6	0	-1.157633	-3.794982	1.692232
9	6	0	0.289435	-1.957607	1.853280
10	6	0	0.644418	-6.148661	-1.421303
11	6	0	2.186588	-6.068037	-1.658815
12	6	0	3.060115	-4.181576	3.483148
13	6	0	2.599982	-5.645820	3.172345
14	6	0	-2.201195	-2.895873	1.535713
15	6	0	-0.807668	-1.119888	1.733974
16	1	0	1.293763	-1.587910	2.013742
17	6	0	-0.185838	-6.297971	-2.687380
18	6	0	0.287523	-7.248083	-0.425704
19	6	0	2.922980	-7.395458	-1.597868
20	6	0	2.539015	-5.326168	-2.949440
21	6	0	2.384570	-3.608118	4.729748
22	6	0	4.565307	-3.989288	3.562190
23	6	0	3.573245	-6.405177	2.274475
24	6	0	2.286358	-6.477389	4.408815
25	7	0	-2.049440	-1.549268	1.569605
26	1	0	-0.641196	-0.045572	1.761568
27	1	0	-1.246824	-6.343336	-2.425504
28	1	0	0.072665	-7.221619	-3.215914

29	1	0	-0.039424	-5.452673	-3.362348
30	1	0	0.485139	-8.236993	-0.849810
31	1	0	0.863476	-7.132646	0.498564
32	1	0	-0.777055	-7.193015	-0.186682
33	1	0	3.989092	-7.229074	-1.776933
34	1	0	2.552575	-8.083639	-2.364746
35	1	0	2.812079	-7.864078	-0.618508
36	1	0	2.289687	-5.915614	-3.836567
37	1	0	2.012718	-4.367898	-3.011512
38	1	0	3.614315	-5.127435	-2.960901
39	1	0	2.593466	-2.536020	4.780920
40	1	0	2.752266	-4.076578	5.647135
41	1	0	1.298718	-3.741404	4.682010
42	1	0	4.986820	-4.574569	4.385928
43	1	0	5.057233	-4.288063	2.634600
44	1	0	4.790113	-2.934411	3.744494
45	1	0	3.103594	-7.347166	1.974713
46	1	0	4.500154	-6.641461	2.806167
47	1	0	3.801001	-5.847161	1.364131
48	1	0	3.172592	-6.576598	5.044384
49	1	0	1.479508	-6.034648	4.995498
50	1	0	1.974191	-7.480310	4.104462
51	6	0	0.805260	-0.731874	-0.920416
52	6	0	0.687257	-2.105498	-0.782013
53	7	0	1.789464	-2.878991	-0.532137
54	6	0	2.999400	-2.208886	-0.359827
55	6	0	3.029052	-0.828677	-0.471223
56	7	0	1.941231	-0.070463	-0.766528
57	1	0	-0.088175	-0.157745	-1.155479
58	1	0	-0.243135	-2.635452	-0.942459
59	6	0	-1.423653	-5.264694	1.777792
60	1	0	-0.533798	-5.843651	1.563486
61	1	0	-1.763578	-5.533275	2.785971
62	1	0	-2.210140	-5.544941	1.074263
63	6	0	-3.613522	-3.390691	1.372180
64	1	0	-3.736118	-3.958305	0.443855
65	1	0	-3.912040	-4.044364	2.197702
66	1	0	-4.282548	-2.530336	1.345614
67	6	0	4.248533	-3.008704	-0.148158
68	1	0	5.033653	-2.374595	0.263418
69	1	0	4.068074	-3.831306	0.538602
70	1	0	4.605255	-3.434807	-1.092354
71	6	0	4.319422	-0.063987	-0.320932
72	1	0	4.746331	-0.182103	0.679979

73	1	0	5.073187	−0.391895	−1.043033
74	1	0	4.113355	0.993275	−0.488736

Int17

Thermal correction to Energy=	0.677441
Thermal correction to Enthalpy=	0.678386
Thermal correction to Gibbs Free Energy=	0.578230
Sum of electronic and zero-point Energies=	-1507.306756
Sum of electronic and thermal Energies=	-1507.271499
Sum of electronic and thermal Enthalpies=	-1507.270554
Sum of electronic and thermal Free Energies=	-1507.370710

Esol = -1507.882143

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.104280	−3.957714	2.582139
2	5	0	1.687803	−4.165369	−1.026427
3	7	0	0.027538	−3.294188	1.916852
4	8	0	0.508188	−4.731914	−1.456155
5	8	0	2.782787	−4.977559	−1.229006
6	8	0	2.347811	−3.372444	2.726193
7	8	0	1.024533	−5.198808	3.175474
8	6	0	−1.274282	−3.797320	1.748791
9	6	0	0.273610	−1.983155	1.319569
10	6	0	0.812701	−6.085056	−1.861970
11	6	0	2.353113	−6.018120	−2.133831
12	6	0	3.030715	−4.144951	3.740836
13	6	0	2.369989	−5.548111	3.570920
14	6	0	−2.292471	−2.934493	1.506434
15	6	0	−0.911067	−1.094326	1.602900
16	1	0	1.178292	−1.562953	1.764998
17	6	0	−0.031074	−6.430957	−3.077876
18	6	0	0.460663	−7.003007	−0.696789
19	6	0	3.116399	−7.290424	−1.807828
20	6	0	2.684210	−5.542219	−3.546328
21	6	0	2.703824	−3.502880	5.087772
22	6	0	4.527890	−4.108039	3.491773
23	6	0	2.980902	−6.353209	2.425504
24	6	0	2.307240	−6.381468	4.839039
25	7	0	−2.103945	−1.544756	1.633050
26	1	0	−0.747615	−0.030367	1.774943

27	1	0	-1.087430	-6.446035	-2.796937
28	1	0	0.233949	-7.421860	-3.460282
29	1	0	0.097796	-5.698798	-3.876644
30	1	0	0.654800	-8.051469	-0.939435
31	1	0	1.035309	-6.736553	0.197104
32	1	0	-0.602563	-6.894702	-0.470135
33	1	0	4.178101	-7.145062	-2.024510
34	1	0	2.755694	-8.124652	-2.417810
35	1	0	3.016588	-7.555156	-0.752992
36	1	0	2.444107	-6.303151	-4.293963
37	1	0	2.136805	-4.626801	-3.791274
38	1	0	3.753724	-5.324449	-3.603674
39	1	0	3.005662	-2.452792	5.060225
40	1	0	3.235030	-3.995069	5.906971
41	1	0	1.629657	-3.544554	5.293138
42	1	0	5.049215	-4.707471	4.245064
43	1	0	4.790464	-4.487880	2.503983
44	1	0	4.886746	-3.077979	3.570176
45	1	0	2.350495	-7.227145	2.237138
46	1	0	3.987312	-6.703665	2.671478
47	1	0	3.031332	-5.759417	1.504543
48	1	0	3.314523	-6.579478	5.218944
49	1	0	1.729232	-5.879164	5.616611
50	1	0	1.829519	-7.341428	4.625440
51	6	0	0.653548	-0.739333	-0.836251
52	6	0	0.515982	-2.108024	-0.213278
53	7	0	1.745803	-2.848363	-0.477444
54	6	0	2.928497	-2.125413	-0.235770
55	6	0	2.894638	-0.771842	-0.308648
56	7	0	1.763558	-0.109224	-0.823511
57	1	0	-0.213411	-0.267950	-1.299179
58	1	0	-0.324298	-2.652408	-0.650201
59	6	0	-3.717370	-3.364455	1.271503
60	1	0	-4.164406	-3.835120	2.154545
61	1	0	-4.312604	-2.481989	1.030363
62	1	0	-3.805967	-4.070354	0.440013
63	6	0	-1.496818	-5.269629	1.922916
64	1	0	-1.543349	-5.536136	2.983940
65	1	0	-2.434763	-5.568950	1.453174
66	1	0	-0.679709	-5.842607	1.486426
67	6	0	4.185167	-2.890452	0.048625
68	1	0	4.664953	-3.229731	-0.874926
69	1	0	4.892606	-2.265417	0.596669
70	1	0	3.956760	-3.772220	0.647131

71	6	0	4.081839	0.109720	−0.021515
72	1	0	4.909273	−0.060969	−0.719241
73	1	0	3.775245	1.152704	−0.118338
74	1	0	4.469180	−0.038121	0.991698

TS19

Thermal correction to Energy=	0.673271
Thermal correction to Enthalpy=	0.674215
Thermal correction to Gibbs Free Energy=	0.573546
Sum of electronic and zero-point Energies=	-1507.256019
Sum of electronic and thermal Energies=	-1507.220512
Sum of electronic and thermal Enthalpies=	-1507.219567
Sum of electronic and thermal Free Energies=	-1507.320236

Esol = -1507.834495

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.098511	−3.984716	2.461483
2	5	0	1.691559	−4.158552	−0.994432
3	7	0	−0.033852	−3.246148	1.958258
4	8	0	0.536934	−4.725911	−1.481018
5	8	0	2.781883	−4.997501	−1.062889
6	8	0	2.326291	−3.381775	2.646966
7	8	0	1.051073	−5.274900	2.936796
8	6	0	−1.355783	−3.740980	1.830231
9	6	0	0.131776	−1.882705	1.691121
10	6	0	0.850827	−6.099398	−1.812091
11	6	0	2.407083	−6.060024	−1.969686
12	6	0	3.009458	−4.195184	3.631618
13	6	0	2.389680	−5.606364	3.375128
14	6	0	−2.390744	−2.865118	1.679398
15	6	0	−0.994726	−1.058148	1.666920
16	1	0	1.130369	−1.488852	1.830062
17	6	0	0.095272	−6.477937	−3.075180
18	6	0	0.404145	−6.971110	−0.645206
19	6	0	3.127208	−7.330804	−1.554364
20	6	0	2.850479	−5.624975	−3.364578
21	6	0	2.637150	−3.629720	5.001231
22	6	0	4.510558	−4.108740	3.421426
23	6	0	3.067849	−6.359479	2.234359
24	6	0	2.290284	−6.487502	4.609110

25	7	0	-2.237936	-1.488359	1.653830
26	1	0	-0.831734	0.016526	1.597810
27	1	0	-0.979039	-6.474250	-2.873287
28	1	0	0.376617	-7.483397	-3.403951
29	1	0	0.291284	-5.773935	-3.885493
30	1	0	0.601673	-8.028949	-0.840019
31	1	0	0.917733	-6.680678	0.278117
32	1	0	-0.671412	-6.845604	-0.499701
33	1	0	4.204458	-7.199169	-1.686891
34	1	0	2.808390	-8.174275	-2.174790
35	1	0	2.938670	-7.572582	-0.506568
36	1	0	2.657912	-6.403403	-4.107872
37	1	0	2.335126	-4.710772	-3.675300
38	1	0	3.924127	-5.421005	-3.345919
39	1	0	2.918783	-2.574272	5.034299
40	1	0	3.157061	-4.153415	5.807860
41	1	0	1.559110	-3.700255	5.177374
42	1	0	5.027595	-4.729351	4.160316
43	1	0	4.808929	-4.436979	2.425363
44	1	0	4.839854	-3.074769	3.556563
45	1	0	2.478158	-7.253559	2.010078
46	1	0	4.076969	-6.678951	2.509968
47	1	0	3.124789	-5.748808	1.325818
48	1	0	3.284938	-6.679759	5.023714
49	1	0	1.670088	-6.027399	5.380144
50	1	0	1.842927	-7.447853	4.339456
51	6	0	0.685646	-0.636320	-0.907497
52	6	0	0.570842	-2.008752	-0.677218
53	7	0	1.739166	-2.775564	-0.594504
54	6	0	2.922765	-2.050321	-0.308279
55	6	0	2.913147	-0.689760	-0.406867
56	7	0	1.803246	0.048526	-0.786798
57	1	0	-0.223348	-0.081703	-1.136612
58	1	0	-0.343717	-2.553744	-0.872542
59	6	0	-3.818524	-3.339962	1.566107
60	1	0	-4.120506	-3.952030	2.421555
61	1	0	-4.467308	-2.464347	1.523397
62	1	0	-3.984760	-3.932096	0.660016
63	6	0	-1.558330	-5.220238	1.930487
64	1	0	-1.519914	-5.562115	2.970394
65	1	0	-2.524293	-5.501037	1.510199
66	1	0	-0.774823	-5.753708	1.394106
67	6	0	4.150539	-2.828483	0.049323
68	1	0	4.669396	-3.202635	-0.839848

69	1	0	4.841407	-2.203494	0.617112
70	1	0	3.880733	-3.688171	0.661208
71	6	0	4.151410	0.127268	-0.133728
72	1	0	5.002801	-0.194957	-0.740956
73	1	0	3.933620	1.169665	-0.369119
74	1	0	4.454910	0.070922	0.917318

Int18

Thermal correction to Energy=	0.677408
Thermal correction to Enthalpy=	0.678352
Thermal correction to Gibbs Free Energy=	0.579196
Sum of electronic and zero-point Energies=	-1507.311452
Sum of electronic and thermal Energies=	-1507.276517
Sum of electronic and thermal Enthalpies=	-1507.275572
Sum of electronic and thermal Free Energies=	-1507.374728

Esol = -1507.883989

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	0.935341	-3.863350	2.616329
2	5	0	-1.564421	-1.859197	-1.636022
3	7	0	-0.197697	-3.285754	1.964380
4	8	0	-1.362271	-0.494163	-1.650868
5	8	0	-2.726226	-2.237809	-2.269093
6	8	0	2.136783	-3.185139	2.670743
7	8	0	0.982964	-5.089657	3.239067
8	6	0	-1.469709	-3.881063	1.820381
9	6	0	0.007127	-1.997706	1.299968
10	6	0	-2.577188	0.102985	-2.155335
11	6	0	-3.204553	-1.071992	-2.977296
12	6	0	3.009352	-3.952110	3.527696
13	6	0	2.386148	-5.382422	3.434119
14	6	0	-2.534045	-3.095092	1.534828
15	6	0	-1.248157	-1.176747	1.419940
16	1	0	0.830358	-1.482189	1.803286
17	6	0	-2.213298	1.326777	-2.979892
18	6	0	-3.424590	0.505308	-0.951850
19	6	0	-4.722965	-1.099388	-2.992862
20	6	0	-2.653554	-1.160242	-4.398599
21	6	0	2.906957	-3.353866	4.927961
22	6	0	4.428952	-3.843664	2.997720

23	6	0	2.853075	-6.147567	2.197842
24	6	0	2.541284	-6.229451	4.684733
25	7	0	-2.412243	-1.688718	1.494559
26	1	0	-1.156015	-0.089636	1.410672
27	1	0	-1.780306	2.090705	-2.328558
28	1	0	-3.105126	1.750253	-3.452851
29	1	0	-1.483619	1.086400	-3.755057
30	1	0	-4.345777	1.005148	-1.264954
31	1	0	-3.674952	-0.358751	-0.329969
32	1	0	-2.850603	1.202894	-0.335208
33	1	0	-5.068151	-1.955207	-3.579275
34	1	0	-5.118847	-0.188978	-3.454068
35	1	0	-5.130227	-1.188121	-1.984180
36	1	0	-3.022427	-0.343493	-5.025172
37	1	0	-1.559505	-1.134189	-4.398146
38	1	0	-2.971602	-2.107459	-4.841887
39	1	0	3.160775	-2.291800	4.878400
40	1	0	3.594513	-3.841835	5.624507
41	1	0	1.888984	-3.444539	5.318771
42	1	0	5.102274	-4.497137	3.561627
43	1	0	4.476952	-4.113025	1.940828
44	1	0	4.784475	-2.815248	3.106441
45	1	0	2.224601	-7.034634	2.077464
46	1	0	3.892960	-6.472645	2.295783
47	1	0	2.758177	-5.533002	1.295588
48	1	0	3.600394	-6.390484	4.909728
49	1	0	2.064632	-5.760788	5.547554
50	1	0	2.076089	-7.206044	4.525838
51	6	0	1.710360	-2.909069	-0.320407
52	6	0	0.427997	-2.127230	-0.198403
53	7	0	-0.604507	-2.736901	-1.039366
54	6	0	-0.584829	-4.139607	-1.159507
55	6	0	0.562252	-4.819729	-0.926661
56	7	0	1.764240	-4.146257	-0.622700
57	1	0	2.642615	-2.386064	-0.104806
58	1	0	0.596448	-1.105401	-0.553025
59	6	0	-3.943168	-3.545262	1.276461
60	1	0	-4.070635	-4.627158	1.294885
61	1	0	-4.619037	-3.108333	2.019252
62	1	0	-4.270941	-3.180687	0.294972
63	6	0	-1.541776	-5.367120	2.013723
64	1	0	-0.737301	-5.853217	1.455910
65	1	0	-1.408255	-5.638979	3.064518
66	1	0	-2.496473	-5.763211	1.671827

67	6	0	−1.853338	−4.825270	−1.572277
68	1	0	−2.699471	−4.429764	−1.005137
69	1	0	−2.074522	−4.661813	−2.631515
70	1	0	−1.779944	−5.898325	−1.392170
71	6	0	0.697855	−6.315541	−1.061941
72	1	0	0.331805	−6.683316	−2.025613
73	1	0	1.756356	−6.572574	−0.987990
74	1	0	0.165473	−6.867768	−0.278387

TS19

Thermal correction to Energy=	0.674581
Thermal correction to Enthalpy=	0.675525
Thermal correction to Gibbs Free Energy=	0.578010
Sum of electronic and zero-point Energies=	-1507.278166
Sum of electronic and thermal Energies=	-1507.243656
Sum of electronic and thermal Enthalpies=	-1507.242712
Sum of electronic and thermal Free Energies=	-1507.340226

Esol = -1507.851837

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.012122	−3.931400	2.626290
2	5	0	−1.601832	−1.827192	−1.776574
3	7	0	−0.198075	−3.373695	2.062589
4	8	0	−1.324394	−0.475551	−1.767289
5	8	0	−2.782354	−2.133844	−2.411701
6	8	0	2.148139	−3.153034	2.713730
7	8	0	1.141364	−5.148980	3.251337
8	6	0	−1.395411	−4.071662	1.798598
9	6	0	−0.134944	−2.044425	1.616579
10	6	0	−2.523893	0.194545	−2.214529
11	6	0	−3.228762	−0.921061	−3.056966
12	6	0	3.048678	−3.833159	3.613559
13	6	0	2.550861	−5.314794	3.531185
14	6	0	−2.439726	−3.423431	1.206594
15	6	0	−1.304936	−1.424370	1.188531
16	1	0	0.717780	−1.475191	1.959856
17	6	0	−2.124677	1.427927	−3.007771
18	6	0	−3.318104	0.591543	−0.972837
19	6	0	−4.746705	−0.882855	−3.018514
20	6	0	−2.729654	−0.978687	−4.498902

21	6	0	2.846996	-3.215802	4.995215
22	6	0	4.473770	-3.616378	3.134193
23	6	0	3.155560	-6.082794	2.358968
24	6	0	2.698669	-6.104308	4.820894
25	7	0	-2.403499	-2.077917	0.872121
26	1	0	-1.271876	-0.360889	0.958880
27	1	0	-1.632902	2.144795	-2.344724
28	1	0	-3.008795	1.912233	-3.434728
29	1	0	-1.433380	1.181271	-3.815470
30	1	0	-4.233344	1.127026	-1.241418
31	1	0	-3.570208	-0.287692	-0.372148
32	1	0	-2.703518	1.260509	-0.362965
33	1	0	-5.149533	-1.693236	-3.632232
34	1	0	-5.119133	0.065282	-3.419403
35	1	0	-5.118591	-1.006957	-1.999855
36	1	0	-3.081658	-0.123697	-5.082839
37	1	0	-1.636068	-1.000320	-4.534306
38	1	0	-3.103976	-1.894002	-4.964881
39	1	0	3.020725	-2.138604	4.929212
40	1	0	3.541486	-3.634116	5.729095
41	1	0	1.824274	-3.375385	5.349955
42	1	0	5.177442	-4.190958	3.744958
43	1	0	4.589470	-3.912971	2.090052
44	1	0	4.733741	-2.557835	3.222075
45	1	0	2.640831	-7.044356	2.272225
46	1	0	4.219966	-6.279050	2.517494
47	1	0	3.016847	-5.537958	1.420200
48	1	0	3.752529	-6.173559	5.109088
49	1	0	2.138981	-5.647268	5.638845
50	1	0	2.320176	-7.119281	4.673321
51	6	0	1.541351	-3.070712	-0.247763
52	6	0	0.516449	-2.217981	-0.649639
53	7	0	-0.604240	-2.761281	-1.296048
54	6	0	-0.715257	-4.166693	-1.291650
55	6	0	0.266825	-4.922237	-0.719456
56	7	0	1.411558	-4.378296	-0.158411
57	1	0	2.451205	-2.629533	0.153089
58	1	0	0.687740	-1.163030	-0.813774
59	6	0	-3.753802	-4.095611	0.897073
60	1	0	-3.633503	-5.105135	0.497612
61	1	0	-4.394537	-4.159899	1.784159
62	1	0	-4.277229	-3.489788	0.153585
63	6	0	-1.454136	-5.493382	2.258342
64	1	0	-0.621159	-6.070196	1.847429

65	1	0	−1.361559	−5.550792	3.347681
66	1	0	−2.393848	−5.959427	1.966201
67	6	0	−1.888374	−4.753229	−2.011864
68	1	0	−2.830791	−4.369764	−1.614228
69	1	0	−1.863791	−4.476328	−3.071072
70	1	0	−1.883989	−5.839705	−1.940100
71	6	0	0.220437	−6.430000	−0.693791
72	1	0	−0.760079	−6.820581	−0.410847
73	1	0	0.484630	−6.860878	−1.666391
74	1	0	0.954978	−6.781766	0.034012

TS19a

Thermal correction to Energy=	0.673271
Thermal correction to Enthalpy=	0.674215
Thermal correction to Gibbs Free Energy=	0.573546
Sum of electronic and zero-point Energies=	-1507.256019
Sum of electronic and thermal Energies=	-1507.220512
Sum of electronic and thermal Enthalpies=	-1507.219567
Sum of electronic and thermal Free Energies=	-1507.320236

Esol = -1507.834495

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.098511	−3.984716	2.461483
2	5	0	1.691559	−4.158552	−0.994432
3	7	0	−0.033852	−3.246148	1.958258
4	8	0	0.536934	−4.725911	−1.481018
5	8	0	2.781883	−4.997501	−1.062889
6	8	0	2.326291	−3.381775	2.646966
7	8	0	1.051073	−5.274900	2.936796
8	6	0	−1.355783	−3.740980	1.830231
9	6	0	0.131776	−1.882705	1.691121
10	6	0	0.850827	−6.099398	−1.812091
11	6	0	2.407083	−6.060024	−1.969686
12	6	0	3.009458	−4.195184	3.631618
13	6	0	2.389680	−5.606364	3.375128
14	6	0	−2.390744	−2.865118	1.679398
15	6	0	−0.994726	−1.058148	1.666920
16	1	0	1.130369	−1.488852	1.830062
17	6	0	0.095272	−6.477937	−3.075180
18	6	0	0.404145	−6.971110	−0.645206

19	6	0	3.127208	-7.330804	-1.554364
20	6	0	2.850479	-5.624975	-3.364578
21	6	0	2.637150	-3.629720	5.001231
22	6	0	4.510558	-4.108740	3.421426
23	6	0	3.067849	-6.359479	2.234359
24	6	0	2.290284	-6.487502	4.609110
25	7	0	-2.237936	-1.488359	1.653830
26	1	0	-0.831734	0.016526	1.597810
27	1	0	-0.979039	-6.474250	-2.873287
28	1	0	0.376617	-7.483397	-3.403951
29	1	0	0.291284	-5.773935	-3.885493
30	1	0	0.601673	-8.028949	-0.840019
31	1	0	0.917733	-6.680678	0.278117
32	1	0	-0.671412	-6.845604	-0.499701
33	1	0	4.204458	-7.199169	-1.686891
34	1	0	2.808390	-8.174275	-2.174790
35	1	0	2.938670	-7.572582	-0.506568
36	1	0	2.657912	-6.403403	-4.107872
37	1	0	2.335126	-4.710772	-3.675300
38	1	0	3.924127	-5.421005	-3.345919
39	1	0	2.918783	-2.574272	5.034299
40	1	0	3.157061	-4.153415	5.807860
41	1	0	1.559110	-3.700255	5.177374
42	1	0	5.027595	-4.729351	4.160316
43	1	0	4.808929	-4.436979	2.425363
44	1	0	4.839854	-3.074769	3.556563
45	1	0	2.478158	-7.253559	2.010078
46	1	0	4.076969	-6.678951	2.509968
47	1	0	3.124789	-5.748808	1.325818
48	1	0	3.284938	-6.679759	5.023714
49	1	0	1.670088	-6.027399	5.380144
50	1	0	1.842927	-7.447853	4.339456
51	6	0	0.685646	-0.636320	-0.907497
52	6	0	0.570842	-2.008752	-0.677218
53	7	0	1.739166	-2.775564	-0.594504
54	6	0	2.922765	-2.050321	-0.308279
55	6	0	2.913147	-0.689760	-0.406867
56	7	0	1.803246	0.048526	-0.786798
57	1	0	-0.223348	-0.081703	-1.136612
58	1	0	-0.343717	-2.553744	-0.872542
59	6	0	-3.818524	-3.339962	1.566107
60	1	0	-4.120506	-3.952030	2.421555
61	1	0	-4.467308	-2.464347	1.523397
62	1	0	-3.984760	-3.932096	0.660016

63	6	0	−1.558330	−5.220238	1.930487
64	1	0	−1.519914	−5.562115	2.970394
65	1	0	−2.524293	−5.501037	1.510199
66	1	0	−0.774823	−5.753708	1.394106
67	6	0	4.150539	−2.828483	0.049323
68	1	0	4.669396	−3.202635	−0.839848
69	1	0	4.841407	−2.203494	0.617112
70	1	0	3.880733	−3.688171	0.661208
71	6	0	4.151410	0.127268	−0.133728
72	1	0	5.002801	−0.194957	−0.740956
73	1	0	3.933620	1.169665	−0.369119
74	1	0	4.454910	0.070922	0.917318

Int18a

Thermal correction to Energy=	0.335799
Thermal correction to Enthalpy=	0.336744
Thermal correction to Gibbs Free Energy=	0.273664
Sum of electronic and zero-point Energies=	-753.629426
Sum of electronic and thermal Energies=	-753.612119
Sum of electronic and thermal Enthalpies=	-753.611175
Sum of electronic and thermal Free Energies=	-753.674254

Esol = -753.9335337

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	−6.587001	−1.707178	2.936284
2	8	0	−7.344200	−2.758119	2.477362
3	8	0	−5.765121	−1.166490	1.981852
4	6	0	−4.955218	−1.889172	−0.172661
5	1	0	−5.216508	−2.412168	−1.097946
6	1	0	−4.577762	−0.897962	−0.437356
7	1	0	−4.155235	−2.437001	0.328194
8	6	0	−5.783917	−4.202402	1.384565
9	1	0	−5.385084	−4.564046	0.432964
10	1	0	−4.951512	−3.849848	2.001232
11	1	0	−6.260947	−5.039352	1.900596
12	6	0	−6.817076	−3.099262	1.173990
13	6	0	−6.175551	−1.748676	0.719434
14	6	0	−7.954347	−3.590534	0.296196
15	1	0	−7.601946	−3.761655	−0.725814
16	1	0	−8.336873	−4.537255	0.686640

17	1	0	−8.777494	−2.874550	0.270263
18	6	0	−7.190615	−0.792610	0.099436
19	1	0	−6.734187	0.196166	0.006393
20	1	0	−7.498945	−1.126752	−0.894963
21	1	0	−8.081045	−0.701570	0.729060
22	6	0	−7.633246	−1.718265	6.470928
23	6	0	−7.500993	−2.047540	5.161167
24	7	0	−6.694054	−1.279813	4.314449
25	6	0	−6.058625	−0.163272	4.896095
26	6	0	−6.248759	0.093553	6.238661
27	7	0	−7.024110	−0.659346	7.062413
28	1	0	−8.265143	−2.334849	7.104504
29	1	0	−7.991448	−2.897460	4.707950
30	6	0	−5.583833	1.275065	6.904042
31	1	0	−4.493600	1.232159	6.822380
32	1	0	−5.912950	2.225743	6.472979
33	1	0	−5.852291	1.265098	7.960661
34	6	0	−5.214630	0.693633	4.005353
35	1	0	−5.796094	1.079788	3.162140
36	1	0	−4.810328	1.538624	4.560037
37	1	0	−4.381548	0.128187	3.576797

Int19

Thermal correction to Energy=	0.675291
Thermal correction to Enthalpy=	0.676235
Thermal correction to Gibbs Free Energy=	0.577007
Sum of electronic and zero-point Energies=	-1507.319530
Sum of electronic and thermal Energies=	-1507.284196
Sum of electronic and thermal Enthalpies=	-1507.283251
Sum of electronic and thermal Free Energies=	-1507.382479

Esol = -1507.892405

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.500004	−0.666952	0.934992
2	5	0	−2.327582	0.844984	3.737368
3	8	0	2.011099	0.237083	0.025965
4	8	0	1.618885	−1.977463	0.518749
5	8	0	−2.813431	2.121870	4.150879
6	8	0	−3.301380	−0.144757	4.056471
7	6	0	4.232515	−0.512965	−0.406848

8	1	0	4.557438	0.526115	-0.305247
9	1	0	4.308640	-0.990708	0.575157
10	1	0	4.911866	-1.023270	-1.095286
11	6	0	3.108296	-3.108249	-0.995466
12	1	0	3.589029	-3.068645	-1.978191
13	1	0	3.880626	-3.097559	-0.224424
14	1	0	2.566351	-4.055001	-0.921155
15	6	0	-5.243187	-0.314603	5.454575
16	1	0	-6.100046	0.227048	5.868916
17	1	0	-5.618051	-1.218175	4.964809
18	1	0	-4.588458	-0.619830	6.272993
19	6	0	-3.384157	1.710283	6.442394
20	1	0	-4.188657	1.578877	7.172449
21	1	0	-2.706077	0.853565	6.499465
22	1	0	-2.820177	2.608208	6.711077
23	6	0	-3.923958	1.876458	5.020933
24	6	0	-4.493743	0.542766	4.446563
25	6	0	2.133684	-1.952565	-0.828800
26	6	0	2.791662	-0.530642	-0.913892
27	6	0	2.698487	0.131095	-2.277893
28	1	0	3.155388	1.123978	-2.234947
29	1	0	3.232550	-0.457510	-3.030716
30	1	0	1.659088	0.244110	-2.591562
31	6	0	0.951157	-2.121702	-1.778165
32	1	0	1.284359	-2.202889	-2.817245
33	1	0	0.423965	-3.043427	-1.515209
34	1	0	0.254189	-1.283727	-1.692286
35	6	0	-4.876182	3.059897	4.951773
36	1	0	-5.787561	2.861046	5.525420
37	1	0	-4.394889	3.945130	5.377725
38	1	0	-5.151777	3.287121	3.919982
39	6	0	-5.354919	0.773271	3.203234
40	1	0	-5.536414	-0.188582	2.714278
41	1	0	-6.323496	1.214787	3.456782
42	1	0	-4.846270	1.431672	2.492477
43	6	0	0.261292	-1.319277	2.951781
44	6	0	-0.635465	-0.945929	3.864000
45	6	0	0.177579	1.287092	3.787614
46	6	0	1.086338	0.938060	2.857661
47	1	0	0.542055	-2.349366	2.765852
48	7	0	-0.918935	0.424121	4.080047
49	6	0	-1.909124	-0.666850	0.157615
50	6	0	-2.394073	-0.364620	1.414561
51	6	0	-1.545895	1.781099	1.225145

52	6	0	−1.042270	1.434365	−0.047399
53	7	0	−2.189458	0.851287	1.953468
54	1	0	−1.183747	−1.660721	4.467564
55	6	0	0.256259	2.503557	4.669096
56	1	0	−0.741462	2.930112	4.792117
57	1	0	0.607188	2.217520	5.667854
58	1	0	0.918982	3.275408	4.275710
59	6	0	2.349249	1.692196	2.552720
60	1	0	3.209844	1.015835	2.613796
61	1	0	2.344508	2.100186	1.537923
62	1	0	2.509650	2.506721	3.258268
63	7	0	0.938168	−0.326810	2.194933
64	7	0	−1.216400	0.219306	−0.561215
65	6	0	−1.377454	3.179985	1.737533
66	1	0	−1.780555	3.287725	2.741139
67	1	0	−0.319808	3.460023	1.729099
68	1	0	−1.906089	3.875501	1.075183
69	6	0	−0.253584	2.421177	−0.855632
70	1	0	−0.069108	2.003516	−1.845498
71	1	0	−0.779504	3.374834	−0.959142
72	1	0	0.712864	2.615999	−0.379010
73	1	0	−2.930117	−1.073547	2.032502
74	1	0	−2.063181	−1.651031	−0.274682

TS20

Thermal correction to Energy=	0.674350
Thermal correction to Enthalpy=	0.675294
Thermal correction to Gibbs Free Energy=	0.577113
Sum of electronic and zero-point Energies=	-1507.319808
Sum of electronic and thermal Energies=	-1507.284985
Sum of electronic and thermal Enthalpies=	-1507.284041
Sum of electronic and thermal Free Energies=	-1507.382222

Esol = -1507.892456

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.344730	−4.246533	2.014736
2	5	0	−2.360558	−1.265386	0.392902
3	7	0	0.138374	−3.519928	2.208864
4	8	0	−2.507652	0.141900	0.330324
5	8	0	−3.332535	−1.888280	−0.421081

6	8	0	1.344904	-5.604009	1.765948
7	8	0	2.614067	-3.710918	2.089146
8	6	0	-1.103455	-4.136159	1.904720
9	6	0	0.034969	-2.223865	2.817367
10	6	0	-3.777704	0.392708	-0.287576
11	6	0	-3.945878	-0.857640	-1.206828
12	6	0	2.713287	-5.995351	1.529261
13	6	0	3.520783	-4.827671	2.198348
14	6	0	-2.164507	-3.374605	1.644497
15	1	0	-1.129887	-5.219115	1.932728
16	6	0	-1.052155	-1.474385	2.556952
17	6	0	-3.716951	1.722157	-1.022218
18	6	0	-4.829980	0.443281	0.820563
19	6	0	-5.387909	-1.252299	-1.484960
20	6	0	-3.174031	-0.717477	-2.519499
21	6	0	2.916464	-6.074489	0.019125
22	6	0	2.941704	-7.360373	2.160221
23	6	0	3.763767	-5.052104	3.689679
24	6	0	4.818451	-4.470339	1.494551
25	7	0	-2.058109	-1.962836	1.670144
26	1	0	-3.137541	-3.789327	1.406399
27	1	0	-3.601059	2.536079	-0.300684
28	1	0	-4.639168	1.897894	-1.585870
29	1	0	-2.870828	1.756226	-1.711393
30	1	0	-5.821811	0.693070	0.431939
31	1	0	-4.884235	-0.515897	1.344296
32	1	0	-4.540375	1.209582	1.545170
33	1	0	-5.410510	-2.125880	-2.143005
34	1	0	-5.926313	-0.438870	-1.982527
35	1	0	-5.910815	-1.509857	-0.562040
36	1	0	-3.657772	-0.006491	-3.196089
37	1	0	-2.147732	-0.385991	-2.337659
38	1	0	-3.139404	-1.691420	-3.016775
39	1	0	2.173758	-6.762422	-0.395321
40	1	0	3.911613	-6.456441	-0.228063
41	1	0	2.785195	-5.094635	-0.447831
42	1	0	3.994123	-7.651040	2.079829
43	1	0	2.652419	-7.371080	3.212524
44	1	0	2.342441	-8.109151	1.635094
45	1	0	4.148329	-4.126707	4.127124
46	1	0	4.491529	-5.848762	3.867384
47	1	0	2.832670	-5.310163	4.204337
48	1	0	5.512778	-5.316598	1.510082
49	1	0	4.637721	-4.181819	0.457496

50	1	0	5.294236	−3.630095	2.008416
51	6	0	1.676081	−1.846623	−0.429148
52	6	0	0.490783	−1.116669	−0.193588
53	7	0	−0.696928	−1.668123	−0.484323
54	6	0	−0.718520	−2.886096	−1.048025
55	6	0	0.456098	−3.574267	−1.288190
56	7	0	1.647009	−3.065197	−0.963806
57	1	0	−1.698340	−3.290643	−1.272696
58	1	0	0.441485	−4.564211	−1.734926
59	6	0	−1.389492	−0.163181	3.209911
60	1	0	−1.726540	0.551643	2.456077
61	1	0	−2.222352	−0.303386	3.909052
62	1	0	−0.549520	0.273228	3.750775
63	6	0	1.102009	−1.889987	3.820631
64	1	0	2.070003	−1.720473	3.340944
65	1	0	0.842504	−1.009457	4.406878
66	1	0	1.238025	−2.730095	4.511655
67	6	0	0.557967	0.273908	0.363691
68	1	0	1.078688	0.274252	1.326594
69	1	0	1.126370	0.918871	−0.316040
70	1	0	−0.439468	0.690918	0.485923
71	6	0	3.014386	−1.283325	−0.053594
72	1	0	3.160851	−0.279629	−0.463957
73	1	0	3.109494	−1.221551	1.035547
74	1	0	3.797906	−1.941594	−0.429415

Int20

Thermal correction to Energy=	0.575875
Thermal correction to Enthalpy=	0.576820
Thermal correction to Gibbs Free Energy=	0.462173
Sum of electronic and zero-point Energies=	-2664.985615
Sum of electronic and thermal Energies=	-2664.947870
Sum of electronic and thermal Enthalpies=	-2664.946926
Sum of electronic and thermal Free Energies=	-2665.061572

Esol = -2665.751989

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.039350	−2.291775	−2.126942
2	6	0	−1.831167	−0.901127	−1.483626
3	6	0	0.362166	−2.428886	−0.816719

4	1	0	0.683835	-2.773394	-2.853161
5	6	0	-1.485908	-1.071413	-0.182422
6	1	0	-2.728979	-0.333015	-1.697997
7	1	0	1.219874	-2.996418	-0.478110
8	1	0	-2.057561	-0.654484	0.638300
9	7	0	-0.360626	-1.795807	0.184630
10	6	0	1.425946	-2.196142	3.326096
11	6	0	0.529566	-0.941940	3.609997
12	5	0	0.184707	-1.696598	1.522641
13	8	0	1.343885	-2.316299	1.882901
14	8	0	-0.435528	-1.000062	2.522838
15	6	0	-0.216475	-0.987740	4.931208
16	1	0	0.490532	-1.040590	5.764993
17	1	0	-0.809781	-0.077376	5.050590
18	1	0	-0.889529	-1.844957	4.984347
19	6	0	0.848199	-3.482326	3.908867
20	1	0	1.401404	-4.333113	3.503495
21	1	0	0.933692	-3.501279	4.998569
22	1	0	-0.205680	-3.599741	3.638742
23	6	0	2.883725	-2.034809	3.717657
24	1	0	2.973399	-1.845926	4.791978
25	1	0	3.427743	-2.954671	3.487534
26	1	0	3.352389	-1.213579	3.172974
27	6	0	1.285653	0.373877	3.458516
28	1	0	0.574398	1.202450	3.521147
29	1	0	2.024485	0.501215	4.254366
30	1	0	1.788162	0.429705	2.488526
31	6	0	-1.051831	-1.465498	-2.543809
32	6	0	1.627897	0.435241	-3.727508
33	6	0	2.113955	0.167129	-2.445117
34	6	0	3.247021	-0.629847	-2.263717
35	6	0	3.898713	-1.157659	-3.370495
36	6	0	3.413828	-0.897642	-4.653030
37	6	0	2.283175	-0.103402	-4.830973
38	1	0	0.736030	1.038453	-3.860958
39	1	0	3.591400	-0.832773	-1.254804
40	1	0	4.780130	-1.775914	-3.236398
41	1	0	3.918373	-1.318094	-5.517259
42	1	0	1.903837	0.091700	-5.828837
43	6	0	1.415828	0.636458	-1.220564
44	8	0	0.435303	1.527612	-1.563978
45	8	0	1.657333	0.310780	-0.089280
46	8	0	-0.293620	1.885577	-0.412513
47	6	0	-1.576846	2.196950	-0.778350

48	6	0	−2.397423	2.421018	0.439578
49	6	0	−2.013596	1.927863	1.690485
50	6	0	−3.600056	3.113382	0.282690
51	6	0	−2.842806	2.139162	2.786635
52	1	0	−1.093870	1.360166	1.796068
53	6	0	−4.416030	3.328591	1.386277
54	1	0	−3.877282	3.474558	−0.702206
55	6	0	−4.036764	2.842318	2.636682
56	1	0	−2.559885	1.748814	3.758637
57	1	0	−5.348373	3.871249	1.272197
58	1	0	−4.678153	3.007037	3.496699
59	8	0	−1.947491	2.287174	−1.915567
60	6	0	−1.315682	−1.176068	−3.929842
61	6	0	−2.134746	−0.088404	−4.316291
62	6	0	−0.732398	−1.924676	−4.979289
63	6	0	−2.307281	0.154019	−5.664881
64	1	0	−2.569904	0.585287	−3.589439
65	6	0	−0.999284	−1.548036	−6.279979
66	1	0	−0.099673	−2.781788	−4.791407
67	7	0	−1.767422	−0.537567	−6.659481
68	17	0	−3.310454	1.508493	−6.148881
69	17	0	−0.260317	−2.464616	−7.582843

TS21

Thermal correction to Energy=	0.572241
Thermal correction to Enthalpy=	0.573185
Thermal correction to Gibbs Free Energy=	0.464586
Sum of electronic and zero-point Energies=	-2664.964546
Sum of electronic and thermal Energies=	-2664.928099
Sum of electronic and thermal Enthalpies=	-2664.927155
Sum of electronic and thermal Free Energies=	-2665.035754

Esol = -2665.721974

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−1.119572	−0.565315	3.454532
2	6	0	−2.589246	1.312182	3.776625
3	6	0	−0.684271	−0.411856	4.741345
4	1	0	−0.723848	−1.385757	2.868426
5	6	0	−2.126673	1.404774	5.067201
6	1	0	−3.317628	2.043323	3.444140

7	1	0	0.080309	-1.041013	5.183164
8	1	0	-2.520040	2.120373	5.781194
9	7	0	-1.157393	0.571589	5.554763
10	6	0	0.483216	-0.068570	8.541757
11	6	0	-0.330687	1.177069	9.022561
12	5	0	-0.321775	1.087584	6.749170
13	8	0	0.727438	0.244022	7.159244
14	8	0	-1.102947	1.493625	7.853173
15	6	0	-1.282352	0.905880	10.176330
16	1	0	-0.736960	0.541996	11.053262
17	1	0	-1.792495	1.832016	10.457959
18	1	0	-2.040100	0.170133	9.900537
19	6	0	-0.344429	-1.352557	8.589335
20	1	0	0.192338	-2.138823	8.050819
21	1	0	-0.510323	-1.692338	9.615818
22	1	0	-1.316121	-1.205802	8.107225
23	6	0	1.815579	-0.267946	9.244827
24	1	0	1.669722	-0.407128	10.321024
25	1	0	2.309855	-1.160948	8.851694
26	1	0	2.477848	0.584992	9.085885
27	6	0	0.571452	2.368134	9.345407
28	1	0	-0.048834	3.262472	9.454361
29	1	0	1.120692	2.214655	10.279168
30	1	0	1.287048	2.548679	8.538984
31	6	0	-2.063617	0.345392	2.901142
32	6	0	0.247422	2.659297	2.466523
33	6	0	0.765250	2.334755	3.733945
34	6	0	1.777174	1.361727	3.864153
35	6	0	2.246135	0.711740	2.737265
36	6	0	1.712826	1.014957	1.478047
37	6	0	0.726131	1.992972	1.346694
38	1	0	-0.540925	3.401445	2.385515
39	1	0	2.157298	1.125250	4.854245
40	1	0	3.025353	-0.037658	2.830190
41	1	0	2.076472	0.495778	0.596468
42	1	0	0.317020	2.222644	0.368057
43	6	0	0.234500	2.929087	4.935494
44	8	0	-0.275273	4.176324	4.746558
45	8	0	0.338762	2.457695	6.096944
46	8	0	-1.193108	4.476701	5.783801
47	6	0	-2.450432	4.651679	5.251583
48	6	0	-3.427901	4.805632	6.358653
49	6	0	-3.197568	4.242981	7.618605
50	6	0	-4.613617	5.490326	6.081801

51	6	0	−4.167225	4.383392	8.606484
52	1	0	−2.291045	3.672431	7.807009
53	6	0	−5.567363	5.635412	7.080505
54	1	0	−4.769267	5.902174	5.090019
55	6	0	−5.342361	5.083093	8.341456
56	1	0	−4.006757	3.940686	9.583832
57	1	0	−6.486674	6.174285	6.877324
58	1	0	−6.091836	5.192959	9.118889
59	8	0	−2.681284	4.676822	4.075372
60	6	0	−2.441039	0.289078	1.491345
61	6	0	−3.633926	0.859311	1.012237
62	6	0	−1.603367	−0.335039	0.549126
63	6	0	−3.898620	0.771393	−0.343418
64	1	0	−4.349857	1.333445	1.671257
65	6	0	−2.000691	−0.333099	−0.777174
66	1	0	−0.650901	−0.765183	0.830530
67	7	0	−3.117848	0.196232	−1.245330
68	17	0	−5.385929	1.459042	−0.954762
69	17	0	−0.948246	−1.070689	−1.966090

Int21

Thermal correction to Energy=	0.109845
Thermal correction to Enthalpy=	0.110789
Thermal correction to Gibbs Free Energy=	0.069432
Sum of electronic and zero-point Energies=	-419.879117
Sum of electronic and thermal Energies=	-419.871827
Sum of electronic and thermal Enthalpies=	-419.870883
Sum of electronic and thermal Free Energies=	-419.912240

Esol = -420.0643127

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.446398	−2.975236	−3.298304
2	6	0	1.095745	−1.714822	−3.474221
3	6	0	0.435618	−1.024838	−2.345338
4	6	0	0.200440	−1.686429	−1.138630
5	6	0	0.054862	0.305770	−2.521761
6	6	0	−0.422919	−1.005681	−0.099455
7	1	0	0.502242	−2.722760	−1.014357
8	6	0	−0.567810	0.979629	−1.478679
9	1	0	0.252176	0.791166	−3.472158

10	6	0	−0.805438	0.323873	−0.271111
11	1	0	−0.610647	−1.509550	0.842567
12	1	0	−0.868328	2.014320	−1.604424
13	1	0	−1.292310	0.852642	0.542165
14	8	0	1.358843	−1.249611	−4.566816

Int22

Thermal correction to Energy=	0.462027
Thermal correction to Enthalpy=	0.462972
Thermal correction to Gibbs Free Energy=	0.370724
Sum of electronic and zero-point Energies=	-2245.168270
Sum of electronic and thermal Energies=	-2245.139424
Sum of electronic and thermal Enthalpies=	-2245.138480
Sum of electronic and thermal Free Energies=	-2245.230728

Esol = -2245.770147

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.881927	−4.213535	−1.692298
2	6	0	−2.356862	−2.324552	−1.833014
3	6	0	−0.012520	−3.427462	−0.957295
4	1	0	−0.636260	−5.252062	−1.882445
5	6	0	−1.434843	−1.593973	−1.101894
6	1	0	−3.265155	−1.843288	−2.177201
7	1	0	0.920629	−3.800287	−0.549860
8	1	0	−1.569082	−0.552961	−0.837045
9	7	0	−0.291761	−2.147982	−0.680828
10	6	0	0.758328	−1.773368	2.445054
11	6	0	0.431750	−0.260497	2.229109
12	5	0	0.802139	−1.269456	0.207206
13	8	0	1.361097	−2.128389	1.198243
14	8	0	0.074959	−0.221814	0.843405
15	6	0	−0.732412	0.264174	3.055103
16	1	0	−0.533015	0.153566	4.126213
17	1	0	−0.881799	1.327373	2.846214
18	1	0	−1.658862	−0.261338	2.813926
19	6	0	−0.506025	−2.614754	2.638175
20	1	0	−0.244918	−3.672405	2.536264
21	1	0	−0.947240	−2.463594	3.627994
22	1	0	−1.261482	−2.371808	1.884314
23	6	0	1.746964	−2.057118	3.565784

24	1	0	1.367696	−1.689535	4.525116
25	1	0	1.905031	−3.136061	3.654714
26	1	0	2.712298	−1.589144	3.364611
27	6	0	1.662193	0.626367	2.425505
28	1	0	1.436853	1.625835	2.043866
29	1	0	1.941023	0.711976	3.480257
30	1	0	2.514736	0.231978	1.864813
31	6	0	−2.083486	−3.658785	−2.142984
32	6	0	2.656369	1.167660	−3.633586
33	6	0	2.816859	0.338624	−2.522149
34	6	0	4.091962	−0.085430	−2.143905
35	6	0	5.201678	0.319636	−2.879156
36	6	0	5.039788	1.145937	−3.989391
37	6	0	3.766485	1.570432	−4.366618
38	1	0	1.654936	1.485262	−3.904293
39	1	0	4.201610	−0.726141	−1.276067
40	1	0	6.193947	−0.007795	−2.585535
41	1	0	5.907414	1.460970	−4.561028
42	1	0	3.641760	2.215312	−5.230614
43	6	0	1.595016	−0.072132	−1.759420
44	8	0	0.480880	0.310506	−2.065871
45	8	0	1.856049	−0.887291	−0.751209
46	6	0	−3.048100	−4.469343	−2.926486
47	6	0	−4.422395	−4.315429	−2.735716
48	6	0	−2.599309	−5.399518	−3.865973
49	6	0	−5.267733	−5.110141	−3.500294
50	1	0	−4.823736	−3.623374	−2.005464
51	6	0	−3.562295	−6.121679	−4.560686
52	1	0	−1.545230	−5.542154	−4.071628
53	7	0	−4.866327	−5.994930	−4.394489
54	17	0	−6.990094	−4.958815	−3.285658
55	17	0	−3.049214	−7.287915	−5.749211

TS22

Thermal correction to Energy=	0.460109
Thermal correction to Enthalpy=	0.461054
Thermal correction to Gibbs Free Energy=	0.369188
Sum of electronic and zero-point Energies=	-2245.152746
Sum of electronic and thermal Energies=	-2245.123954
Sum of electronic and thermal Enthalpies=	-2245.123010
Sum of electronic and thermal Free Energies=	-2245.214875

Esol = -2245.754276

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	−2.095964	−6.303924	6.934605
2	8	0	−1.549797	−5.383521	7.812770
3	8	0	−3.472712	−6.257362	6.877453
4	6	0	−5.194684	−5.291761	8.246248
5	1	0	−5.478462	−4.428890	8.857571
6	1	0	−5.974220	−5.447709	7.495438
7	1	0	−5.154727	−6.178111	8.881453
8	6	0	−2.796152	−5.565912	9.837544
9	1	0	−3.580675	−5.145935	10.473449
10	1	0	−3.022841	−6.619608	9.649797
11	1	0	−1.846825	−5.513669	10.376903
12	6	0	−2.658107	−4.797517	8.524715
13	6	0	−3.864061	−5.044715	7.552270
14	6	0	−2.353450	−3.334205	8.799224
15	1	0	−3.210173	−2.841954	9.270639
16	1	0	−1.501880	−3.259118	9.481212
17	1	0	−2.102899	−2.800145	7.880519
18	6	0	−4.022593	−3.940139	6.508509
19	1	0	−4.726585	−4.280005	5.743440
20	1	0	−4.421100	−3.026024	6.958500
21	1	0	−3.072523	−3.709133	6.022450
22	6	0	0.662319	−5.690623	1.399129
23	6	0	0.573671	−6.878642	0.670990
24	6	0	1.366021	−6.993640	−0.463227
25	6	0	2.244103	−4.940317	−0.211524
26	6	0	1.523126	−4.688472	0.949614
27	6	0	−0.126026	−5.532273	2.644592
28	6	0	−1.448637	−5.974476	2.714338
29	6	0	−2.115914	−5.899889	3.930646
30	6	0	−0.281382	−4.979265	4.970549
31	6	0	0.454910	−4.989807	3.793235
32	1	0	−0.055516	−7.697502	0.999456
33	1	0	1.617566	−3.741992	1.468534
34	1	0	−1.949709	−6.378465	1.841145
35	1	0	1.482154	−4.640597	3.787558
36	7	0	−1.531079	−5.441592	5.040004
37	7	0	2.184477	−6.058879	−0.911536
38	1	0	0.141408	−4.627971	5.908599
39	1	0	−3.136257	−6.255696	4.046002
40	17	0	3.318671	−3.709135	−0.820780

41	17	0	1.312155	−8.478180	−1.378196
42	8	0	−1.321588	−7.448332	6.639310
43	6	0	−1.660117	−8.309335	5.660487
44	8	0	−2.788591	−8.680224	5.449382
45	6	0	−0.494827	−8.729070	4.822223
46	6	0	0.793186	−8.245590	5.057946
47	6	0	−0.740795	−9.563718	3.727527
48	6	0	1.831116	−8.592851	4.196140
49	1	0	0.970740	−7.598973	5.910240
50	6	0	0.296876	−9.909382	2.870672
51	1	0	−1.751413	−9.923563	3.564371
52	6	0	1.583449	−9.418461	3.102107
53	1	0	2.832884	−8.216489	4.377030
54	1	0	0.107510	−10.556584	2.019761
55	1	0	2.391948	−9.681862	2.426743

TS23

Thermal correction to Energy=	0.107893
Thermal correction to Enthalpy=	0.108837
Thermal correction to Gibbs Free Energy=	0.066226
Sum of electronic and zero-point Energies=	-419.865858
Sum of electronic and thermal Energies=	-419.858456
Sum of electronic and thermal Enthalpies=	-419.857512
Sum of electronic and thermal Free Energies=	-419.900123

Esol = -420.0560773

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.528898	2.144005	−2.489594
2	6	0	2.429072	1.459797	−2.114033
3	8	0	2.978558	0.777100	−1.306884
4	6	0	3.659349	1.454498	−3.628120
5	6	0	4.832291	0.754453	−3.466848
6	6	0	3.263846	2.151195	−4.746179
7	6	0	5.701990	0.761882	−4.561614
8	1	0	5.063557	0.230955	−2.547462
9	6	0	4.157426	2.136171	−5.821463
10	1	0	2.318389	2.677769	−4.786616
11	6	0	5.364639	1.447153	−5.726804
12	1	0	6.643740	0.226432	−4.493206
13	1	0	3.899571	2.668676	−6.731534

14	1	0	6.048845	1.444206	-6.568850

Int23

Thermal correction to Energy=	0.092784
Thermal correction to Enthalpy=	0.093728
Thermal correction to Gibbs Free Energy=	0.060416
Sum of electronic and zero-point Energies=	-231.377642
Sum of electronic and thermal Energies=	-231.373301
Sum of electronic and thermal Enthalpies=	-231.372357
Sum of electronic and thermal Free Energies=	-231.405670

Esol = -231.4839326

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.416876	-1.007114	-2.309421
2	6	0	0.206574	-1.700422	-1.139705
3	6	0	0.060955	0.302613	-2.535421
4	6	0	-0.421928	-1.006875	-0.099541
5	1	0	0.509971	-2.735813	-1.019449
6	6	0	-0.566247	0.976749	-1.481794
7	1	0	0.252947	0.798483	-3.481895
8	6	0	-0.804186	0.322564	-0.273828
9	1	0	-0.611193	-1.508590	0.844953
10	1	0	-0.867439	2.012532	-1.608439
11	1	0	-1.291267	0.852821	0.538133

Int24

Thermal correction to Energy=	0.443534
Thermal correction to Enthalpy=	0.444479
Thermal correction to Gibbs Free Energy=	0.357673
Sum of electronic and zero-point Energies=	-2056.622955
Sum of electronic and thermal Energies=	-2056.596546
Sum of electronic and thermal Enthalpies=	-2056.595602
Sum of electronic and thermal Free Energies=	-2056.682408

Esol = -2057.145875

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	5	0	-5.431903	-2.541642	2.703564
2	8	0	-6.071071	-3.247253	1.621100
3	8	0	-5.205656	-1.183537	2.296443
4	6	0	-4.137900	-1.405436	0.142668
5	1	0	-4.244297	-1.244316	-0.934620
6	1	0	-3.363795	-0.727333	0.514915
7	1	0	-3.802757	-2.434424	0.303941
8	6	0	-6.511153	-2.865893	-0.711721
9	1	0	-6.739180	-2.107491	-1.468213
10	1	0	-5.550306	-3.325478	-0.953528
11	1	0	-7.281115	-3.641061	-0.767526
12	6	0	-6.497669	-2.258088	0.683028
13	6	0	-5.444865	-1.121030	0.889028
14	6	0	-7.906625	-1.810192	1.077530
15	1	0	-8.336258	-1.114615	0.349903
16	1	0	-8.549810	-2.692644	1.136006
17	1	0	-7.896822	-1.332376	2.061751
18	6	0	-5.942797	0.274320	0.541131
19	1	0	-5.138970	1.001637	0.690227
20	1	0	-6.259617	0.329107	-0.505869
21	1	0	-6.780470	0.560826	1.179563
22	6	0	-0.103762	-5.125414	3.312426
23	6	0	0.348128	-6.070657	2.389479
24	6	0	1.597965	-6.635736	2.611881
25	6	0	1.938685	-5.449553	4.491208
26	6	0	0.712828	-4.801857	4.397723
27	6	0	-1.428049	-4.478580	3.142890
28	6	0	-2.517105	-5.197742	2.643854
29	6	0	-3.738517	-4.560449	2.497956
30	6	0	-2.868887	-2.566642	3.300454
31	6	0	-1.617660	-3.133919	3.473686
32	1	0	-0.233625	-6.341874	1.516979
33	1	0	0.401850	-4.094769	5.157167
34	1	0	-2.425691	-6.247402	2.388237
35	1	0	-0.797333	-2.524985	3.836419
36	7	0	2.386530	-6.345249	3.630366
37	7	0	-3.898487	-3.274759	2.826081
38	6	0	-7.340371	-4.026176	5.780146
39	6	0	-6.793263	-3.860545	4.509540
40	6	0	-5.929434	-1.719010	5.146999
41	6	0	-6.471905	-1.872497	6.421491
42	1	0	-7.901125	-4.925224	6.020575
43	1	0	-6.943990	-4.630368	3.755059
44	17	0	2.987097	-5.082881	5.833542

45	17	0	2.203996	−7.816033	1.482248
46	1	0	−3.080456	−1.524783	3.515841
47	1	0	−4.620234	−5.052404	2.102216
48	1	0	−5.401122	−0.801747	4.894466
49	1	0	−6.353753	−1.087312	7.163203
50	6	0	−6.070673	−2.710645	4.168394
51	6	0	−7.175795	−3.031552	6.742330
52	1	0	−7.601960	−3.154948	7.733629

TS24

Thermal correction to Energy=	0.442428
Thermal correction to Enthalpy=	0.443372
Thermal correction to Gibbs Free Energy=	0.355895
Sum of electronic and zero-point Energies=	-2056.617962
Sum of electronic and thermal Energies=	-2056.591599
Sum of electronic and thermal Enthalpies=	-2056.590654
Sum of electronic and thermal Free Energies=	-2056.678131

Esol = -2057.142554

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	−1.573343	−6.217128	6.904623
2	8	0	−1.211897	−4.980065	7.428203
3	8	0	−2.944526	−6.404201	6.907902
4	6	0	−4.792537	−5.415951	8.083660
5	1	0	−5.229506	−4.479709	8.445978
6	1	0	−5.543027	−5.926532	7.473629
7	1	0	−4.561674	−6.052106	8.939760
8	6	0	−2.370139	−4.738427	9.495534
9	1	0	−3.211399	−4.289105	10.030973
10	1	0	−2.390978	−5.821045	9.651988
11	1	0	−1.440742	−4.353098	9.922904
12	6	0	−2.400016	−4.404411	8.004604
13	6	0	−3.553893	−5.143966	7.242182
14	6	0	−2.371208	−2.897375	7.805457
15	1	0	−3.291690	−2.438547	8.180851
16	1	0	−1.530044	−2.471301	8.359478
17	1	0	−2.254719	−2.634064	6.752120
18	6	0	−3.960698	−4.447027	5.944631
19	1	0	−4.585477	−5.130276	5.362252
20	1	0	−4.537590	−3.539537	6.146877

21	1	0	−3.091567	−4.182981	5.339623
22	6	0	−0.196824	−9.817096	6.512627
23	6	0	−1.064858	−8.729317	6.577438
24	6	0	0.786196	−7.270049	7.042480
25	6	0	1.660718	−8.351163	6.980060
26	1	0	−0.583275	−10.812219	6.312385
27	6	0	0.116501	−4.721246	0.763184
28	6	0	0.428458	−5.738211	−0.142019
29	6	0	0.844891	−5.362002	−1.412656
30	6	0	0.666416	−3.169440	−0.958758
31	6	0	0.238735	−3.394568	0.343442
32	6	0	−0.332303	−5.043513	2.140516
33	6	0	−1.151173	−6.148102	2.389729
34	6	0	−1.540748	−6.412049	3.696954
35	6	0	−0.385727	−4.599555	4.497708
36	6	0	0.055161	−4.253815	3.225760
37	1	0	0.376115	−6.784112	0.134479
38	1	0	−0.011584	−2.565243	0.993615
39	1	0	−1.498590	−6.781107	1.580118
40	1	0	0.709847	−3.399417	3.090881
41	7	0	−1.167762	−5.653939	4.726820
42	7	0	0.966940	−4.115035	−1.830206
43	1	0	−0.109745	−4.022899	5.377672
44	1	0	−2.175868	−7.262123	3.934166
45	17	0	0.825712	−1.526504	−1.522832
46	17	0	1.253851	−6.602558	−2.568360
47	1	0	−2.132453	−8.879263	6.434307
48	1	0	1.170178	−6.275691	7.258280
49	1	0	2.724234	−8.202884	7.143101
50	6	0	−0.588646	−7.438656	6.837460
51	6	0	1.168977	−9.627889	6.712042
52	1	0	1.848488	−10.473700	6.664567

CO_2

Thermal correction to Energy=	0.014496
Thermal correction to Enthalpy=	0.015440
Thermal correction to Gibbs Free Energy=	-0.009489
Sum of electronic and zero-point Energies=	-188.497426
Sum of electronic and thermal Energies=	-188.494797
Sum of electronic and thermal Enthalpies=	-188.493853
Sum of electronic and thermal Free Energies=	-188.518782

Esol = -188.6011327

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.362971	2.131497	-2.345105
2	6	0	2.137137	1.468675	-1.785573
3	8	0	2.911304	0.805853	-1.226041

S1

Thermal correction to Energy=	0.226911
Thermal correction to Enthalpy=	0.227856
Thermal correction to Gibbs Free Energy=	0.165241
Sum of electronic and zero-point Energies=	-839.820246
Sum of electronic and thermal Energies=	-839.805410
Sum of electronic and thermal Enthalpies=	-839.804466
Sum of electronic and thermal Free Energies=	-839.867081

Esol = -840.1693289

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.119062	-3.461101	-0.926819
2	6	0	-0.818680	-2.250771	-0.934286
3	6	0	-0.133451	-1.034125	-0.940764
4	6	0	1.255636	-1.026490	-0.939785
5	6	0	1.956781	-2.231080	-0.932367
6	6	0	1.271084	-3.444256	-0.925902
7	1	0	-0.656000	-4.403268	-0.921766
8	1	0	-0.702701	-0.110679	-0.946489
9	1	0	1.791780	-0.083430	-0.944810
10	1	0	3.042269	-2.224653	-0.931627
11	1	0	1.820141	-4.379817	-0.920125
12	6	0	-2.304784	-2.183594	-0.935756
13	8	0	-2.819329	-3.453310	-0.929506
14	8	0	-2.975293	-1.190586	-0.941465
15	8	0	-4.227175	-3.376361	-0.930966
16	6	0	-4.741720	-4.646077	-0.924835
17	6	0	-6.227824	-4.578900	-0.926289
18	6	0	-6.927442	-3.368570	-0.933724
19	6	0	-6.913053	-5.795546	-0.919831
20	6	0	-8.317588	-3.385415	-0.934630
21	1	0	-6.390504	-2.426403	-0.938765

22	6	0	−8.302140	−5.803180	−0.920797
23	1	0	−6.343803	−6.718992	−0.914131
24	6	0	−9.003285	−4.598590	−0.928183
25	1	0	−8.866645	−2.449854	−0.940383
26	1	0	−8.838284	−6.746241	−0.915787
27	1	0	−10.088773	−4.605017	−0.928914
28	8	0	−4.071211	−5.639086	−0.919220

1d

Thermal correction to Energy=	0.131749
Thermal correction to Enthalpy=	0.132693
Thermal correction to Gibbs Free Energy=	0.094222
Sum of electronic and zero-point Energies=	-417.681296
Sum of electronic and thermal Energies=	-417.674806
Sum of electronic and thermal Enthalpies=	-417.673862
Sum of electronic and thermal Free Energies=	-417.712333

Esol = -417.8510744

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.913185	−1.231603	−0.009792
2	6	0	−1.634745	−0.004046	−0.016010
3	6	0	0.324202	1.145271	−0.012043
4	6	0	1.043752	−0.078883	−0.005850
5	6	0	2.460700	−0.055696	−0.000672
6	1	0	2.984519	−1.005918	0.003982
7	6	0	3.123496	1.144753	−0.001615
8	6	0	2.404818	2.367473	−0.007727
9	6	0	1.033571	2.372179	−0.012883
10	1	0	4.208476	1.165622	0.002320
11	1	0	2.950878	3.305194	−0.008320
12	1	0	0.457713	3.291817	−0.017596
13	7	0	−1.039864	1.161118	−0.017159
14	7	0	0.394206	−1.278489	−0.004801
15	1	0	−2.722341	−0.016901	−0.019954
16	1	0	−1.453269	−2.175638	−0.009076

TS25

Thermal correction to Energy=	0.654355
Thermal correction to Enthalpy=	0.655300

Thermal correction to Gibbs Free Energy=	0.559269
Sum of electronic and zero-point Energies=	-1657.241606
Sum of electronic and thermal Energies=	-1657.207925
Sum of electronic and thermal Enthalpies=	-1657.206981
Sum of electronic and thermal Free Energies=	-1657.303011

Esol = -1657.856719

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.464342	-4.257831	1.769811
2	5	0	1.613091	-4.410106	-0.186415
3	7	0	0.149786	-3.417776	1.859316
4	8	0	0.412341	-4.870453	-0.810264
5	8	0	2.668652	-5.321412	-0.481781
6	8	0	2.597405	-3.560221	2.277809
7	8	0	1.398025	-5.547967	2.378913
8	6	0	-1.141757	-3.924787	1.706616
9	6	0	0.284483	-2.085896	1.852107
10	6	0	0.706581	-6.126883	-1.440897
11	6	0	2.252174	-6.049042	-1.644770
12	6	0	3.004183	-4.243004	3.470616
13	6	0	2.575989	-5.718674	3.177733
14	6	0	-2.220813	-3.014183	1.551392
15	6	0	-0.829394	-1.230160	1.717680
16	1	0	1.287265	-1.705996	2.011670
17	6	0	-0.100107	-6.224163	-2.727478
18	6	0	0.316935	-7.254330	-0.487231
19	6	0	2.968711	-7.389438	-1.658409
20	6	0	2.633551	-5.232074	-2.881487
21	6	0	2.229982	-3.636523	4.642998
22	6	0	4.498384	-4.037905	3.659899
23	6	0	3.612945	-6.483585	2.357752
24	6	0	2.203352	-6.521524	4.417191
25	7	0	-2.055727	-1.654438	1.562297
26	1	0	-0.656944	-0.156586	1.742405
27	1	0	-1.166367	-6.267039	-2.487173
28	1	0	0.159748	-7.131058	-3.283954
29	1	0	0.067486	-5.357276	-3.369774
30	1	0	0.489883	-8.236800	-0.937263
31	1	0	0.886824	-7.176382	0.444559
32	1	0	-0.747813	-7.168754	-0.254166
33	1	0	4.039466	-7.231689	-1.818334

34	1	0	2.594896	-8.026162	-2.467204
35	1	0	2.840616	-7.911902	-0.708544
36	1	0	2.425923	-5.777693	-3.807014
37	1	0	2.089143	-4.282951	-2.912000
38	1	0	3.704036	-5.011082	-2.843449
39	1	0	2.420263	-2.559797	4.672750
40	1	0	2.537197	-4.066288	5.601066
41	1	0	1.152833	-3.792586	4.523495
42	1	0	4.865588	-4.605930	4.521167
43	1	0	5.052351	-4.347331	2.771335
44	1	0	4.704226	-2.978027	3.835870
45	1	0	3.172156	-7.433206	2.039108
46	1	0	4.508147	-6.702730	2.948289
47	1	0	3.888274	-5.929150	1.458418
48	1	0	3.051475	-6.590723	5.106792
49	1	0	1.357112	-6.075007	4.942637
50	1	0	1.922846	-7.537299	4.123883
51	6	0	0.926186	-0.752059	-0.940552
52	6	0	0.821930	-2.152767	-0.802686
53	7	0	1.889952	-2.911777	-0.527687
54	6	0	3.109552	-2.254577	-0.346716
55	6	0	3.146823	-0.840987	-0.479372
56	7	0	2.041511	-0.090056	-0.784839
57	1	0	0.027734	-0.192110	-1.190106
58	1	0	-0.108544	-2.680714	-0.977997
59	6	0	4.298406	-2.956160	-0.052101
60	6	0	5.479255	-2.265117	0.099014
61	6	0	5.524027	-0.862087	-0.029598
62	6	0	4.376658	-0.163759	-0.312805
63	1	0	4.258849	-4.031145	0.049794
64	1	0	6.387776	-2.812503	0.328243
65	1	0	6.465372	-0.337347	0.096709
66	1	0	4.366130	0.915455	-0.421455
67	6	0	-2.689216	-5.768195	1.590936
68	6	0	-1.397937	-5.310597	1.728399
69	6	0	-3.533022	-3.519579	1.405112
70	6	0	-3.764882	-4.872635	1.424076
71	1	0	-2.877483	-6.836913	1.608748
72	1	0	-0.571066	-5.994002	1.858802
73	1	0	-4.332043	-2.795876	1.284905
74	1	0	-4.774380	-5.254808	1.313446

1e

Thermal correction to Energy=	0.064764
Thermal correction to Enthalpy=	0.065708
Thermal correction to Gibbs Free Energy=	0.026632
Sum of electronic and zero-point Energies=	-1183.292227
Sum of electronic and thermal Energies=	-1183.285899
Sum of electronic and thermal Enthalpies=	-1183.284955
Sum of electronic and thermal Free Energies=	-1183.324030

Esol = -1183.498551

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.040985	0.169556	0.001530
2	6	0	1.347512	0.171702	−0.000361
3	7	0	2.035764	1.315702	−0.001679
4	6	0	1.353481	2.438433	−0.001095
5	6	0	−0.053889	2.436256	0.000964
6	7	0	−0.732730	1.311444	0.002195
7	1	0	−0.610386	−0.753845	0.002490
8	1	0	1.919729	−0.749959	−0.000811
9	17	0	−0.958720	3.913410	0.002007
10	17	0	2.253683	3.918410	−0.003043

TS26

Thermal correction to Energy=	0.520158
Thermal correction to Enthalpy=	0.521102
Thermal correction to Gibbs Free Energy=	0.424145
Sum of electronic and zero-point Energies=	-3188.433141
Sum of electronic and thermal Energies=	-3188.399757
Sum of electronic and thermal Enthalpies=	-3188.398813
Sum of electronic and thermal Free Energies=	-3188.495770

Esol = -3189.124524

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	5	0	1.480892	−4.226946	1.853695
2	5	0	1.549825	−4.469173	−0.193389
3	7	0	0.108054	−3.476818	1.879370
4	8	0	0.301877	−4.814813	−0.766950
5	8	0	2.510061	−5.456140	−0.470039

6	8	0	2.551805	-3.410806	2.283563
7	8	0	1.538966	-5.491586	2.459091
8	6	0	-1.126638	-4.038619	1.718172
9	6	0	0.166339	-2.115419	1.839354
10	6	0	0.487471	-6.072299	-1.458054
11	6	0	2.037062	-6.124257	-1.652010
12	6	0	3.081710	-4.043962	3.465932
13	6	0	2.768099	-5.554097	3.203470
14	6	0	-2.203031	-3.232434	1.363550
15	6	0	-0.961736	-1.364386	1.565961
16	1	0	1.136001	-1.680561	2.049417
17	6	0	-0.315743	-6.030507	-2.748923
18	6	0	-0.008625	-7.200169	-0.561440
19	6	0	2.635644	-7.520262	-1.688930
20	6	0	2.502079	-5.321253	-2.868708
21	6	0	2.307358	-3.487731	4.661504
22	6	0	4.557424	-3.706536	3.584989
23	6	0	3.821648	-6.238056	2.336759
24	6	0	2.518879	-6.370346	4.463959
25	7	0	-2.140875	-1.910784	1.277863
26	1	0	-0.896473	-0.280835	1.561789
27	1	0	-1.382781	-5.982177	-2.513872
28	1	0	-0.140154	-6.932699	-3.344154
29	1	0	-0.060251	-5.157030	-3.352192
30	1	0	0.103812	-8.170172	-1.054718
31	1	0	0.542868	-7.208256	0.383825
32	1	0	-1.068671	-7.049660	-0.345894
33	1	0	3.717352	-7.448826	-1.833437
34	1	0	2.218814	-8.102543	-2.517285
35	1	0	2.451465	-8.052234	-0.754241
36	1	0	2.240622	-5.822271	-3.805424
37	1	0	2.059201	-4.319845	-2.881347
38	1	0	3.589176	-5.213005	-2.825875
39	1	0	2.410263	-2.398915	4.675659
40	1	0	2.687387	-3.880188	5.608944
41	1	0	1.242555	-3.733955	4.589189
42	1	0	4.997966	-4.208214	4.452807
43	1	0	5.106132	-4.003730	2.690295
44	1	0	4.678461	-2.627217	3.716538
45	1	0	3.438982	-7.216786	2.034317
46	1	0	4.754871	-6.385985	2.889138
47	1	0	4.017215	-5.665869	1.427955
48	1	0	3.400454	-6.359946	5.113646
49	1	0	1.662175	-5.990956	5.024088

50	1	0	2.311909	-7.408533	4.190123
51	6	0	1.078315	-0.771937	-0.805055
52	6	0	0.904196	-2.143760	-0.807434
53	7	0	1.933567	-2.981095	-0.493143
54	6	0	3.146571	-2.395827	-0.254699
55	6	0	3.232199	-1.010072	-0.189073
56	7	0	2.221549	-0.190496	-0.451152
57	1	0	0.250895	-0.125324	-1.080406
58	1	0	-0.027951	-2.627462	-1.073263
59	17	0	-1.338790	-5.691662	2.095982
60	17	0	-3.755579	-3.943441	1.059183
61	17	0	4.546340	-3.375897	-0.156986
62	17	0	4.740566	-0.251002	0.208226

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