Electronic Supplementary Information

for

Metal π-Lewis Base Activation Model in Pd-Catalyzed Hydroamination of Amine and 1,3-Dienes

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1. Alternative transition states structures in the π-Lewis base activation step

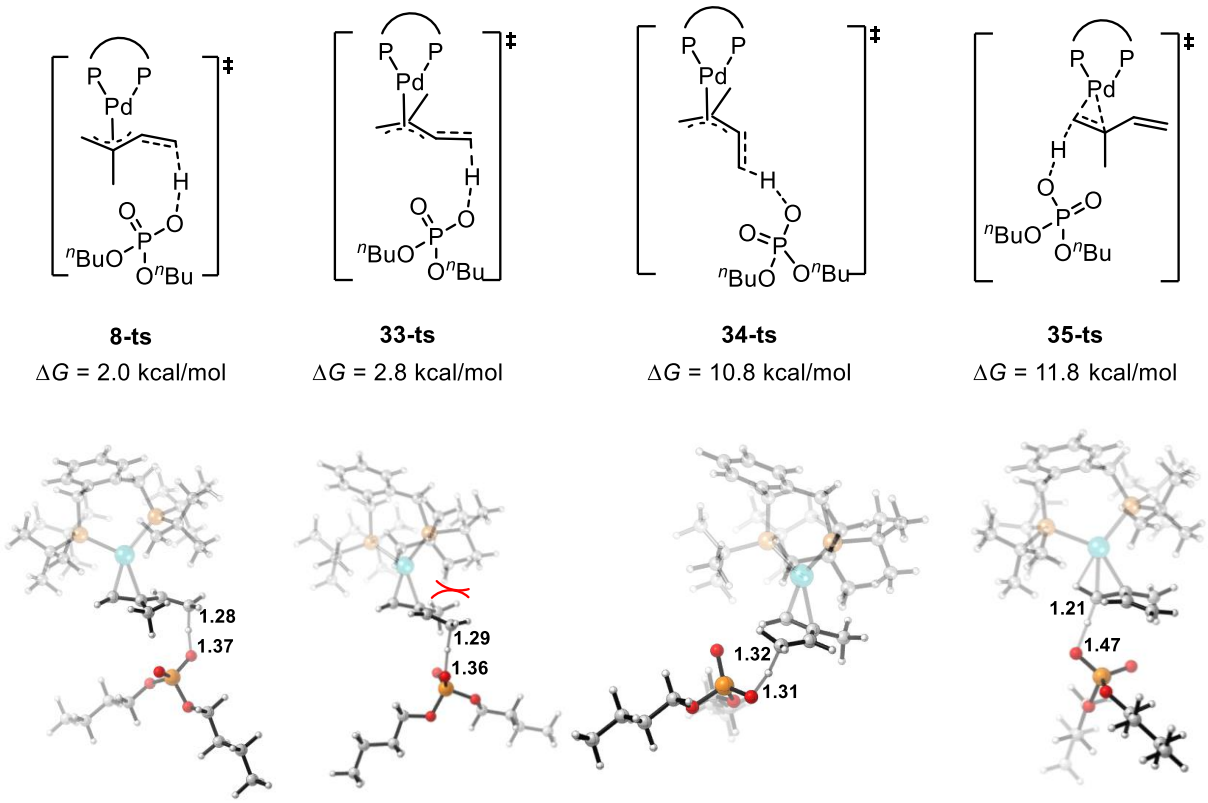


Fig. S1. The structure and energy difference of various π-lewis base activation transition states in Pd-catalyzed hydroamination of indazoles with isoprene.

As shown in **Fig. S1**, alternative transition state structures in the π-Lewis base activation step were considered. Due to the steric hindrance between methyl at isoprene and ligand, the relative free energy of **33-ts** is 0.8 kcal/mol higher than that of **8-ts**. Meanwhile, the cis-conformation isoprene involved transition state **34-ts** is 8.8 kcal/mol higher than that of **8-ts**. In **35-ts**, phosphoric acid reacts with the adjacent carbon atom. and the relative free energy of **35-ts** is 9.8 kcal/mol higher than that of **8-ts**, indicating the vinylogy activation of diene is more favorable. It is consistent with the orbital analysis in Figure 2.

2. Alternative transition states structures in the LLHT step

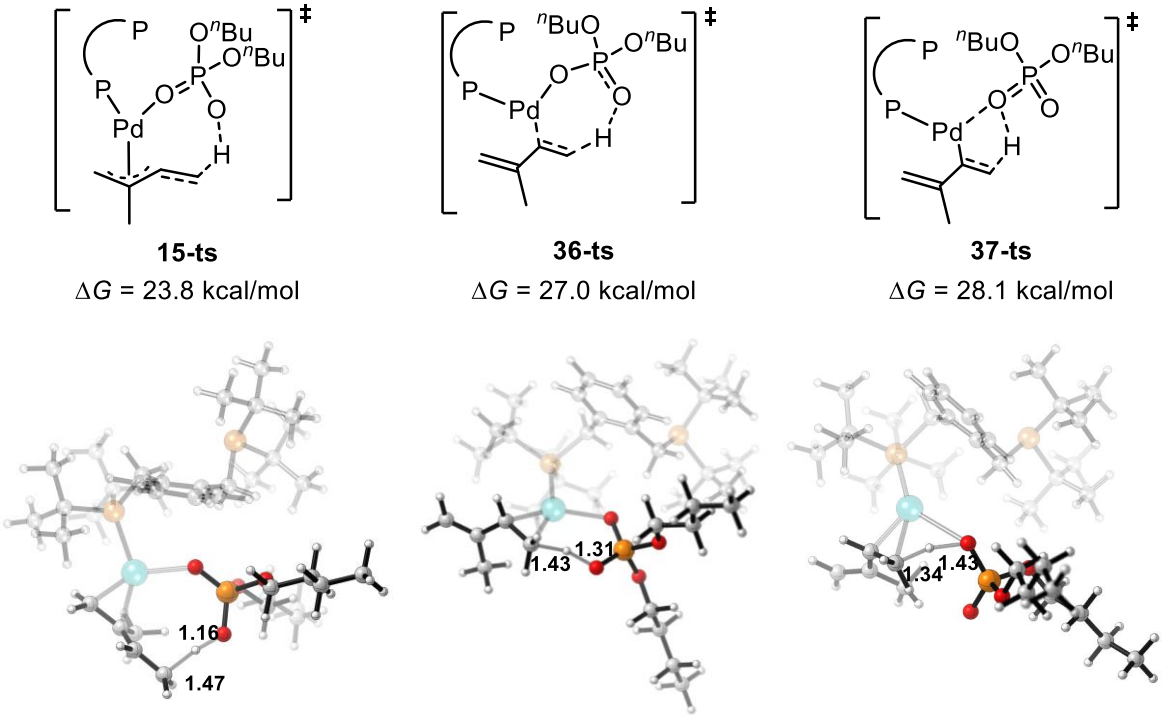


Fig. S2. The structure and energy difference of various LLHT transition state in Pd-catalyzed hydroamination of indazoles with isoprene.

As shown in **Fig. S2**, alternative transition state structures in the LLHT step were considered. Calculated results showed that all of these are much higher than that of **8-ts** for the π-Lewis base activation process.

3. BEt_3 mediated generation Pd(II)-H species

The ancillary Lewis acid BEt_3 could facilitate the Pd(0)-catalyzed hydroamination of indazoles with isoprene to get N^1-functionalized product **3b** (**Scheme 2a**). For this Brønsted acid absent system, a **BEt_3** activating Pd(0) mechanism was proposed in the previous report. A small amount of **BEt_3** was expected to undergo oxidative addition with Pd(0) and the subsequent hydride elimination to deliver the Et_2B-Pd(II)-H species. To evaluate the possibility of this pathway, we have calculated the free energy profile. As shown in Figure S3, the activation free energy of this pathway is up to 66.9 kcal/mol (referring to **7→39-ts**). The extremely high activation free energy suggests this process is hard to occur in this reaction condition. Thus the possibility of the BEt_3 mediated generation Pd(II)-H species pathway was excluded.

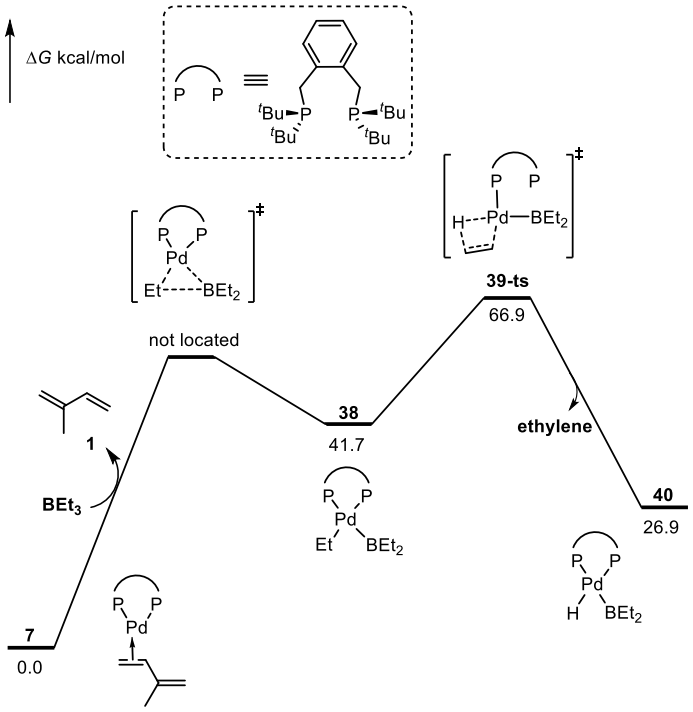


Fig. S3. Free energy profile of the pathway for BEt_3 mediated generation Pd(II)-H species.

4. The initial cycle of cationic Pd(II)−π-allyl mediated Pd-catalyzed hydroamination

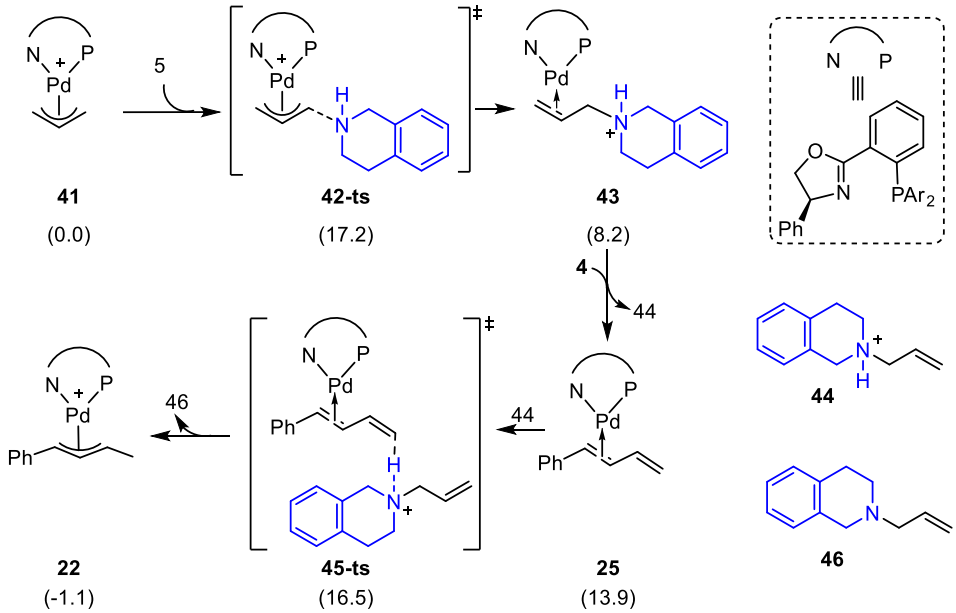


Fig. S4. The initial cycle of cationic Pd(II)−π-allyl mediated Pd-catalyzed hydroamination of aliphatic amine with diene. The data in parentheses represent the relative free energy, which is given in kcal/mol.

The main reaction mechanism of cationic Pd(II)−π-allyl mediated Pd-catalyzed hydroamination of aliphatic amine with diene was given in the text. The active complex **22** could be generated through

the initial cycle of cationic Pd(II)−π-allyl mediated Pd-catalyzed hydroamination (Figure S4). The reaction starts from the amine **5** nucleophilic attack of the Pd(II)-π-allyl species **41** to give Pd(0) complex **25** and quaternary ammonium salt cation **44**. Subsequently, the formation of Pd(II)-π-allyl species **22** via the π-Lewis base activation process between **44** and **25**. The activation free energy for the initial cycle of cationic Pd(II)−π-allyl mediated Pd-catalyzed hydroamination is 17.2 kcal/mol (referring to **41→42-ts**), indicating this process could proceed smoothly in the reaction condition.

5. Alternative transition states structures for the oxidative protonation process

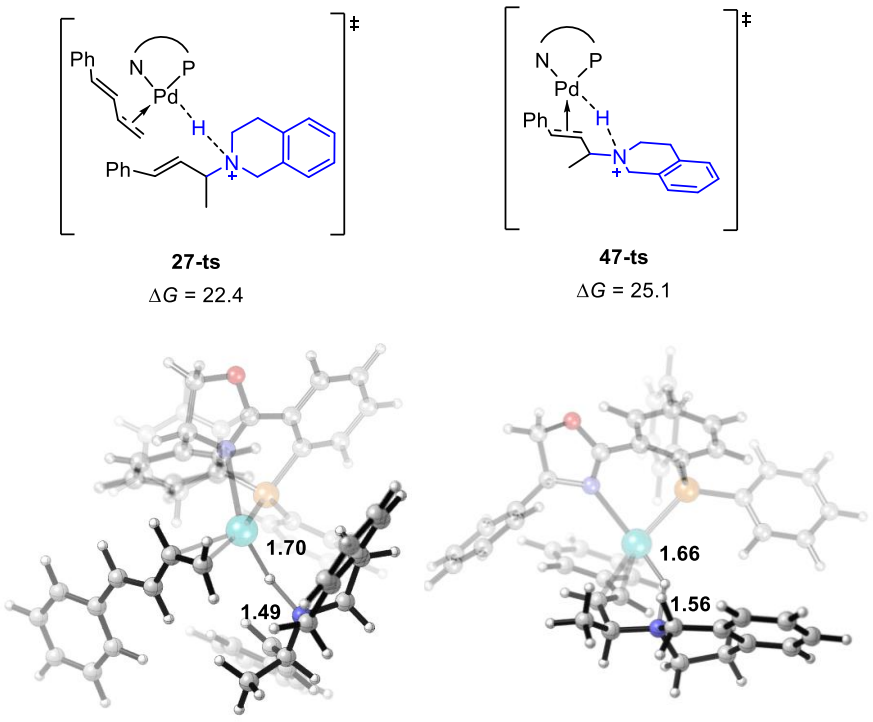


Fig. S5. The structure and energy of different transition states for the generation of Pd(II)-H species via the oxidative protonation process.

As shown in **Fig. S5**, alternative transition state structures in the generation of Pd(II)-H species via the oxidative protonation process were considered. Calculated results showed that all of these are much higher than that of **26-ts** for the π-Lewis base activation process.

6. Neutral pathway for the Pd-catalyzed hydroamination of aliphatic amine with diene

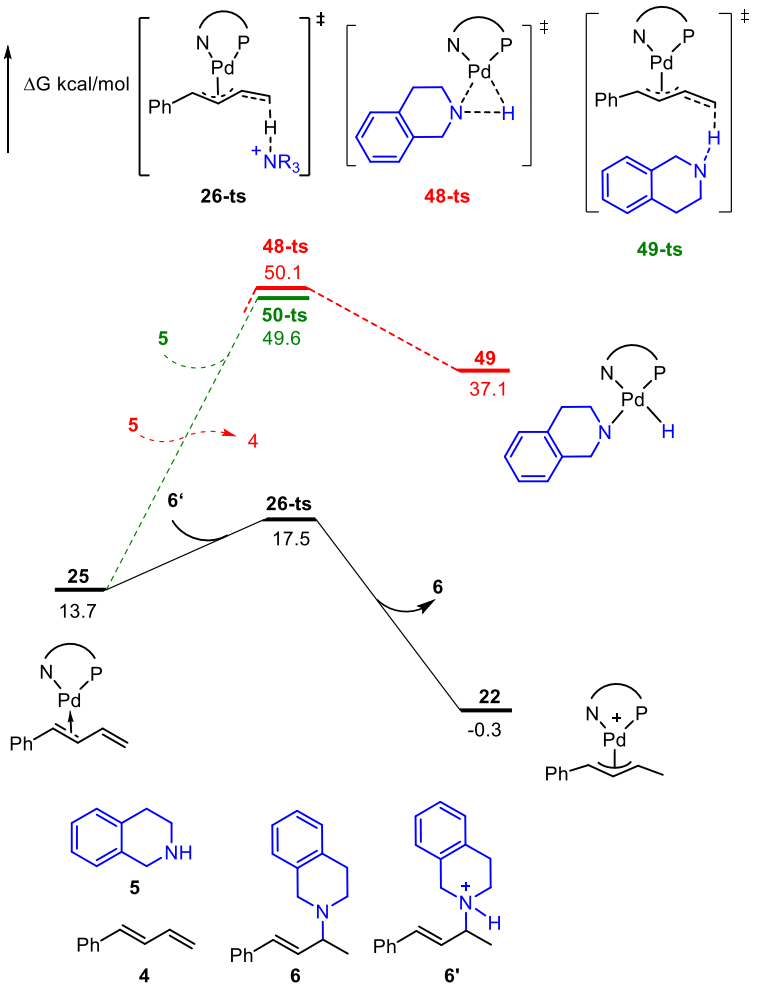


Fig. S6. Free energy profile of the neutral pathway for the Pd-catalyzed hydroamination of aliphatic amine with diene.

Neutral aliphatic amine **5** direct oxidation addition with Pd complexes in hydroamination reaction was discussed. As shown in Figure S6, calculated results show that the energy barrier of oxidation addition with neutral amine **5** is up to 50.1 kcal/mol (referring to **25→48-ts**). It suggests that the neutral amine **5** is insufficient to oxidize Pd(0) species. Moreover, the aliphatic amine **5** involved π-Lewis base activation process needs to overcome a high energy barrier of 49.6 kcal/mol (referring to **25→50-ts**). These results emphasize the critical role of the cationic Pd(II) pre-catalyst triggered ammonium salt **6′**.

7. The pre-activation of [Pd(π-allyl)Cl]$_2$ in the neutral catalytic system

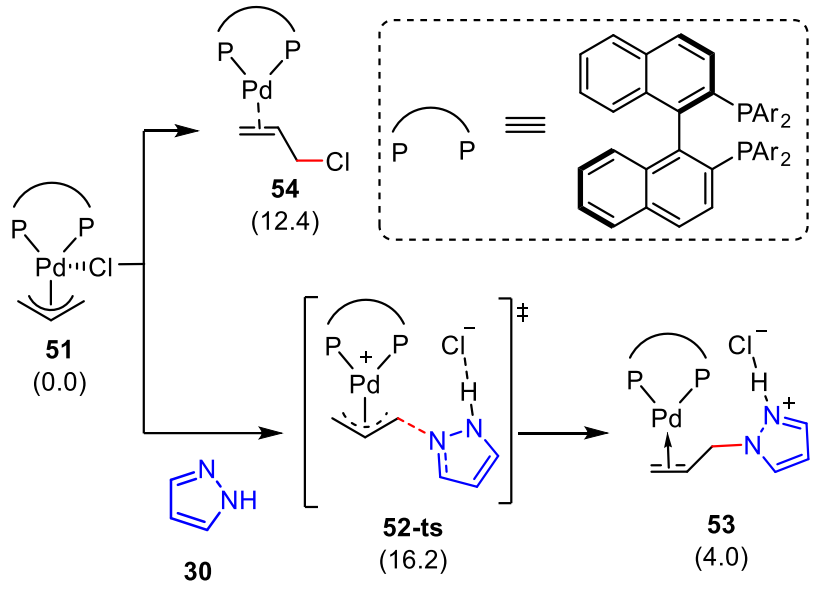
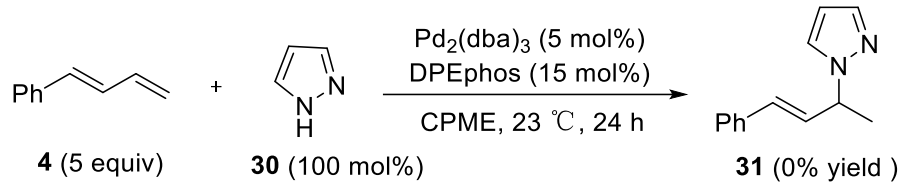


Fig. S7. The pre-activation of [Pd(π-allyl)Cl]$_2$ in the neutral catalytic system. The data in parentheses represent the relative free energy, which is given in kcal/mol.

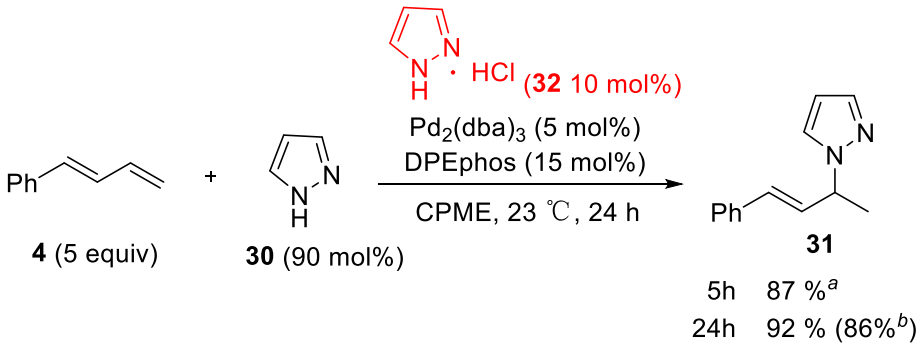
In addition, the neutral [Pd(π-allyl)Cl]$_2$ catalyst was also sufficient to mediate hydroamination reactions. Based on the above results, we anticipated that the pyrazole hydrochloride generated through reductive elimination with pyrazole could serve as an initial electrophile of the π-Lewis base activation mode. To validate this issue, we have calculated the pre-activation of [Pd(π-allyl)Cl]$_2$ in this neutral catalytic system. As shown in Figure S7, [Pd(π-allyl)Cl]$_2$ **51** could directly afford allyl chloride (**54**) with an endothermic by 12.4 kcal/mol. However, the formation of pyrazole hydrochloride **53** via **52-ts** is only endothermic by 4.0 kcal/mol. It suggests that the formation of pyrazole hydrochloride **53** is more thermodynamically favorable. And the generated pyrazole hydrochloride could drive the catalytic cycle via the π-Lewis base activation process to obtain desired hydroaminated products.

8. Control experiments



When the catalyst was changed from $[Pd(\eta^3\text{-}C_3H_5)Cl]_2$ to $Pd_2(dba)_3$, the reaction could not proceed normally and no target product was detected. The detailed operations are as follows:

Procedure: In a N_2-filled glovebox, an oven dried vial equipped with a magnetic stir bar was charged with $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol), DPEphos (16.2 mg, 0.03 mmol) and CPME (1.0 mL). The resulting mixture was stirred for 10 mins and then (*E*)-buta-1,3-dien-1-ylbenzene **4** (130.2 mg, 140.2 μL, 1.0 mmol) followed by a solution of freshly recrystallized pyrazole **30** (13.6 mg, 0.2 mmol) in CPME (1.0 mL) were added dropwise. The mixture was removed from the glovebox and stirred at 23 ºC for 24 h. TLC and ^{1}H-NMR analysis showed that no target product **31** was formed.

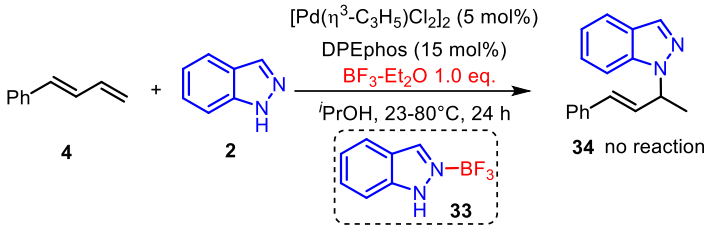


[a]The yield was determined by 1H-NMR with mesitylene as the internal standard.
[b]isolated yield.

However, when a catalytic amount of pyrazole hydrochloride **32** was added, the reaction was back on track and the target product was obtained in a high isolated yield of 87%. Increasing the reaction time to 24 hours could obtain a slightly higher yield of 92% (86% isolated yield).The detailed operations are as follows:

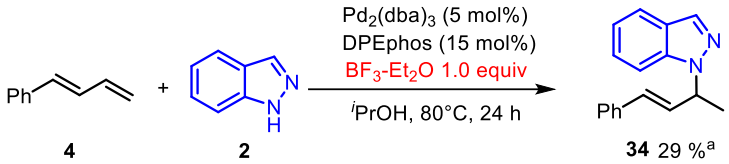
Procedure: In a N_2-filled glovebox, an oven dried vial equipped with a magnetic stir bar was charged with $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol), DPEphos (16.2 mg, 0.03 mmol) and CPME (1.0 mL). The resulting mixture was stirred for 10 mins and then (*E*)-buta-1,3-dien-1-ylbenzene **4** (130.2 mg, 140.2 μL, 1.0 mmol) followed by a solution of freshly recrystallized pyrazole **30** (12.3 mg, 0.18 mmol) and pyrazole hydrochloride **32** (2.1 mg, 0.02 mmol) in CPME (1.0 mL) were added dropwise. The mixture was removed from the glovebox and stirred at 23 ºC until no starting material was

observed by TLC. After completion, the mixture was concentrated and purified by flash chromatography on silica gel (EtOAc:petroleum ether = 1:10) to give the product **31** (34.1 mg, 0.172 mmol), as a white solid, yielding 86%. The structure of product **31** was identified by comparison with the NMR spectra of the previous report (*Angew. Chem. Int. Ed.* **2021**, *60*, 19660).



Moreover, when 1.0 equiv BF_3 additive was added, the neutral [Pd(π-allyl)Cl]$_2$ catalyzed hydroamination of indazole **2** was completely quenched at 23ºC or 80ºC. We speculate that the combination of **2** and BF_3 generates Lewis acid-base adduct **33**. So that the reductive amination of indazole **2** and [Pd(π-allyl)Cl]$_2$ was inhibited, and the active Pd(0)-intermediate cannot generate to realize the catalytic process.

Procedure: In a N_2-filled glovebox, an oven dried vial equipped with a magnetic stir bar was charged with [Pd(π-allyl)Cl]$_2$ (1.83mg, 0.005 mmol), DPEphos (8.1 mg, 0.015 mmol) and ^{i}PrOH (0.50 mL). The resulting mixture was stirred for 10 mins and then (*E*)-buta-1,3-dien-1-ylbenzene **4** (56 µL, 0.4 mmol) followed by a solution of freshly recrystallized indazole **2** (23.6 mg, 0.2 mmol) and BF_3-Et_2O (46.5%, 0.2mmol, 25µL) in ^{i}PrOH (0.50 mL) were added dropwise. The mixture was removed from the glovebox and stirred at 80 ºC until no starting material was observed by TLC. The structure of product **34** was identified by comparison with the NMR spectra of the previous report (*Org. Lett.* **2022**, *24,* 2452).



Meanwhile, the controlled trial (Fig 7e) showed that the corresponding transformation can proceed smoothly when Pd(0)-catalyst ($Pd_2(dba)_3$, 5 mol %) was used. It suggests that the BF_3 additive only intervenes in the reductive amination process. On the other hand, it can facilitate the Pd(0)-catalyzed hydroamination as a Lewis acid co-catalyst.

Procedure: In a N_2-filled glovebox, an oven dried vial equipped with a magnetic stir bar was charged with $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol), DPEphos (16.2 mg, 0.03 mmol) and ^{i}PrOH (0.50 mL). The resulting mixture was stirred for 10 mins and then (*E*)-buta-1,3-dien-1-ylbenzene **4** (140 µL, 1

mmol) followed by a solution of freshly recrystallized indazole **2** (23.6 mg, 0.2 mmol) and BF_3-Et_2O (46.5%, 0.2mmol, 25μL) in ^{i}PrOH (0.50 mL) were added dropwise. The mixture was removed from the glovebox and stirred at 80 ºC until no starting material was observed by TLC. The structure of product **34** was identified by comparison with the NMR spectra of the previous report (*Org. Lett.* **2022**, *24,* 2452).

The above control experiments demonstrate that the in situ generated pyrazole hydrochloride is the key to this Pd-catalyzed hydroamination, which is corroborate with our calculation results.

9. Detection the complex II and IV by ^{1}H NMR experiments

we have found the interaction of 1,3-diene with Pd(0)-catalyst via ^{1}H NMR experiments. As shown below, The ^{1}H NMR experiments showed that the diene moiety in **4** experienced apparent high-field shifts when Pd(0)-catalyst and ligand were added, potentially supporting the electron-donating effect of Pd(0) in 1,3-diene coordinated η^2-Pd(0)-complex (**II**) (The similar phenomenon was observed in our previous report: *J. Am. Chem. Soc.*, 2021, **143**, 4809). These results provide reliable evidence for the HOMO-raised η^2-complexes with Pd(0) achieving π-Lewis base activation.

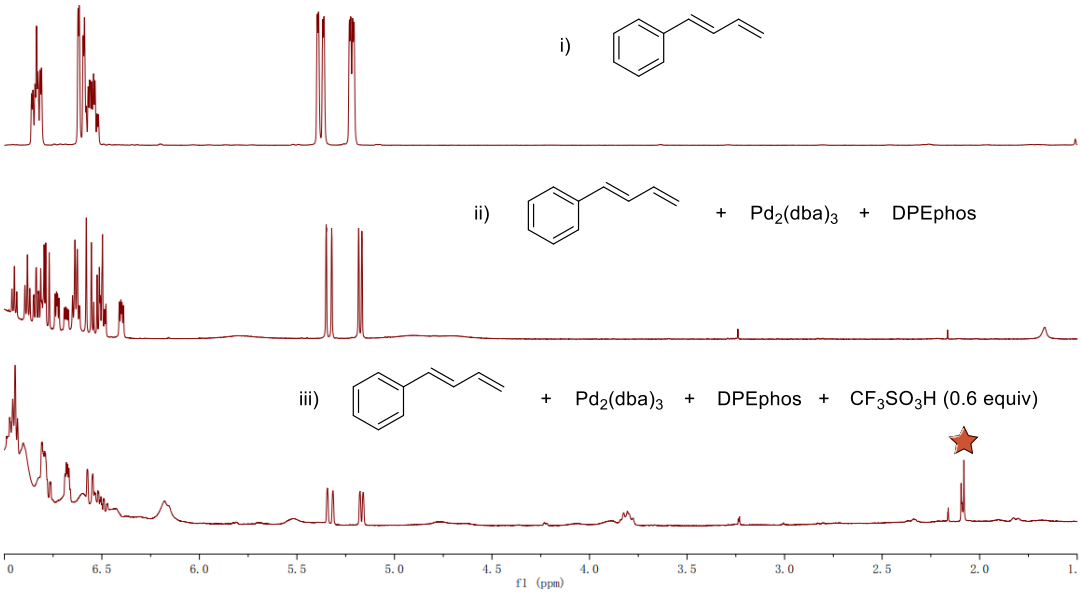


Fig. S8 The ^{1}H NMR experiments of 1,3-diene **4** with adding $Pd_2(dba)_3$, DPEphos, and CF_3SO_3H to trace the **complex IV**.

Complex **III** was considered a transition state, so it cannot be detected by experimental methods. Pd-π-allyl complex **IV** is well known in the Pd-catalyzed reactions. We also try to detect Pd-π-allyl complex **IV** in the reaction system. The 1H NMR experiments showed that when Brønsted acid CF_3SO_3H is added, the characteristic signal for the alkyl group was apparently observed. We

speculate this could be methyl of Pd-π-allyl complex **IV**. This result provides reliable evidence for the Pd-π-allyl complex **IV** could potentially be considered as the reaction intermediate.

10. Reaction scope of alkyl amine

we have evaluated the reactivity of simple alkyl amine with our developed Pd(0)-catalyzed hydroamination of 1,3-diene. The reaction result showed that alkyl amine **35** exhibits lower reactivity compared with pyrazole. It's worth noting that this reaction could proceed with the assistance of pyrazole hydrochloride so that the preparation of other hydrochloride is unnecessary. Moreover, the yield of this reaction can be raised to 74% in the presence of the $AgPF_6$ additive.

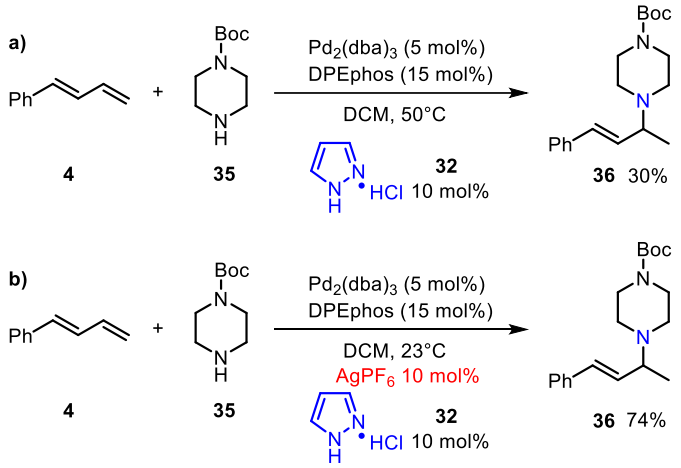


Fig. S9 The reaction scope of alkyl amine.

Procedure: In a N_2-filled glovebox, an oven dried vial equipped with a magnetic stir bar was charged with $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol), DPEphos (16.2 mg, 0.03 mmol) and DCM (0.5 mL). The resulting mixture was stirred for 10 mins and then (*E*)-buta-1,3-dien-1-ylbenzene **4** (130.2 mg, 140.2 µL, 1.0 mmol) followed by a solution of freshly recrystallized piperazine **35** (37.2 mg, 0.2 mmol) and pyrazole hydrochloride **32** (2.1 mg, 0.02 mmol) in DCM (1.0 mL) were added dropwise. The mixture was removed from the glovebox and stirred at 50 ºC until no starting material was observed by TLC. The structure of product **36** was identified by comparison with the NMR spectra of the previous report (*J. Am. Chem. Soc.* **2017***, 139,* 7180).

11. Complete References for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.;

Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

12. Calculated energy and geometry for all intermediates and transition states

1

Zero-point correction= 0.114116 (Hartree/Particle)
Thermal correction to Energy= 0.119951
Thermal correction to Enthalpy= 0.120895
Thermal correction to Gibbs Free Energy= 0.085640
E(solv) = -195.38939962

C	0.65954100	1.40247800	0.00007100
C	0.51598000	-0.10056500	-0.00007700
H	0.18162900	1.84598300	-0.88273700
H	0.17795400	1.84634200	0.88060300
H	1.71227800	1.69922300	0.00218900
C	1.58984500	-0.90969300	-0.00012100
H	2.60314500	-0.51765200	0.00011800
H	1.48668400	-1.99204000	0.00009500
C	-0.83343700	-0.67948900	0.00015600
C	-1.98629500	0.00466400	-0.00006200
H	-2.02058600	1.09056200	-0.00014600
H	-2.94379200	-0.50785400	-0.00016700
H	-0.87112000	-1.76892700	0.00024700

2

Zero-point correction= 0.118564 (Hartree/Particle)
Thermal correction to Energy= 0.124689
Thermal correction to Enthalpy= 0.125633
Thermal correction to Gibbs Free Energy= 0.088311
E(solv)= -379.98585428

C	-0.50801500	0.60256100	0.00000000
C	0.00000000	-0.72265000	0.00000000
C	1.37760700	-0.99669700	0.00000000
C	2.23453700	0.09315200	0.00000000
C	1.74836100	1.42296900	0.00000000
C	0.38851900	1.68815000	0.00000000
C	-1.92804400	0.43453100	0.00000000
H	1.75688100	-2.01457300	0.00000000
H	3.30803100	-0.07587900	0.00000000
H	2.45934000	2.24429900	0.00000000
H	0.02030400	2.71053300	0.00000000
H	-2.69865300	1.19440500	0.00000000
N	-2.26949000	-0.84183900	0.00000000
N	-1.10006500	-1.53633600	0.00000000
H	-1.13680800	-2.54366200	0.00000000

3a

Zero-point correction= 0.236593 (Hartree/Particle)
Thermal correction to Energy= 0.249038
Thermal correction to Enthalpy= 0.249983
Thermal correction to Gibbs Free Energy= 0.197293
E(solv)= -575.39747912

H	-3.46392000	0.56300000	2.09960100
C	-2.37236100	0.03882300	-2.01262800
C	-2.79690800	-0.18875100	-0.58223800
H	-2.39019100	1.10627400	-2.27303400
H	-1.34751900	-0.31402100	-2.17855700
H	-3.03097400	-0.49075700	-2.70698300
C	-3.79882200	-1.01237400	-0.26426500
H	-4.34691300	-1.54646400	-1.03594400
H	-4.10809600	-1.19826500	0.75854100
C	-2.03570400	0.61895900	0.46447600

C	-2.40614700	0.34517100	1.92469500
H	-2.20514900	-0.69764300	2.18197700
H	-1.81025700	0.98446400	2.58336800
H	-2.20993200	1.68254600	0.25040600
C	1.56696200	0.79660100	-0.06002600
C	1.27470300	-0.58365600	0.21530600
C	2.31523800	-1.54734600	0.24205400
C	3.59884500	-1.11540000	-0.00253100
C	3.89178800	0.25535500	-0.27633500
C	2.90045500	1.21011300	-0.30827900
C	0.31664500	1.42026500	-0.00218800
H	2.08913300	-2.58859100	0.45049600
H	4.41732100	-1.83041800	0.01133400
H	4.92301500	0.54306100	-0.46253400
H	3.13276800	2.25104900	-0.51723400
H	0.01171800	2.44769200	-0.13940600
N	-0.58193000	0.44652400	0.28365800
N	-0.04509300	-0.78059200	0.42344600

3b

Zero-point correction=0.236598 (Hartree/Particle)

Thermal correction to Energy=0.249124

Thermal correction to Enthalpy=0.250068

Thermal correction to Gibbs Free Energy=0.196789

E(Solv)= -575.40256649

C	2.11670700	-0.56320900	-1.94419700
C	2.61121600	-0.32242900	-0.53841200
H	1.63381400	-1.54575700	-2.03759300
H	1.37010400	0.18657700	-2.23143400
H	2.93910800	-0.51855000	-2.66414800
C	3.88111700	0.00268400	-0.28275600
H	4.60459400	0.10076300	-1.08794100
H	4.25109800	0.19268500	0.71902100
C	1.57272900	-0.51725100	0.56313300
C	2.04749300	-0.22215400	1.99008400
H	2.34581600	0.82543500	2.08566000
H	2.89418000	-0.86103000	2.25941200
H	1.24898600	-1.56574900	0.51573800
C	-1.72952100	0.96371000	-0.08696300
C	-0.93469000	-0.18989300	0.14729900
C	-1.50163000	-1.47557700	0.21558700
C	-2.87368500	-1.57326400	0.04275800
C	-3.67915800	-0.43309400	-0.19308000
C	-3.12040800	0.83258100	-0.25964500
C	-0.79103200	2.03822800	-0.07973200
H	-0.89849600	-2.36009500	0.39710200
H	-3.34450200	-2.55156900	0.08997300
H	-4.75024100	-0.55965600	-0.32256000
H	-3.74025900	1.70670500	-0.44042900
H	-0.97207800	3.09608600	-0.22187100
N	0.43949300	1.60667000	0.13364100
N	0.35894900	0.25426600	0.26608500
H	1.23396000	-0.41437700	2.69653600

4

Zero-point correction= 0.167365 (Hartree/Particle)

Thermal correction to Energy= 0.176323

Thermal correction to Enthalpy= 0.177268

Thermal correction to Gibbs Free Energy= 0.132588

E(solv)= -387.20701714

C	-0.89639100	-0.66149100	-0.00011300
C	-1.98196100	0.14281400	0.00003100
H	-1.06886200	-1.73856300	-0.00028400
H	-1.86416800	1.22590300	0.00022200
C	-3.34610600	-0.35165400	-0.00004200
C	-4.43904200	0.42949000	0.00011300
H	-3.46700500	-1.43551200	-0.00024500
C	0.51375100	-0.26592200	-0.00006000
C	1.50040000	-1.27030700	0.00003000
C	0.94328900	1.07659900	-0.00010500
C	2.85755500	-0.95313300	0.00009600
H	1.19080700	-2.31303800	0.00005800
C	2.29795800	1.39403300	-0.00003700
H	0.21127000	1.87888100	-0.00021500
C	3.26380800	0.38210600	0.00006700
H	3.59745400	-1.74924200	0.00016700
H	2.60440100	2.43689800	-0.00007100
H	4.32067700	0.63430000	0.00011400
H	-5.44056300	0.01050500	0.00005400
H	-4.36358500	1.51466000	0.00031800

5

Zero-point correction= 0.183110 (Hartree/Particle)

Thermal correction to Energy= 0.190826

Thermal correction to Enthalpy= 0.191771

Thermal correction to Gibbs Free Energy= 0.150823

E(solv) = -404.49274818

C	-1.18463300	1.45974300	-0.04489200

C	0.12353900	0.69091400	0.00165400
C	0.13143100	-0.71314000	0.04183200
C	-1.17190100	-1.48764900	0.10214800
C	-2.36057700	-0.62953100	-0.33739800
H	1.32781000	2.47376400	-0.06960800
H	-1.32190000	1.84418900	-1.07721500
C	1.33928200	1.38564500	-0.03874400
C	1.36108500	-1.38627500	0.04265700
H	-1.10476700	-2.38948100	-0.52002300
H	-3.30152100	-1.13704600	-0.09852300
C	2.56668500	-0.68943200	0.00475900
C	2.55592500	0.70737800	-0.03637700
H	1.36672100	-2.47427100	0.07210300
H	3.50901200	-1.23103300	0.00508200
H	3.48940900	1.26329600	-0.06382000
N	-2.30838000	0.63521200	0.39534300
H	-3.17459900	1.15231900	0.26527100
H	-1.11914800	2.33886600	0.60848500
H	-2.33015300	-0.48953000	-1.43641000
H	-1.34721700	-1.82346800	1.13342700

6

Zero-point correction= 0.243101 (Hartree/Particle)

Thermal correction to Energy= 0.256411

Thermal correction to Enthalpy= 0.257355

Thermal correction to Gibbs Free Energy= 0.200191

E(Solv)= -613.52886444

C	3.80322000	-1.51756500	-0.57991900
C	2.51082900	-1.00182400	-0.61655200
C	2.20941500	0.23764100	-0.02064200
C	3.25404600	0.93133200	0.61578500
C	4.54939100	0.41632600	0.65347200
C	4.83073000	-0.81183800	0.05422400
H	4.01090100	-2.47718700	-1.04624800
H	1.72771400	-1.57131400	-1.10849800
H	3.04237400	1.88953300	1.08530700
H	5.33756800	0.97482100	1.15159700
H	5.83803200	-1.21829700	0.08170200
C	0.86491100	0.83844800	-0.02836400
H	0.78972400	1.76999000	0.53003100
C	-0.22993500	0.36691900	-0.64329700
H	-0.17612000	-0.56296100	-1.20768800
C	-1.60564200	1.00077600	-0.63611800
C	-1.69215600	2.34178800	0.11792600
H	-1.45265800	2.21130200	1.17818500
H	-1.00127900	3.07741000	-0.30839100
H	-1.86813400	1.19977700	-1.68938500
C	-3.87142200	-1.48727300	0.94709700
C	-2.59035600	-0.89061900	0.93644500
C	-2.62445600	0.01368700	-0.11355500
N	-3.87620200	-0.09850100	-0.64273500
H	-4.25332400	-2.25042400	1.61309400
H	-1.75359100	-1.08632900	1.59105200
N	-4.65677600	-1.00664800	-0.01609700
H	-2.70663100	2.74800300	0.05357800
H	-4.25517600	0.40493200	-1.43151300

7

Zero-point correction= 0.750691 (Hartree/Particle)

Thermal correction to Energy= 0.792039

Thermal correction to Enthalpy= 0.792983

Thermal correction to Gibbs Free Energy= 0.681307

E(solv)= -1947.68693849

Pd	-0.40337300	-0.95832000	-0.49870200
P	1.87911400	-0.75359000	0.23858700
P	-1.54384200	0.99473500	0.32848600
C	2.32495500	0.84139500	1.17855600
C	2.07505900	2.19682500	0.54366800
C	3.18022600	2.91197200	0.04904300
C	3.07078700	4.19294100	-0.48502300
C	1.82485500	4.81551900	-0.50276800
C	0.72670400	4.14274600	0.02503700
C	0.81101500	2.83718200	0.54151000
C	-0.43157700	2.27012700	1.20042100
C	3.16153700	-0.83237400	-1.20806000
C	2.57763400	0.06145100	-2.32708400
C	4.58924000	-0.34751400	-0.88919900
C	3.25454800	-2.27404400	-1.74959800
C	2.37070800	-2.05603000	1.59539300
C	1.63220700	-1.68703500	2.90209900
C	3.87531800	-2.15776700	1.90924900
C	1.84801900	-3.44297700	1.16488600
C	-2.41252100	2.00385400	-1.07408300
C	-1.32370900	2.25925500	-2.14318800
C	-3.04111600	3.34096600	-0.64220500
C	-3.50139100	1.14502600	-1.75141100
C	-2.77148700	0.68570400	1.80222400
C	-3.14853800	1.92632700	2.63852700

C	-4.06822200	0.02004900	1.30092500
C	-2.05955100	-0.32089300	2.73240100
H	1.72687900	0.76742400	2.09102400
H	3.37339300	0.78920200	1.49293500
H	4.16485700	2.45992000	0.11435000
H	3.95414200	4.70399100	-0.85804200
H	1.71067000	5.82263100	-0.89433100
H	-0.23264300	4.65225200	0.05749500
H	-1.05570500	3.11322900	1.50918000
H	-0.14617400	1.75377000	2.12422500
H	1.58279000	-0.28078900	-2.62884400
H	2.49480900	1.10747900	-2.01813200
H	3.23839400	0.02192000	-3.20441400
H	4.61599600	0.70353000	-0.59936200
H	5.07362400	-0.93099600	-0.10373900
H	5.20561600	-0.44419000	-1.79369600
H	3.79804700	-2.26045500	-2.70418800
H	3.80675400	-2.93576700	-1.07513100
H	2.26955100	-2.70943300	-1.93271300
H	0.56819600	-1.50116500	2.72836400
H	1.71218400	-2.52656300	3.60538900
H	2.06473100	-0.81281600	3.39907400
H	4.31773700	-1.19072700	2.17246200
H	4.01950700	-2.82425600	2.77100900
H	4.44583700	-2.58130500	1.07807700
H	2.30421600	-3.80081700	0.23931100
H	2.07781800	-4.17461700	1.95181900
H	0.76447900	-3.42510700	1.01972600
H	-1.78322700	2.75622200	-3.00870700
H	-0.51317900	2.89589400	-1.78482700
H	-0.88507500	1.31600500	-2.48668400
H	-3.90726800	3.19305500	0.01035600
H	-2.33650300	4.00031400	-0.12648100
H	-3.39617000	3.87981700	-1.53149100
H	-3.79484400	1.62680500	-2.69413600
H	-3.13356200	0.14319000	-1.98301600
H	-4.40250600	1.04476700	-1.14422200
H	-3.87593700	1.62849700	3.40612200
H	-2.29093400	2.35795300	3.16362100
H	-3.61363400	2.71499200	2.04088600
H	-3.87925500	-0.79372300	0.59418100
H	-4.60771400	-0.40084200	2.16073700
H	-4.73968900	0.74227000	0.82774500
H	-1.82129900	-1.24874000	2.20347200
H	-1.12993300	0.08057500	3.15081900
H	-2.71765200	-0.56401800	3.57792300
C	-2.50332900	-3.88366600	0.17197800
C	-2.85827700	-2.95808000	-0.97041400
H	-1.89869800	-4.73152100	-0.17539200
H	-1.91053100	-3.36303000	0.93440300
H	-3.40241300	-4.28764600	0.64761900
C	-4.14565600	-2.79236600	-1.33174900
H	-4.95509600	-3.29328300	-0.80739200
H	-4.42756800	-2.15691300	-2.16789700
C	-1.76781500	-2.28629800	-1.70597300
C	-0.42828800	-2.73135100	-1.73270900
H	-2.10898900	-1.69825600	-2.55734700
H	0.16295300	-2.53558500	-2.62547300
H	-0.12892100	-3.62327200	-1.18714800

8-ts

Zero-point correction= 1.026340 (Hartree/Particle)

Thermal correction to Energy= 1.085841

Thermal correction to Enthalpy= 1.086786

Thermal correction to Gibbs Free Energy= 0.926309

E(solv)= -2906.62578869

Pd	1.31511000	0.07065000	-0.19985800
P	2.87615700	1.88195400	0.02274000
P	2.66773000	-1.90758800	-0.71728700
C	4.70198300	1.35459700	0.00075200
C	5.22130800	0.29458000	0.95758200
C	5.94059700	0.71331300	2.09028200
C	6.54255700	-0.17943800	2.97282600
C	6.47245600	-1.54440300	2.70825800
C	5.80249000	-1.97787600	1.56777200
C	5.15169400	-1.09554300	0.68841200
C	4.54348500	-1.67029700	-0.57638400
C	2.69963100	2.92241200	1.64584300
C	2.44929700	1.89935100	2.77765100
C	3.92886300	3.77665200	2.02000300
C	1.48916500	3.87724200	1.56611800
C	2.85318600	3.07703600	-1.50710100
C	3.36974000	2.29822100	-2.73614000
C	3.70893600	4.34863900	-1.34772500
C	1.39662900	3.47843000	-1.82392800
C	2.25347800	-3.32152100	0.52877600
C	2.16606300	-2.64761900	1.91846500
C	3.26562900	-4.48085700	0.61133000

C	0.86851400	-3.90686400	0.18880500
C	2.56482100	-2.58574300	-2.53312800
C	3.10813500	-4.01425900	-2.72905700
C	1.09458300	-2.53259700	-2.99353300
C	3.36754700	-1.64739600	-3.46127400
H	4.85386400	1.00792800	-1.02433100
H	5.31473100	2.25540200	0.11126800
H	6.06649800	1.77565900	2.26785900
H	7.08493500	0.19344200	3.83706200
H	6.95778300	-2.26433500	3.36114300
H	5.81095900	-3.03714200	1.33229800
H	5.02626800	-2.62927000	-0.79393700
H	4.78493700	-1.01240200	-1.41543700
H	1.54233200	1.31486200	2.59895500
H	3.28327900	1.20033800	2.89206600
H	2.32881200	2.43538300	3.72865500
H	4.80884500	3.17319600	2.23974300
H	4.19549700	4.50403700	1.25079000
H	3.69462500	4.33991200	2.93295800
H	1.29216000	4.27499000	2.57027100
H	1.68281700	4.73439100	0.91454900
H	0.57799800	3.38569800	1.22433900
H	2.84061800	1.34861500	-2.85610600
H	3.18445400	2.89585700	-3.63780500
H	4.44554800	2.10109300	-2.69931800
H	4.74750700	4.12838200	-1.07871900
H	3.73040900	4.88524800	-2.30567300
H	3.29873500	5.03718500	-0.60455100
H	0.90975200	4.01587300	-1.00834600
H	1.39278100	4.13810400	-2.70167300
H	0.79025100	2.60043600	-2.06285600
H	1.87516100	-3.40025700	2.66375200
H	3.12225600	-2.21971300	2.23215300
H	1.41569700	-1.85139800	1.93105700
H	3.36816700	-5.02867200	-0.32670600
H	4.25689800	-4.15051200	0.92479500
H	2.91463000	-5.19539400	1.36783400
H	0.53473000	-4.53951700	1.02182000
H	0.11763800	-3.12798100	0.03995000
H	0.89155800	-4.53711000	-0.70531500
H	3.11346200	-4.24782700	-3.80223200
H	4.13655000	-4.12777900	-2.36927100
H	2.48578600	-4.76831400	-2.24085500
H	0.70750900	-1.50996400	-2.96155200
H	1.02797500	-2.88917500	-4.03017400
H	0.43535700	-3.15485000	-2.38605300
H	3.10506800	-0.59652000	-3.31145800
H	4.44989800	-1.75772400	-3.34252600
H	3.13163800	-1.89732200	-4.50351200
C	-1.36005300	-0.88172300	1.55889400
C	-0.96873700	-0.19280800	0.26980400
H	-2.44445800	-0.76009200	1.69137300
H	-1.13765800	-1.95370900	1.54938500
H	-0.84366800	-0.43384100	2.41476500
C	-0.46032000	1.14082200	0.29546300
H	-0.67679100	1.79897900	-0.54423000
H	-0.45722500	1.64330300	1.25897100
C	-1.31810800	-0.74701400	-0.98360200
C	-2.09891800	-1.91157600	-1.22058100
H	-1.99442800	-2.35620100	-2.21295800
H	-2.14486900	-2.65204400	-0.42062600
H	-1.11933600	-0.11451900	-1.84981000
P	-5.18162300	-0.27030600	-0.24827400
O	-4.45316100	-0.25314800	1.06254100
O	-4.62014800	-1.12456600	-1.39906600
H	-3.29804800	-1.46351000	-1.26905600
O	-6.76233100	-0.66308000	-0.05082700
O	-5.37605100	1.22026200	-0.88263700
C	-7.05860900	-1.85920300	0.67743100
H	-6.57466800	-1.81848000	1.66188600
H	-6.65422600	-2.72655900	0.13600300
C	-8.57128100	-1.97674400	0.81610700
H	-8.94768000	-1.08102900	1.32867200
H	-9.01813200	-1.97473500	-0.18706400
C	-9.00041400	-3.23619700	1.57941600
H	-8.53833000	-3.23426700	2.57697700
H	-8.60985700	-4.12589000	1.06497600
C	-10.52119300	-3.35939700	1.72349100
H	-10.80004100	-4.26710500	2.27155400
H	-10.93784400	-2.50102300	2.26488900
H	-11.00934500	-3.39842600	0.74185100
C	-5.86316100	2.26455200	-0.03133100
H	-6.91204200	2.06331100	0.22545600
H	-5.28295200	2.27911900	0.89999200
C	-5.73737200	3.58852700	-0.77494800
H	-6.28896400	3.51518300	-1.72175800
H	-4.68246300	3.74554200	-1.03923100
C	-6.25554200	4.77814100	0.04319400

H	-7.30830100	4.60703700	0.30926200
H	-5.70733900	4.83437900	0.99458700
C	-6.12968200	6.11435800	-0.69666900
H	-6.69630200	6.10091400	-1.63588600
H	-6.50774800	6.94603400	-0.09050100
H	-5.08350300	6.33146400	-0.94634300

9

Zero-point correction=0.765533 (Hartree/Particle)

Thermal correction to Energy=0.807061

Thermal correction to Enthalpy=0.808005

Thermal correction to Gibbs Free Energy=0.696417

E(solv)= -1948.17224206

Pd	-0.26012100	-1.13831900	-0.38489200
P	1.94493700	-0.37243300	0.23771200
P	-1.73374000	0.69200600	0.35592400
C	2.01790600	1.32503900	1.07382400
C	1.49660700	2.60095200	0.43902100
C	2.42042600	3.52061700	-0.08550600
C	2.04189700	4.77736400	-0.55099000
C	0.70949800	5.16702800	-0.44716500
C	-0.21247200	4.28697400	0.11346100
C	0.14130900	2.99483100	0.53601500
C	-0.90679100	2.14915800	1.22956500
C	3.16483900	-0.23647300	-1.25866800
C	2.36047600	0.41387300	-2.40677600
C	4.40413700	0.63846400	-0.97272900
C	3.68338900	-1.61329000	-1.72255600
C	2.70450700	-1.44501400	1.66840100
C	1.85483100	-1.22108400	2.94088700
C	4.17295800	-1.09517200	1.98812300
C	2.62163900	-2.94815200	1.33809500
C	-2.66050600	1.47813300	-1.14366400
C	-1.59193200	1.69732200	-2.24019100
C	-3.35432000	2.82258600	-0.84653600
C	-3.72135100	0.51102400	-1.69763400
C	-2.96081000	0.14490500	1.74954200
C	-4.10432600	1.14308800	2.01612400
C	-3.56480100	-1.22432900	1.39028500
C	-2.15574500	-0.03859000	3.05677200
H	1.49120500	1.16484600	2.01738100
H	3.06784400	1.47801700	1.33980800
H	3.47556200	3.27096200	-0.08377000
H	2.78976200	5.45580400	-0.95026500
H	0.39352600	6.15665400	-0.76313300
H	-1.23023500	4.63096500	0.26527900
H	-1.71166500	2.80395400	1.57808600
H	-0.47227000	1.70376300	2.12847600
H	1.51109000	-0.20510800	-2.71191000
H	1.98053700	1.40305800	-2.13421800
H	3.01614000	0.53788100	-3.27789700
H	4.14648200	1.68024200	-0.79535100
H	5.00254100	0.27841200	-0.13404000
H	5.04711100	0.61817000	-1.86121800
H	4.27376300	-1.46446600	-2.63507500
H	4.34664400	-2.07695300	-0.98690700
H	2.88824600	-2.31613000	-1.96768300
H	0.78561400	-1.35698400	2.74686300
H	2.14836300	-1.96383600	3.69244300
H	2.00899700	-0.23712700	3.39218300
H	4.32751000	-0.03349600	2.20211800
H	4.47372100	-1.64863200	2.88642200
H	4.85469400	-1.39134700	1.18668400
H	3.15423000	-3.21971700	0.42414100
H	3.07974800	-3.51170000	2.16011300
H	1.58343800	-3.27792200	1.25324900
H	-2.07682100	2.11419500	-3.13214200
H	-0.81221600	2.39710100	-1.92904400
H	-1.11095200	0.75622700	-2.52946400
H	-4.14590900	2.73888900	-0.10025900
H	-2.65578400	3.59355500	-0.52605600
H	-3.81956500	3.18068100	-1.77354600
H	-4.14121800	0.93949200	-2.61620800
H	-3.29110400	-0.45716700	-1.95500500
H	-4.55358600	0.35491200	-1.00510600
H	-4.66098400	0.81183900	2.90185500
H	-3.74773100	2.15705700	2.22268300
H	-4.81670700	1.18847600	1.18827600
H	-2.78401400	-1.98225000	1.27554000
H	-4.23086300	-1.54645300	2.20060300
H	-4.15493700	-1.19744600	0.47274500
H	-1.26847000	-0.66411800	2.91113600
H	-1.84620300	0.91066800	3.50268100
H	-2.79342800	-0.54377500	3.79224600
C	-0.96020100	-4.42468600	0.00197200
C	-0.78587800	-3.33041800	-1.02815900
H	-1.72275700	-4.18410400	0.74875600
H	-1.27623300	-5.34883700	-0.49856900

H	-0.02359300	-4.63762900	0.52213900
C	0.51806800	-2.87019500	-1.38563200
H	1.36890700	-3.40853900	-0.98832300
H	0.66499300	-2.47780000	-2.39171300
C	-1.87652600	-2.68644600	-1.60787400
C	-3.29735800	-3.14731400	-1.43566600
H	-3.51063400	-3.52425700	-0.43331300
H	-4.02333700	-2.36814400	-1.67454700
H	-1.67831200	-2.08023800	-2.49139700
H	-3.48032600	-3.97376400	-2.13930000

10-ts

Zero-point correction= 0.884580 (Hartree/Particle)

Thermal correction to Energy= 0.933326

Thermal correction to Enthalpy= 0.934271

Thermal correction to Gibbs Free Energy= 0.804430

E(Solv)= -2328.13125863

Pd	-0.16740700	-0.10479700	0.02020400
P	-1.22030900	2.03516000	0.40902500
P	-1.96540800	-1.75667700	0.41032500
C	-3.09835800	1.97727500	0.67011700
C	-4.00894500	1.32136400	-0.35387000
C	-4.73208200	2.14660700	-1.23207100
C	-5.66371700	1.64588100	-2.13754300
C	-5.92914300	0.27927700	-2.15149900
C	-5.25775500	-0.54921800	-1.25665400
C	-4.28381300	-0.06843700	-0.36494700
C	-3.70047200	-1.03636900	0.64665900
C	-0.97057900	3.31327900	-1.02289000
C	-1.16998600	2.52555300	-2.33828200
C	-1.95151400	4.50459200	-1.01538500
C	0.45728200	3.90036800	-1.00590800
C	-0.66455100	2.83420200	2.08851500
C	-1.22587300	1.97762600	3.24386200
C	-1.13458900	4.28751800	2.29630400
C	0.87342700	2.77586800	2.20393800
C	-2.12375000	-2.92112000	-1.12140200
C	-2.03871600	-2.00028300	-2.36148100
C	-3.41832500	-3.75217100	-1.21659100
C	-0.92576300	-3.88962900	-1.15818800
C	-1.83692300	-2.81365300	2.03440200
C	-2.75922000	-4.04703000	2.08817500
C	-0.37731800	-3.27225300	2.21815100
C	-2.18337500	-1.90929500	3.23810900
H	-3.21022000	1.46094800	1.62669200
H	-3.44042300	3.00362000	0.83790500
H	-4.59367800	3.22077500	-1.17843000
H	-6.19773700	2.32306800	-2.79763100
H	-6.67411000	-0.13617400	-2.82374200
H	-5.52597300	-1.60012300	-1.22325300
H	-4.39583300	-1.87268900	0.77362900
H	-3.64504500	-0.54014300	1.61884000
H	-0.44917100	1.70829600	-2.43456000
H	-2.17429700	2.09864600	-2.41343700
H	-1.03174300	3.20489300	-3.18966200
H	-1.90444900	5.09488300	-0.09866400
H	-1.68927700	5.17307800	-1.84553800
H	-2.98426800	4.19786300	-1.17369500
H	0.61822200	4.45014400	-1.94219300
H	0.59991400	4.61340200	-0.18895300
H	1.23416900	3.13843100	-0.93587700
H	-0.98084900	0.91967100	3.11367300
H	-0.76946700	2.30935800	4.18498900
H	-2.30854700	2.07652900	3.36400400
H	-2.21764300	4.40098900	2.18416500
H	-0.88334200	4.59854400	3.31874200
H	-0.64196800	4.98886000	1.61832300
H	1.38530300	3.32833400	1.41352900
H	1.17475400	3.21681300	3.16307200
H	1.22578700	1.73990400	2.18395200
H	-2.06374800	-2.61706300	-3.26973200
H	-2.87479700	-1.29803600	-2.41315500
H	-1.10964200	-1.42108700	-2.36838000
H	-3.53489400	-4.46058200	-0.39515600
H	-4.31264100	-3.13011600	-1.26057200
H	-3.39108400	-4.33505900	-2.14654400
H	-0.90156300	-4.39316700	-2.13331500
H	0.02324900	-3.36163300	-1.03258400
H	-0.99662500	-4.67023000	-0.39473800
H	-2.70055800	-4.49197900	3.09017900
H	-3.80993600	-3.79724600	1.90897700
H	-2.46262000	-4.82176400	1.37641100
H	0.30970000	-2.41931600	2.21775600
H	-0.27630200	-3.78937100	3.18115800
H	-0.06221800	-3.97194700	1.44088300
H	-1.62519200	-0.96911000	3.22150200
H	-3.25091700	-1.68033000	3.30182900
H	-1.91430200	-2.43410000	4.16328100

H	1.75910300	-3.48647300	0.38758700
C	1.92676700	-1.36951100	-2.18343700
C	1.90520200	-0.80442000	-0.77064500
H	2.93327600	-1.30507300	-2.62795200
H	1.60756700	-2.41426000	-2.23975000
H	1.26369000	-0.79348800	-2.83477600
C	1.70791500	0.60511500	-0.60136100
H	1.65260400	1.20521000	-1.50707500
H	2.21813100	1.11394100	0.21580000
C	2.60205900	-1.52337900	0.27965700
C	2.74213900	-3.03020800	0.25766500
H	3.14023100	-3.39648000	-0.69445900
H	3.39058000	-3.37702000	1.06589400
H	2.45190400	-1.11584900	1.27744000
C	6.19445900	0.30038700	0.39717400
C	6.32455000	-0.51630100	-0.75713300
C	7.44856500	-0.45758400	-1.59642800
C	8.43408400	0.44927500	-1.24454900
C	8.32199800	1.27860600	-0.09875900
C	7.21625100	1.21673300	0.72720000
C	4.95063800	-0.07113500	0.97118900
H	7.54261400	-1.08766500	-2.47485000
H	9.32191300	0.52940600	-1.86445500
H	9.12574500	1.97173400	0.12791700
H	7.13349300	1.85002400	1.60484400
H	4.45505900	0.30833900	1.85415400
N	4.38596400	-1.03091300	0.24997900
N	5.18989100	-1.28173600	-0.81753100
H	4.99016200	-2.07132800	-1.41332300

10-ts-iso

Zero-point correction= 0.885154 (Hartree/Particle)

Thermal correction to Energy= 0.933640

Thermal correction to Enthalpy= 0.934584

Thermal correction to Gibbs Free Energy= 0.805712

E(Solv) = -2328.12742014

Pd	-0.16073100	0.05783700	-0.15316400
P	-1.52221400	1.94618500	0.49658600
P	-1.54663800	-1.91722900	0.38513900
C	-3.29993200	1.52675000	1.00477800
C	-4.21264100	0.73797100	0.08155200
C	-5.19602100	1.43436400	-0.64166100
C	-6.14322500	0.79022400	-1.43318800
C	-6.15318600	-0.60106700	-1.48156600
C	-5.21642100	-1.31068400	-0.73527200
C	-4.22538300	-0.67797200	0.03433500
C	-3.33009900	-1.54377200	0.90050100
C	-1.71818300	3.28604600	-0.88685000
C	-1.95665900	2.51091200	-2.20314900
C	-2.89049200	4.26891100	-0.68260500
C	-0.43547500	4.13300300	-1.03162900
C	-0.88701000	2.78852600	2.12559800
C	-1.11597300	1.81255700	3.29983100
C	-1.57880300	4.12259600	2.46913900
C	0.63677800	3.01512800	2.03099400
C	-1.71312800	-3.04773400	-1.17034800
C	-1.96643700	-2.09306900	-2.36084900
C	-2.84365900	-4.09458400	-1.13257600
C	-0.38356300	-3.78610600	-1.41801400
C	-0.98633100	-2.97363500	1.91497000
C	-1.64808000	-4.36078400	2.02842400
C	0.54385100	-3.14977500	1.86869800
C	-1.31230300	-2.18555300	3.20307700
H	-3.17775800	0.97399500	1.93949200
H	-3.79584900	2.46579400	1.27079100
H	-5.25103500	2.51350700	-0.55007600
H	-6.88383400	1.37105300	-1.97501100
H	-6.90097100	-1.13239800	-2.06289800
H	-5.28128500	-2.39360500	-0.71891500
H	-3.83275200	-2.50025700	1.07838900
H	-3.22360900	-1.07243700	1.88077200
H	-1.12021500	1.84692000	-2.44104000
H	-2.86567400	1.90375800	-2.16298900
H	-2.07004000	3.22679700	-3.02786700
H	-2.82329800	4.83089600	0.25042300
H	-2.87685500	4.99836400	-1.50264100
H	-3.86066700	3.77570900	-0.71748300
H	-0.51485000	4.73022900	-1.94917900
H	-0.30935000	4.83571500	-0.20324000
H	0.47035000	3.53052000	-1.10930800
H	-0.70614800	0.82179200	3.08411800
H	-0.59711400	2.19822300	4.18631700
H	-2.17060800	1.70691200	3.56996900
H	-2.66917500	4.03429400	2.51173300
H	-1.24403300	4.44927400	3.46222200
H	-1.32396400	4.92042000	1.76717600
H	0.92380200	3.67279000	1.20799000
H	0.98514500	3.48225100	2.96111700

H	1.16750900	2.06521300	1.91503600
H	-2.02027000	-2.67994400	-3.28741000
H	-2.90709300	-1.54542100	-2.25884700
H	-1.15890900	-1.36144100	-2.46783500
H	-2.72713100	-4.82323400	-0.32914600
H	-3.83050200	-3.64063100	-1.04250400
H	-2.83537700	-4.65071100	-2.07906300
H	-0.40946200	-4.24688400	-2.41390400
H	0.46966900	-3.10367000	-1.39034300
H	-0.21148500	-4.58987700	-0.69596800
H	-1.35799200	-4.81581800	2.98452000
H	-2.74157100	-4.30920200	2.01654800
H	-1.32611100	-5.04402400	1.23836000
H	1.05292200	-2.18093300	1.83064600
H	0.87656700	-3.67234800	2.77492700
H	0.86895300	-3.74588500	1.01340900
H	-0.94276400	-1.15721600	3.16117400
H	-2.38252700	-2.16355400	3.42709900
H	-0.81926200	-2.67640400	4.05140100
H	2.38349700	-2.92742700	-0.33832200
C	1.81361800	-0.75306800	-2.66068200
C	1.88204600	-0.22124700	-1.23318700
H	2.76617600	-0.62239700	-3.19941900
H	1.57461100	-1.81853700	-2.70941300
H	1.04458400	-0.22180100	-3.22889400
C	1.44768400	1.12614300	-0.96781600
H	1.14890600	1.72760900	-1.82508400
H	1.94668000	1.69878700	-0.18644000
C	2.81304000	-0.83461400	-0.30833800
C	3.24479000	-2.27173300	-0.48588200
H	3.63802200	-2.45035400	-1.48980200
H	4.00879900	-2.55760000	0.23952800
H	2.71724600	-0.50469300	0.72182000
C	6.62400000	0.81631100	-0.72765100
C	5.74863100	-0.08655900	-0.03644800
C	6.23557500	-0.91034100	1.00680000
C	7.57523500	-0.81421000	1.31350700
C	8.45350300	0.07234900	0.62365900
C	7.99797900	0.88728200	-0.38618500
C	5.80577800	1.47506700	-1.65608200
H	5.58155000	-1.58107200	1.55266700
H	7.98011400	-1.43066600	2.11061200
H	9.49961200	0.10156400	0.91134600
H	8.66421900	1.56788200	-0.90698000
H	6.01468600	2.24323800	-2.38650300
N	4.57146400	0.97278400	-1.50161100
N	4.49257200	0.03582700	-0.53843600
H	3.70707600	1.24600000	-1.95838600

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Zero-point correction= 0.886879 (Hartree/Particle)

Thermal correction to Energy= 0.935272

Thermal correction to Enthalpy= 0.936216

Thermal correction to Gibbs Free Energy= 0.808188

E(Solv)= -2328.13979717

Pd	-0.13775500	-0.03257600	0.11792600
P	-1.48897500	1.98252700	0.52164700
P	-1.77783000	-1.87247600	0.31433000
C	-3.36815300	1.74012500	0.62345800
C	-4.10131300	1.04651100	-0.51087700
C	-4.85151500	1.83395300	-1.40109900
C	-5.61281700	1.28560200	-2.42972900
C	-5.67125800	-0.09878800	-2.56546100
C	-4.97820200	-0.89747300	-1.65996500
C	-4.17751000	-0.36263400	-0.63631000
C	-3.58841200	-1.31382800	0.38874100
C	-1.26621000	3.33641900	-0.84729600
C	-1.28361100	2.58484700	-2.19857700
C	-2.35776600	4.42623700	-0.88584600
C	0.09082000	4.05813300	-0.70020000
C	-1.14875100	2.78092300	2.25830800
C	-1.71417000	1.83858000	3.34236500
C	-1.76826000	4.17629600	2.46834300
C	0.37504100	2.85853100	2.49468300
C	-1.70434200	-3.03611300	-1.22668900
C	-1.59777300	-2.09740000	-2.45145000
C	-2.90514400	-3.97989100	-1.43830200
C	-0.42823200	-3.89737400	-1.16331300
C	-1.73612300	-2.94251900	1.94056800
C	-2.55278300	-4.24831800	1.89113800
C	-0.27254700	-3.28404400	2.27653500
C	-2.27786900	-2.09065800	3.10989800
H	-3.50909100	1.16868100	1.54462600
H	-3.82938500	2.71743600	0.79843300
H	-4.87212900	2.90939700	-1.26143700
H	-6.17586800	1.93423400	-3.09443900
H	-6.27791000	-0.55673800	-3.34126700
H	-5.09398000	-1.97401600	-1.72772100

H	-4.21031500	-2.21435200	0.42457500
H	-3.67148400	-0.85301600	1.37541500
H	-0.48682800	1.83743600	-2.25764500
H	-2.23479000	2.07346400	-2.37098800
H	-1.13969700	3.30517500	-3.01498000
H	-2.44298800	4.98332900	0.04875400
H	-2.10063800	5.14823000	-1.67199200
H	-3.33843300	4.02508800	-1.13711200
H	0.26898800	4.65496600	-1.60433400
H	0.10036200	4.75043200	0.14635600
H	0.93052900	3.37070000	-0.58857700
H	-1.35187200	0.81522500	3.21124100
H	-1.37499700	2.18508800	4.32683900
H	-2.80764000	1.82437700	3.36929500
H	-2.84598200	4.19150300	2.27596700
H	-1.62432400	4.47611900	3.51473800
H	-1.29700200	4.94294900	1.84824300
H	0.88934600	3.49310500	1.76967800
H	0.56161300	3.28040600	3.49091800
H	0.82608400	1.86154600	2.46216000
H	-1.48058900	-2.70233600	-3.36056400
H	-2.49058400	-1.47901600	-2.57614900
H	-0.73417500	-1.43029400	-2.37131600
H	-3.00273000	-4.73102700	-0.65339400
H	-3.85354200	-3.44764700	-1.51731700
H	-2.76301200	-4.51744700	-2.38499200
H	-0.27866600	-4.39085900	-2.13255500
H	0.45801600	-3.29260600	-0.95687200
H	-0.49575800	-4.68626900	-0.40782200
H	-2.56578100	-4.69760200	2.89299300
H	-3.59508900	-4.08521400	1.59920100
H	-2.11669500	-4.98815900	1.21496100
H	0.33416800	-2.37627500	2.36230900
H	-0.23193300	-3.81125800	3.23869000
H	0.18063600	-3.94077200	1.52995800
H	-1.80740100	-1.10493300	3.15328900
H	-3.36277900	-1.95875600	3.07122300
H	-2.05342600	-2.60309700	4.05381300
H	1.88519500	-2.97321500	0.78555300
C	2.13660700	-1.02749500	-1.95813700
C	1.98876100	-0.50102200	-0.53549100
H	3.17212600	-0.93411500	-2.32804200
H	1.85960700	-2.08090600	-2.05485700
H	1.49887200	-0.46275300	-2.64373200
C	1.69213000	0.89022700	-0.35440600
H	1.58069400	1.51836800	-1.23690400
H	2.04069500	1.42134000	0.53352600
C	2.91858000	-1.13817600	0.48344500
C	2.90612100	-2.65966400	0.58283500
H	3.23012300	-3.13293300	-0.34901300
H	3.53217600	-3.02179000	1.40497900
H	2.73779800	-0.69858200	1.46943300
C	6.59109100	-0.58960600	-0.14830500
C	6.00138500	0.67369400	-0.42634900
C	6.75950400	1.77964100	-0.84635500
C	8.12195600	1.57648400	-0.97159000
C	8.73247400	0.32377600	-0.69170000
C	7.98783100	-0.76253700	-0.28160500
C	5.51777500	-1.43106600	0.21842500
H	6.30289300	2.74030100	-1.05908400
H	8.74926100	2.40210200	-1.29350200
H	9.80732600	0.22825300	-0.80563500
H	8.45358400	-1.71912700	-0.06823300
H	5.51839600	-2.46869000	0.51130900
N	4.38218200	-0.73362900	0.16831600
N	4.66364000	0.54440800	-0.19455800
H	3.87318500	1.13860100	-0.43668600

12-ts

Zero-point correction= 0.908227 (Hartree/Particle)

Thermal correction to Energy= 0.961275

Thermal correction to Enthalpy= 0.962219

Thermal correction to Gibbs Free Energy= 0.817393

E(Solv)= -2709.98191475

Pd	-0.08672000	-0.26286500	0.18644300
P	-1.42532600	-0.16021900	2.00335400
P	-1.32882300	-1.11431500	-1.80394100
C	-3.22088700	-0.65084200	1.58377300
C	-4.01560900	0.07934100	0.51177600
C	-4.93430500	1.05863000	0.93007600
C	-5.78280400	1.72613000	0.05148600
C	-5.75806800	1.39020000	-1.29946500
C	-4.88669200	0.39426700	-1.73015500
C	-3.99565100	-0.26616100	-0.86558600
C	-3.16984000	-1.39880700	-1.44998700
C	-1.54917000	1.57513700	2.84358500
C	-1.68003500	2.59041100	1.68461900
C	-2.73050800	1.77068500	3.81502300

C	-0.24643700	1.89393300	3.60792500
C	-1.01183300	-1.50677300	3.33567400
C	-1.34181300	-2.89334900	2.73913900
C	-1.76897600	-1.36377400	4.66968600
C	0.50795000	-1.48706300	3.60601700
C	-1.26451800	0.12381100	-3.27736500
C	-1.47357000	1.52392200	-2.65264100
C	-2.30674900	-0.08309900	-4.39233800
C	0.14946200	0.09836200	-3.89715600
C	-0.80194500	-2.87667200	-2.40172700
C	-1.34786800	-3.31242400	-3.77356300
C	0.74190900	-2.93036200	-2.41585900
C	-1.27997600	-3.89916200	-1.34640700
H	-3.11996300	-1.69904800	1.29240500
H	-3.80366200	-0.64411400	2.51220800
H	-5.00829000	1.28463200	1.98848200
H	-6.47188800	2.47770900	0.42682200
H	-6.42623700	1.87334600	-2.00705700
H	-4.91443200	0.09410200	-2.77325200
H	-3.66745400	-1.76407000	-2.35580000
H	-3.16632200	-2.23449500	-0.74435800
H	-0.83050200	2.51340200	0.99875700
H	-2.59610700	2.44606200	1.10511700
H	-1.69959900	3.60803200	2.09856200
H	-2.66325400	1.13154100	4.69744500
H	-2.72708900	2.81097200	4.16734300
H	-3.69981100	1.59789800	3.34582600
H	-0.27061100	2.95003600	3.90960900
H	-0.14946700	1.30296200	4.52409900
H	0.64875300	1.74343700	2.99949500
H	-0.90704200	-3.01318800	1.74161400
H	-0.91079800	-3.66937300	3.38510500
H	-2.41776000	-3.08621100	2.68024200
H	-2.85465900	-1.30233900	4.53578000
H	-1.56907900	-2.24648100	5.29230800
H	-1.44218000	-0.48988100	5.23977200
H	0.86043800	-0.53388400	4.00443200
H	0.75022000	-2.26754700	4.34062700
H	1.07040100	-1.68839300	2.68985200
H	-1.39899800	2.28426300	-3.44273800
H	-2.45361300	1.62869300	-2.17915900
H	-0.70781000	1.73686900	-1.89965500
H	-2.20567100	-1.04766100	-4.89455400
H	-3.33197900	0.00362500	-4.02559500
H	-2.17266500	0.69693400	-5.15454600
H	0.25212800	0.95765800	-4.57433400
H	0.93148200	0.17148600	-3.13494900
H	0.32192900	-0.80188500	-4.49567700
H	-1.08096700	-4.36310300	-3.95450400
H	-2.44002800	-3.24097700	-3.83138900
H	-0.92178300	-2.72723600	-4.59302800
H	1.15657500	-2.65458500	-1.44151100
H	1.06466600	-3.95310800	-2.65611200
H	1.18194800	-2.26000300	-3.15623300
H	-1.00205600	-3.59570200	-0.33164000
H	-2.36162200	-4.06523500	-1.37776300
H	-0.80009600	-4.86658700	-1.54436800
P	2.91114600	0.67248000	0.02326500
O	1.91787900	0.03542600	-0.94018500
O	2.29258400	0.88750300	1.43595400
H	1.07270300	0.41531300	1.28156100
O	4.29442300	-0.15079700	0.11235300
O	3.54743900	2.05276100	-0.51299600
C	2.77917100	3.26864000	-0.41822100
H	2.52863000	3.45241000	0.63302900
H	1.84384800	3.15564700	-0.98223400
C	3.61871000	4.40088700	-0.99232300
H	3.87924400	4.15601900	-2.03027600
H	4.56255900	4.45611200	-0.43443000
C	2.89368800	5.75207400	-0.93638900
H	2.62789500	5.98186800	0.10515500
H	1.94400900	5.68105900	-1.48566000
C	3.73039100	6.89908100	-1.51324300
H	3.98321500	6.71450100	-2.56443000
H	3.19039000	7.85133100	-1.46155800
H	4.67145000	7.01787700	-0.96259400
C	4.24266900	-1.57853400	0.29960300
H	3.69667000	-2.03166500	-0.53619200
H	3.70243300	-1.80471700	1.22878900
C	5.67244200	-2.09581800	0.36886100
H	6.19326100	-1.81314500	-0.55531800
H	6.19184900	-1.58823300	1.19200400
C	5.73514800	-3.61643700	0.56448100
H	5.20178200	-4.11353200	-0.25825500
H	5.19978600	-3.88949600	1.48505300
C	7.17094900	-4.14748700	0.63453200
H	7.18755500	-5.23436100	0.77422000
H	7.72194500	-3.92007300	-0.28612000

H	7.71986100	-3.69451100	1.46905000

13

Zero-point correction= 0.912443 (Hartree/Particle)

Thermal correction to Energy= 0.965236

Thermal correction to Enthalpy= 0.966180

Thermal correction to Gibbs Free Energy=0.823148

E(Solv)= -2711.23539894

Pd	-0.36198900	0.34059000	0.54218800
P	-2.07187300	1.75899900	0.05777900
P	-1.36448500	-1.89104400	0.81313600
C	-3.80217100	0.99508700	-0.03948200
C	-4.12723900	-0.12969900	-1.00631800
C	-4.86598000	0.18659400	-2.15912400
C	-5.30066300	-0.78021600	-3.06164700
C	-5.03604800	-2.12070300	-2.79583800
C	-4.34956800	-2.45808400	-1.63248500
C	-3.86636400	-1.49541700	-0.72999600
C	-3.23848500	-1.98330500	0.56343200
C	-1.73500400	2.59189300	-1.64565100
C	-1.23881200	1.46590200	-2.58394900
C	-2.96959200	3.26638800	-2.27734400
C	-0.61474600	3.64614600	-1.53441300
C	-2.35946500	3.08475400	1.43649300
C	-2.98938800	2.38148500	2.66031700
C	-3.28978600	4.23691700	1.00598200
C	-1.01059800	3.67436900	1.90139000
C	-0.61737000	-3.18849600	-0.39584100
C	-0.47801200	-2.46667100	-1.75720200
C	-1.47714100	-4.45422000	-0.58436800
C	0.79003500	-3.62377000	0.06500000
C	-1.21920300	-2.49654800	2.64088600
C	-1.63161200	-3.96445100	2.86151600
C	0.22975200	-2.28785700	3.13463800
C	-2.12598400	-1.59985200	3.51391800
H	-3.97686600	0.64676300	0.98218800
H	-4.50929800	1.81449200	-0.20879100
H	-5.14162000	1.22126000	-2.33541900
H	-5.86431400	-0.48720500	-3.94285800
H	-5.38609400	-2.90092500	-3.46582800
H	-4.21283200	-3.50828700	-1.39639000
H	-3.56151400	-3.01445600	0.73988200
H	-3.64029700	-1.39340300	1.39262500
H	-0.29058400	1.04049800	-2.24014600
H	-1.97096100	0.65861400	-2.68346500
H	-1.07574000	1.89113600	-3.58358800
H	-3.40604500	4.04623600	-1.64926900
H	-2.66016100	3.74115100	-3.21722200
H	-3.74831800	2.54681000	-2.52874100
H	-0.33481900	3.95540400	-2.54951500
H	-0.93579600	4.54500200	-0.99844100
H	0.28184300	3.24510800	-1.05515000
H	-2.41801500	1.49632300	2.95612200
H	-2.98058300	3.07742000	3.50863000
H	-4.03132200	2.08997700	2.49563300
H	-4.25378900	3.88589300	0.62218000
H	-3.50126500	4.86672800	1.87999400
H	-2.83105900	4.87952800	0.24978000
H	-0.46577000	4.17451200	1.09857100
H	-1.20645100	4.41805800	2.68542500
H	-0.35868500	2.90100800	2.31549900
H	-0.10219700	-3.18426400	-2.49941900
H	-1.43673500	-2.08561800	-2.12413300
H	0.23310600	-1.63669900	-1.70688200
H	-1.68223500	-4.97792800	0.35285700
H	-2.42691700	-4.24345900	-1.07756200
H	-0.92918300	-5.15045900	-1.23285200
H	1.25476400	-4.19119000	-0.75253400
H	1.43488100	-2.77439200	0.29492800
H	0.75015200	-4.28915600	0.93353100
H	-1.61139300	-4.18340900	3.93772600
H	-2.64699500	-4.17723500	2.50817700
H	-0.94470400	-4.66379700	2.37780600
H	0.55669700	-1.25255600	3.01302400
H	0.27478100	-2.54743300	4.20131200
H	0.95122500	-2.91313400	2.60833800
H	-1.92495700	-0.53746700	3.34322100
H	-3.19357600	-1.78636400	3.35817900
H	-1.91534600	-1.80825100	4.57057800
P	2.64898200	-0.09639200	-0.17559700
O	1.54995400	-0.52210000	0.82542800
O	2.28349300	0.20799200	-1.59688800
H	0.35448300	1.72968100	0.41662400
O	3.51369500	1.12810600	0.49429200
O	3.70826500	-1.32745200	-0.01857400
C	3.52012600	2.43355200	-0.09789600
H	2.60662700	2.96790700	0.19976400
H	3.51686500	2.34436500	-1.18974200

C	4.75248800	3.18240500	0.39535000
H	4.74175200	3.19871800	1.49348300
H	5.64925500	2.62095600	0.09972800
C	4.82890700	4.61474300	-0.14911200
H	3.92318200	5.16540800	0.14374000
H	4.82745200	4.58878800	-1.24809600
C	6.06576000	5.37561300	0.34071700
H	6.09428300	6.39500600	-0.06145500
H	6.07815200	5.44736300	1.43526600
H	6.98884200	4.86928200	0.03289300
C	4.89631100	-1.31413100	-0.82222500
H	5.52197400	-0.46039700	-0.52721800
H	4.62294700	-1.18875900	-1.87761300
C	5.63982300	-2.62498600	-0.60088400
H	5.85277700	-2.73250100	0.47105800
H	4.97660000	-3.45656700	-0.87451300
C	6.94326800	-2.70744700	-1.40584600
H	7.59527600	-1.86551600	-1.13272300
H	6.72086500	-2.58585400	-2.47549700
C	7.69636200	-4.02441300	-1.18904800
H	8.62263300	-4.05671400	-1.77436400
H	7.96310900	-4.15829800	-0.13347000
H	7.08323400	-4.88416500	-1.48620000

14-ts

Zero-point correction= 0.759767 (Hartree/Particle)

Thermal correction to Energy= 0.801255

Thermal correction to Enthalpy= 0.802199

Thermal correction to Gibbs Free Energy= 0.690055

E(Solv)= -1948.13224241

Pd	-0.38672400	-0.95014200	-0.42840500
P	1.87573800	-0.87299200	0.29051800
P	-1.42223400	1.14402000	0.39677800
C	2.41902900	0.70793400	1.16181100
C	2.28664700	2.04894200	0.46538200
C	3.44810200	2.64209200	-0.05691600
C	3.44135300	3.90333700	-0.64671600
C	2.25204400	4.62601100	-0.68586600
C	1.10299200	4.07526700	-0.12390500
C	1.07977200	2.78938800	0.44183600
C	-0.17608000	2.34114500	1.16823400
C	3.02898100	-1.08248400	-1.24037600
C	2.47718700	-0.14719800	-2.34153300
C	4.50257100	-0.71199000	-0.96949800
C	2.99454700	-2.53169000	-1.76790600
C	2.24329000	-2.21333300	1.63207000
C	1.61779200	-1.75350500	2.96736400
C	3.74991000	-2.45165100	1.86334600
C	1.57008200	-3.54640100	1.24234800
C	-2.27993100	2.15225100	-1.00508400
C	-1.35243800	2.04193800	-2.23726100
C	-2.50014900	3.64545600	-0.68725500
C	-3.65240300	1.54417800	-1.35769700
C	-2.62074900	0.89856200	1.89485900
C	-3.41729000	2.16063400	2.28044500
C	-3.59749300	-0.24851700	1.57523500
C	-1.79184600	0.45668700	3.12138700
H	1.83656600	0.71197900	2.08685500
H	3.46273300	0.56014600	1.45961200
H	4.39420400	2.11887000	0.03554700
H	4.36177100	4.32509900	-1.03902700
H	2.22272800	5.62438700	-1.11185100
H	0.20714100	4.68498400	-0.08249600
H	-0.73946200	3.22974500	1.46954800
H	0.11588100	1.84471200	2.09671700
H	1.44978000	-0.40711700	-2.61693600
H	2.49348700	0.90343700	-2.04088600
H	3.10226600	-0.24815900	-3.23767900
H	4.96668900	-1.33130100	-0.20052100
H	5.07087500	-0.86376600	-1.89526100
H	4.62385700	0.33436200	-0.69253300
H	3.53783400	-2.56421100	-2.72006600
H	3.48599500	-3.23695500	-1.09245900
H	1.97933600	-2.89039200	-1.96415800
H	0.56173800	-1.49050100	2.85773000
H	1.67485700	-2.58245000	3.68285800
H	2.14699000	-0.90784400	3.41588200
H	4.29471500	-1.53025700	2.09304200
H	3.86888400	-3.11846700	2.72616600
H	4.23352400	-2.93874100	1.01305200
H	1.92511600	-3.94384900	0.28885700
H	1.79627800	-4.29350600	2.01302700
H	0.48161200	-3.44370100	1.18724400
H	-1.78596300	2.61385100	-3.06755400
H	-0.35467200	2.44577600	-2.04096200
H	-1.23807700	1.00424000	-2.56939300
H	-3.09908800	3.80963100	0.21038600
H	-1.56374900	4.19212800	-0.58284000

H	-3.04114000	4.10077700	-1.52629300
H	-4.00474000	1.99274200	-2.29500200
H	-3.61374700	0.46368900	-1.50189600
H	-4.40669300	1.75676300	-0.59520200
H	-3.97605100	1.95469800	3.20213600
H	-2.77473700	3.02390800	2.48195600
H	-4.14928200	2.44308900	1.51968100
H	-3.06437900	-1.18316600	1.37936700
H	-4.25152700	-0.41127900	2.44131800
H	-4.23697000	-0.04281900	0.71619200
H	-1.13523700	-0.38693700	2.88785500
H	-1.19042600	1.26459600	3.54784600
H	-2.48093600	0.12478500	3.90731600
H	0.32373100	-2.26037600	-0.93296100
C	-2.92527300	-3.84959500	-0.10970500
C	-3.31015500	-2.68047500	-0.98573500
H	-2.50677100	-4.67614100	-0.69832300
H	-2.16648200	-3.56474400	0.63055200
H	-3.79507600	-4.23796400	0.42612700
C	-4.59546200	-2.32174700	-1.15559500
H	-5.40340300	-2.85631000	-0.66493600
H	-4.88404500	-1.50342100	-1.80961700
C	-2.26126500	-1.97389100	-1.74028600
C	-1.04423600	-2.54422800	-2.08903400
H	-0.83666300	-3.58083600	-1.83975100
H	-0.49137400	-2.15044200	-2.93681800
H	-2.57833400	-1.10435500	-2.30797700

15-ts

Zero-point correction=1.024613 (Hartree/Particle)

Thermal correction to Energy=1.084476

Thermal correction to Enthalpy=1.085420

Thermal correction to Gibbs Free Energy=0.925103

E(Solv) = -2906.59529205

Pd	2.49758200	0.71529200	0.46076700
P	2.55791800	-1.49851300	-0.39530400
P	-2.31090500	-2.24764000	-1.61819500
C	1.02320800	-2.63316000	-0.27914400
C	0.20109100	-2.72704400	0.99564700
C	0.68345400	-3.48006400	2.07904000
C	-0.02729800	-3.63458300	3.26695600
C	-1.27574900	-3.03021300	3.39414900
C	-1.79232900	-2.31828700	2.31477200
C	-1.09593800	-2.16510300	1.10143200
C	-1.80008900	-1.39034000	0.00468300
C	3.99864100	-2.56374900	0.34503100
C	4.02491000	-2.26758900	1.86313300
C	3.86677800	-4.08469900	0.12169700
C	5.36202600	-2.12235700	-0.22618100
C	2.73610200	-1.40427800	-2.32253800
C	1.43269500	-0.77440800	-2.86570600
C	2.95890800	-2.76085900	-3.01718000
C	3.87675400	-0.43589000	-2.70366300
C	-3.23577000	-0.75183700	-2.43756500
C	-2.11888600	0.14769200	-3.01640700
C	-4.11618400	0.11374600	-1.51388500
C	-4.09191600	-1.24511500	-3.62069200
C	-3.57234000	-3.61810800	-1.11638100
C	-4.80772200	-3.15968400	-0.32380000
C	-4.02112600	-4.35698700	-2.39771400
C	-2.78388600	-4.64931700	-0.27494600
H	0.37558800	-2.29401500	-1.08562800
H	1.35079300	-3.63775700	-0.56732600
H	1.64215200	-3.97694000	1.98709700
H	0.39125000	-4.22450400	4.07796500
H	-1.85014500	-3.12568700	4.31180500
H	-2.78216400	-1.87537400	2.40058200
H	-1.15502800	-0.56652600	-0.31736400
H	-2.68106700	-0.92106500	0.44974100
H	4.25943600	-1.21648900	2.05045800
H	3.07443400	-2.48015500	2.35664700
H	4.79960800	-2.88479300	2.33914500
H	2.99117500	-4.51688500	0.61173400
H	3.82114300	-4.35065800	-0.93784200
H	4.74863700	-4.58318900	0.54611600
H	6.15967500	-2.58574300	0.37013100
H	5.50546500	-2.44572000	-1.26119900
H	5.49861400	-1.03939900	-0.17542000
H	1.16504900	0.13693800	-2.31973000
H	1.58586900	-0.50049500	-3.91810500
H	0.58089600	-1.45884900	-2.83644100
H	2.18382200	-3.49192900	-2.76435100
H	2.92631600	-2.61890400	-4.10607300
H	3.93453000	-3.19547900	-2.77897700
H	4.86374600	-0.78631200	-2.39814800
H	3.89278300	-0.32231700	-3.79604100
H	3.71202500	0.55162100	-2.26230200
H	-2.57520200	1.00140100	-3.53728600

H	-1.46387900	0.55806900	-2.24136500
H	-1.50010500	-0.39265500	-3.74046000
H	-4.89894700	-0.46426800	-1.01410600
H	-3.53113500	0.63535400	-0.75089600
H	-4.61633000	0.88640500	-2.11530700
H	-4.39110900	-0.38524500	-4.23565100
H	-3.54315800	-1.93910400	-4.26762600
H	-5.01091800	-1.73706200	-3.28803800
H	-5.38867800	-4.03389900	0.00377500
H	-4.53397600	-2.59574100	0.57465900
H	-5.47507700	-2.53638500	-0.92749600
H	-3.16006900	-4.67793300	-2.99519500
H	-4.58498800	-5.25721700	-2.11687400
H	-4.66938300	-3.75411700	-3.03631100
H	-1.86301500	-4.96266500	-0.78075200
H	-2.51634500	-4.27196000	0.71302800
H	-3.40469900	-5.54489300	-0.13337300
C	3.57410100	3.60227400	-0.35288900
C	3.70187700	2.58685200	0.76736300
H	2.54186400	3.94731300	-0.48001300
H	4.19266500	4.48922100	-0.15147000
H	3.90134400	3.17565400	-1.30599900
C	4.46406200	1.38249800	0.58534600
H	5.06869400	1.29863600	-0.31685900
H	4.93246400	0.92811200	1.46019400
C	3.21673200	2.90994200	2.06456000
C	2.45688400	4.02673200	2.42805500
H	3.42109200	2.17134000	2.84141700
P	-0.51400900	2.31668900	0.86049300
O	0.27006600	1.04003800	0.71668000
O	-0.03132200	3.37039500	1.89916700
H	1.09640100	3.57562500	2.11356200
O	-0.65589900	2.99900600	-0.59307900
O	-2.06882400	2.04679100	1.22812700
C	-1.36457600	4.24867000	-0.75394200
H	-0.95959800	4.98274300	-0.04777500
H	-2.42204800	4.08600300	-0.51520400
C	-1.19140400	4.71197300	-2.19290200
H	-0.11950000	4.82698500	-2.40186100
H	-1.56067700	3.92541700	-2.86399800
C	-1.92542400	6.03028000	-2.47389800
H	-1.55820500	6.80697900	-1.78831600
H	-2.99497600	5.90780300	-2.25195300
C	-1.75673400	6.50662400	-3.92058100
H	-2.29014600	7.44795100	-4.09425500
H	-0.69972400	6.67175000	-4.16212100
H	-2.14637700	5.76569400	-4.62920100
C	-2.41688500	1.66070600	2.57901100
H	-1.99580500	0.66874700	2.78140100
H	-1.97261400	2.37837600	3.27732000
C	-3.93396400	1.64994900	2.69767600
H	-4.34752300	0.95288700	1.95650200
H	-4.31560900	2.64643300	2.43876000
C	-4.40480000	1.25739800	4.10491800
H	-4.00574500	0.26566100	4.36090200
H	-3.97986000	1.95538500	4.83971800
C	-5.93129300	1.24305300	4.23827400
H	-6.38366200	0.52872800	3.53953600
H	-6.23955200	0.96029200	5.25108400
H	-6.35650900	2.23088700	4.02312200
H	2.35821500	4.23887800	3.49167300
H	2.48836400	4.90938900	1.78890000

16

Zero-point correction= 0.323415 (Hartree/Particle)
Thermal correction to Energy= 0.340444
Thermal correction to Enthalpy=0.341388
Thermal correction to Gibbs Free Energy=0.278861
E(Solv)= -642.663413811

C	-1.92415000	-0.80823800	-0.37010900
C	-1.90084300	0.46120300	0.26582100
C	-3.07533600	1.12941000	0.64948600
C	-4.27249100	0.48879800	0.37625200
C	-4.31798300	-0.77803500	-0.25842000
C	-3.15953400	-1.43375400	-0.63420400
C	-0.55827900	-1.13683000	-0.58318900
H	-3.04710400	2.09980400	1.13491300
H	-5.20507400	0.97054900	0.65574400
H	-5.28346300	-1.23631600	-0.45008500
H	-3.19664200	-2.40402500	-1.12035300
H	-0.11319500	-2.01103300	-1.03217200
N	0.21852000	-0.16472800	-0.12687600
N	-0.58611800	0.80254600	0.38353100
H	-0.14702900	1.60846300	0.80389700
B	1.86672200	0.02693200	-0.16114700
C	2.18605300	0.95647800	-1.47871900
C	1.65304400	2.39913500	-1.51922400
H	1.84731700	0.43419200	-2.38845000

H	3.28246900	1.00101700	-1.56880900
H	0.55419000	2.43380900	-1.50864100
H	2.00799000	2.98859100	-0.66351300
H	1.97070800	2.93220400	-2.42542000
C	2.27382400	0.74828200	1.25494100
C	2.00251500	-0.04196900	2.54761100
H	1.83049100	1.75694800	1.36274800
H	3.35214000	0.95912300	1.19457300
H	2.32575700	0.49976100	3.44678200
H	0.93432200	-0.26803100	2.67457100
H	2.52804400	-1.00398100	2.54099700
C	2.46184700	-1.48869200	-0.33455900
C	3.99688600	-1.57674300	-0.25817000
H	2.15575000	-1.91334300	-1.30651600
H	2.04415000	-2.16869800	0.42626800
H	4.35881900	-2.60363100	-0.40172800
H	4.47473700	-0.95487600	-1.02499200
H	4.37188200	-1.23418200	0.71424000
H	-0.10501900	-1.60993100	2.17958200
H	1.10842800	-2.73146200	1.55450700
H	1.22132300	-2.13957800	3.21336000
C	1.71243700	-1.28069300	-0.98125000
C	1.43789900	-0.86155300	-2.43627700
H	1.08942200	-2.15678500	-0.74580000
H	2.74019000	-1.67138400	-0.92181300
H	1.57909300	-1.68964800	-3.14409700
H	0.40966800	-0.49844900	-2.56853300
H	2.10449200	-0.04942600	-2.75296100
C	2.59305000	1.16617000	-0.14102000
C	4.07554200	0.79094600	-0.32066600
H	2.56338800	1.90121100	0.68976900
H	2.28150500	1.71873400	-1.04459000
H	4.70997800	1.67510100	-0.46726000
H	4.46126500	0.25355600	0.55356300
H	4.21718800	0.14009500	-1.19086200
H	0.72769500	2.39826500	0.42781200

16-iso

Zero-point correction= 0.323830 (Hartree/Particle)

Thermal correction to Energy= 0.340628

Thermal correction to Enthalpy= 0.341572

Thermal correction to Gibbs Free Energy= 0.279969

E(Solv)=-642.65639320

C	-2.16361500	1.09712000	0.09891600
C	-1.21125000	0.03157100	-0.03223400
C	-1.64976700	-1.29484300	-0.27117900
C	-3.00603500	-1.50778300	-0.37349200
C	-3.95582400	-0.45179300	-0.24518000
C	-3.55359700	0.84168600	-0.01072700
C	-1.39379200	2.24407100	0.32367800
H	-0.93989900	-2.10512800	-0.36575600
H	-3.36890200	-2.51510300	-0.55714100
H	-5.01334300	-0.68205500	-0.33494000
H	-4.27358500	1.64855600	0.08888800
H	-1.66094200	3.27935600	0.47538000
N	-0.11378700	1.84582700	0.31685500
N	0.04889500	0.52421100	0.10484300
B	1.60251700	-0.11983200	0.16246400
C	1.81762800	-0.66103300	1.69580600
C	0.96761300	-1.84490100	2.18580500
H	1.69014900	0.17491500	2.40541300
H	2.87781900	-0.94573400	1.78819200

17-ts

Zero-point correction=1.070491 (Hartree/Particle)

Thermal correction to Energy= 1.130131

Thermal correction to Enthalpy=1.131075

Thermal correction to Gibbs Free Energy= 0.975315

E(Solv)= -2590.33846816

Pd	1.31431100	-0.31721700	0.38428400
P	3.38013700	-1.51816200	0.60166100
P	1.95944200	2.03072600	0.07499900
C	4.94907800	-0.46026800	0.46583300
C	5.24956800	0.40022500	-0.74797900
C	6.20204800	-0.06210400	-1.67235700
C	6.65074100	0.71082100	-2.73988400
C	6.18144100	2.01438700	-2.87524100
C	5.26589900	2.50375900	-1.94773900
C	4.75581400	1.72013400	-0.89812000
C	3.82517800	2.38309400	0.09979400
C	3.62069600	-2.92429700	-0.70233200
C	3.18323800	-2.31631800	-2.05484900
C	5.06097800	-3.45706400	-0.84536100
C	2.70935000	-4.12935500	-0.39091400
C	3.64430800	-2.21448800	2.39608300
C	3.84214200	-1.01494400	3.35159700
C	4.85179000	-3.16081400	2.54684600
C	2.37383000	-2.95029300	2.86825400

C	1.34937200	2.72495600	-1.61859600
C	1.62932900	1.61254600	-2.65552000
C	2.02576500	4.02564700	-2.09437000
C	-0.17087900	2.96772800	-1.57180100
C	1.39402400	3.18903200	1.51772900
C	1.55572200	4.69717400	1.24891000
C	-0.08132000	2.88626600	1.84817600
C	2.22318600	2.82453100	2.77037400
H	4.88613500	0.19004500	1.34157900
H	5.80478500	-1.12079800	0.64047000
H	6.63989700	-1.04392800	-1.52756300
H	7.38607700	0.30872900	-3.43094200
H	6.54351700	2.65685600	-3.67277900
H	4.96234400	3.54299300	-2.01786800
H	3.95974500	3.46767900	0.03283800
H	4.12738400	2.10176500	1.11274400
H	2.14179700	-1.98155700	-2.02677200
H	3.80464200	-1.46362400	-2.34374700
H	3.27535200	-3.07883900	-2.83971000
H	5.76299800	-2.68835400	-1.16670500
H	5.44277000	-3.90927100	0.07178900
H	5.06715000	-4.23634500	-1.61876900
H	2.74746700	-4.82379900	-1.24034000
H	3.04236000	-4.68405600	0.49134500
H	1.66608700	-3.84451700	-0.24890900
H	3.07250400	-0.24967400	3.20716300
H	3.76252500	-1.37121100	4.38638800
H	4.82614800	-0.54750800	3.25060600
H	5.78556400	-2.72394700	2.17813900
H	4.99809300	-3.38141100	3.61252200
H	4.69442300	-4.11727600	2.04084900
H	2.10913600	-3.79978000	2.23491000
H	2.54376800	-3.33680400	3.88162800
H	1.51860800	-2.27115500	2.90890200
H	1.28088900	1.94481400	-3.64252600
H	2.69502000	1.38012700	-2.73834000
H	1.09797500	0.68885000	-2.40229100
H	1.91827600	4.84865000	-1.38501000
H	3.08503700	3.88886600	-2.30872700
H	1.54909400	4.34129400	-3.03181300
H	-0.53404400	3.13319700	-2.59453400
H	-0.71506800	2.11677200	-1.16004200
H	-0.43214900	3.85739000	-0.99114200
H	1.31900700	5.25036500	2.16744800
H	2.57700700	4.97119900	0.96260100
H	0.87210900	5.05523300	0.47467900
H	-0.21631700	1.83255700	2.10573500
H	-0.38728800	3.48915900	2.71320100
H	-0.76151400	3.12007800	1.02788300
H	2.21276200	1.74674200	2.96547100
H	3.26324500	3.15887400	2.70480100
H	1.78072000	3.32002900	3.64372000
C	-1.38035600	-0.89786100	2.24303000
C	-0.91352200	-0.98511800	0.80369800
H	-1.44893300	0.13334500	2.60200600
H	-2.38504700	-1.32976000	2.33711700
H	-0.71205700	-1.44871200	2.91141900
C	0.01094400	-1.99955500	0.41376000
H	0.22651700	-2.78895400	1.12636100
H	-0.00213100	-2.33224600	-0.62539200
C	-1.53888100	-0.19932500	-0.19086800
C	-2.64055300	0.67963800	0.00153700
C	-6.18975700	-2.27643700	-1.40281600
C	-4.89875000	-1.98625400	-0.87112500
C	-3.82287100	-2.88190400	-1.06930300
C	-4.06556600	-4.02996900	-1.80202100
C	-5.34834000	-4.32008400	-2.33757900
C	-6.41145600	-3.45830600	-2.14047100
C	-6.97403400	-1.17808900	-0.99433700
H	-2.84332300	-2.68812600	-0.64292700
H	-3.25628400	-4.73793800	-1.96619600
H	-5.49135200	-5.23793500	-2.90166800
H	-7.39611500	-3.68683200	-2.54071100
H	-8.02029500	-0.97570800	-1.15689600
N	-6.21713400	-0.32600300	-0.29487300
N	-4.94238100	-0.80762300	-0.19252000
H	-3.72783500	-0.02674000	-0.06361800
H	-1.25495600	-0.42492400	-1.21980200
H	-2.81551400	1.40217600	-0.79681100
H	-2.74824200	1.11759000	0.99501700
B	-6.74510000	1.03295300	0.46935000
C	-6.77214300	0.69607500	2.08312900
C	-5.44128800	0.48565000	2.82430800
H	-7.40659700	-0.18954700	2.25574700
H	-7.30268000	1.52491700	2.57928400
H	-4.88121400	-0.35972800	2.40492100
H	-4.79644100	1.37248000	2.75197000
H	-5.58622100	0.28225500	3.89599400

C	-5.74508200	2.27592700	0.08687400
C	-5.60272600	2.60924000	-1.40837000
H	-4.74162700	2.13110900	0.51011800
H	-6.12824400	3.16944700	0.60515800
H	-4.93088100	3.46131900	-1.59511500
H	-5.20902800	1.75431200	-1.97584900
H	-6.57189100	2.86200200	-1.85679800
C	-8.28232100	1.28657900	-0.07427000
C	-8.92559100	2.60199900	0.40033900
H	-8.94411000	0.46344300	0.24691800
H	-8.32357900	1.27916700	-1.17680700
H	-9.96373500	2.70551500	0.05318400
H	-8.94370300	2.67171000	1.49532100
H	-8.37440000	3.47675200	0.03289200

18-ts

Zero-point correction=1.076000 (Hartree/Particle)

Thermal correction to Energy=1.135243

Thermal correction to Enthalpy=1.136187

Thermal correction to Gibbs Free Energy= 0.984666

E(solv)= -2590.34543989

Pd	-0.70881500	0.00574500	-0.28228100
P	-1.86566500	1.97853000	0.46868300
P	-2.22697200	-1.85670700	0.21346100
C	-3.63640200	1.67883700	1.09524600
C	-4.69462200	0.98389200	0.25661100
C	-5.69263200	1.77133500	-0.34358300
C	-6.77144500	1.22414000	-1.03291300
C	-6.90322900	-0.16025900	-1.09549800
C	-5.95156400	-0.95819700	-0.46667900
C	-4.83073400	-0.42542000	0.19311200
C	-3.91610100	-1.38216200	0.93208600
C	-2.06542800	3.33178200	-0.90275500
C	-2.39332200	2.56693400	-2.20504700
C	-3.18556900	4.36263100	-0.65119200
C	-0.75696600	4.12474000	-1.10751400
C	-1.10996700	2.78221800	2.06438500
C	-1.28967600	1.78678900	3.23261900
C	-1.74667000	4.12691000	2.46882100
C	0.40896600	2.97813300	1.88211900
C	-2.65267100	-2.86517800	-1.37747600
C	-2.96952500	-1.81638200	-2.46965300
C	-3.83761500	-3.84448300	-1.27215900
C	-1.41248800	-3.65702600	-1.83122500
C	-1.61253200	-3.04113800	1.62058300
C	-2.39603000	-4.36065800	1.75631500
C	-0.12230400	-3.36340400	1.39580100
C	-1.71044300	-2.27904300	2.96185800
H	-3.47999100	1.09961400	2.00877700
H	-4.03414100	2.64707200	1.41563500
H	-5.64850100	2.84874200	-0.22909700
H	-7.51544300	1.87557200	-1.48264300
H	-7.75162300	-0.61744400	-1.59685900
H	-6.10054600	-2.03306700	-0.45775400
H	-4.46805700	-2.30561400	1.13681100
H	-3.66945200	-0.95399400	1.90724200
H	-1.58844400	1.87930400	-2.48067000
H	-3.31709300	1.98627100	-2.11744200
H	-2.52593300	3.28627700	-3.02453500
H	-4.17694100	3.91389200	-0.68858100
H	-3.07974400	4.89121600	0.29820800
H	-3.14856000	5.11644000	-1.44878000
H	-0.84821900	4.71352500	-2.02983100
H	-0.57310300	4.83073900	-0.29267400
H	0.12167400	3.48777500	-1.21110300
H	-0.92929800	0.78808700	2.96909100
H	-0.69221000	2.13318000	4.08497300
H	-2.32587500	1.71127000	3.57726200
H	-2.83476500	4.07041300	2.57985700
H	-1.33962400	4.42938900	3.44264500
H	-1.51237600	4.92776600	1.76225000
H	0.66337900	3.63266700	1.04672200
H	0.81580800	3.43637800	2.79288500
H	0.92109300	2.02447500	1.74308900
H	-3.15960000	-2.33410900	-3.41976400
H	-3.85526900	-1.22204000	-2.23118900
H	-2.12979700	-1.13019700	-2.61845800
H	-3.66518400	-4.64525100	-0.55103600
H	-4.77242000	-3.34684400	-1.01251800
H	-3.98956900	-4.31652400	-2.25214900
H	-1.59303200	-4.06090900	-2.83629300
H	-0.52729300	-3.01914600	-1.88354400
H	-1.19490800	-4.50578100	-1.17586400
H	-2.05897500	-4.88257600	2.66179200
H	-3.47607700	-4.20756900	1.85577100
H	-2.21910000	-5.03552900	0.91419000
H	0.48392400	-2.45424600	1.36733400
H	0.24254800	-3.98072900	2.22682300

H	0.05403800	-3.92208800	0.47451100
H	-1.24771200	-1.28932500	2.90390100
H	-2.74096900	-2.16667000	3.31274600
H	-1.16933000	-2.84607600	3.72950900
C	0.93399400	-0.59114700	-3.05182400
C	1.23751900	-0.35529800	-1.57972900
H	1.80371700	-0.34229700	-3.67164100
H	0.65393100	-1.62610500	-3.26978300
H	0.10884800	0.04957500	-3.37882600
C	1.02124000	0.95475100	-1.04529400
H	1.63959000	1.27636800	-0.21061800
H	0.81433400	1.74011800	-1.76780200
C	2.01427100	-1.28614900	-0.83590500
C	2.32757700	-2.67383400	-1.31809000
H	3.13578100	-3.10305000	-0.72692500
H	1.44668800	-3.31868700	-1.21860300
H	2.10373500	-1.11556200	0.22556300
H	2.62167600	-2.68316400	-2.37082500
C	5.49446400	1.09360700	-1.49814800
C	4.64616300	0.02079700	-1.90414100
C	4.50060800	-0.28211200	-3.27814000
C	5.17335000	0.50351000	-4.19618900
C	6.00080500	1.58478700	-3.79134700
C	6.17409400	1.88043300	-2.45276500
C	5.43744100	1.04457300	-0.09233400
H	3.90511100	-1.12816300	-3.60568200
H	5.08068800	0.28078000	-5.25642500
H	6.51366000	2.17179000	-4.54854400
H	6.82540800	2.69296800	-2.14026500
H	5.96357800	1.63588500	0.63881000
N	4.62905000	0.04607100	0.28717900
N	4.12779900	-0.60549100	-0.81029800
B	4.43216500	-0.46228200	1.84981000
C	4.36748400	-2.10418200	1.84042900
C	5.57885700	-2.84519900	1.24761000
H	3.45474200	-2.47595100	1.34503000
H	4.25666500	-2.42312300	2.88919200
H	5.48225400	-3.93876500	1.32024400
H	5.71799500	-2.59797600	0.18789900
H	6.50493200	-2.57010900	1.76757500
C	5.75504400	0.03521700	2.71449700
C	5.80228900	1.45917100	3.30714600
H	6.67727700	-0.13072600	2.13499500
H	5.84530800	-0.65981300	3.56473000
H	6.73115200	1.64087000	3.86665600
H	5.73336300	2.24978500	2.54729300
H	4.97139900	1.63353300	4.00143500
C	3.04390400	0.21734500	2.42877200
C	2.66869700	-0.20659000	3.86110400
H	2.17441500	-0.00870300	1.78821800
H	3.13421600	1.31582700	2.40276900
H	1.77596000	0.31611800	4.23715400
H	2.46210000	-1.28286700	3.91646800
H	3.48148200	-0.00518700	4.56914900

18-ts-iso

Zero-point correction= 1.075911 (Hartree/Particle)

Thermal correction to Energy=1.135180

Thermal correction to Enthalpy=1.136124

Thermal correction to Gibbs Free Energy=0.984026

E(Solv)= -2590.34275158

Pd	1.01452100	-0.08280700	-0.39278100
P	2.23454500	-1.93114300	0.52370000
P	2.33783400	1.91976700	0.14560900
C	3.95704300	-1.48212700	1.18667300
C	4.97047200	-0.77389300	0.30412300
C	6.00207200	-1.53463400	-0.27276300
C	7.03170700	-0.96547000	-1.01724000
C	7.07498600	0.41799400	-1.16661600
C	6.08760100	1.19343400	-0.56550900
C	5.01692700	0.63487300	0.15369000
C	4.06166500	1.57921200	0.85777500
C	2.55980000	-3.39519300	-0.70117700
C	2.96008600	-2.74564500	-2.04588700
C	3.67670900	-4.37243300	-0.27849200
C	1.28154300	-4.23353100	-0.91823400
C	1.41120000	-2.61793600	2.14174000
C	1.51559700	-1.53336200	3.23545000
C	2.04828100	-3.91234800	2.68397400
C	-0.09559300	-2.85262900	1.90046200
C	2.66779300	2.92308100	-1.47083400
C	3.01773700	1.87584100	-2.55409700
C	3.80273200	3.96380600	-1.41183600
C	1.37365600	3.64178800	-1.89962300
C	1.65308200	3.10395100	1.52345100
C	2.31816000	4.49282400	1.58224800
C	0.13538200	3.27936100	1.32036700
C	1.85166100	2.42690800	2.89788100

H	3.73858900	-0.85083500	2.05130400
H	4.41443800	-2.39413600	1.58425100
H	6.02134600	-2.60554600	-0.10318000
H	7.80513400	-1.59649900	-1.44588900
H	7.88248300	0.89434600	-1.71539600
H	6.16804900	2.27389600	-0.62675900
H	4.56495800	2.54065400	1.00623300
H	3.85322300	1.18980700	1.85751000
H	2.17251300	-2.08891800	-2.42612900
H	3.87738900	-2.15558800	-1.96135400
H	3.13696200	-3.53461700	-2.78929300
H	4.65462800	-3.89574800	-0.22020000
H	3.47722500	-4.86214400	0.67633000
H	3.75295600	-5.16107700	-1.03870200
H	1.45014200	-4.91206200	-1.76490600
H	1.04506500	-4.85637200	-0.05094600
H	0.40604800	-3.62782500	-1.15258700
H	1.13655000	-0.57178800	2.87926400
H	0.89498000	-1.83284000	4.08907400
H	2.53440700	-1.39735100	3.61169200
H	3.12989400	-3.82334600	2.83212000
H	1.60587900	-4.14054900	3.66255400
H	1.85720600	-4.77361700	2.03862900
H	-0.29930100	-3.57647000	1.10929900
H	-0.54459900	-3.24141200	2.82336000
H	-0.61070900	-1.92021900	1.65425000
H	3.16593800	2.38743600	-3.51490200
H	3.93618700	1.33036400	-2.32078500
H	2.21243400	1.14460300	-2.67759200
H	3.62072600	4.75522200	-0.68318200
H	4.77151400	3.51339300	-1.19246700
H	3.89004200	4.44207500	-2.39664800
H	1.49529100	4.01890600	-2.92365800
H	0.51443900	2.96659100	-1.89394600
H	1.14361800	4.50155900	-1.26354100
H	1.94608200	5.02629900	2.46701500
H	3.40825500	4.43734700	1.67442000
H	2.07567300	5.10939600	0.71270900
H	-0.38682600	2.31850200	1.33801700
H	-0.27002200	3.89367000	2.13471200
H	-0.10669600	3.78318000	0.38252400
H	1.48117600	1.39863000	2.90803800
H	2.89630300	2.42706900	3.22402400
H	1.28020100	2.98478000	3.65007300
C	-0.78208100	0.55194700	-3.14280900
C	-0.93545200	0.10115900	-1.69925400
H	-1.70633000	0.37536000	-3.71059900
H	-0.55086500	1.61707100	-3.23555100
H	0.01854000	-0.00691000	-3.63786000
C	-0.51114600	-1.21210700	-1.31899900
H	-1.08897100	-1.73161400	-0.55827900
H	-0.14856300	-1.85908600	-2.11571200
C	-1.79609200	0.80511200	-0.80961800
C	-2.36606900	2.15689300	-1.12894100
H	-1.58040300	2.92042700	-1.08160100
H	-2.79122200	2.18161400	-2.13626900
H	-1.76510400	0.52342400	0.23038700
H	-3.14505300	2.42386700	-0.41343700
C	-5.37972500	-0.77916800	-2.22761800
C	-5.88819900	-0.24295500	-1.00655100
C	-7.28505800	-0.09704700	-0.82955400
C	-8.11450700	-0.48388300	-1.86488500
C	-7.60864600	-1.02327800	-3.07781700
C	-6.25046200	-1.17465200	-3.26739300
C	-3.98355700	-0.74901500	-2.04921000
H	-7.69375700	0.31722500	0.08192700
H	-9.18951700	-0.36928800	-1.74987700
H	-8.30412500	-1.31450200	-3.86060800
H	-5.85567400	-1.58386500	-4.19428200
H	-3.19311900	-1.04402300	-2.72486900
N	-3.69201300	-0.26293900	-0.83994500
N	-4.83647500	0.05239900	-0.17465200
B	-4.93114200	0.44601300	1.43966200
C	-5.91306700	-0.66824000	2.15355000
C	-5.50859900	-2.14304000	1.97971700
H	-6.96185200	-0.56559900	1.83697400
H	-5.93723500	-0.44360600	3.23113600
H	-6.17546900	-2.83135100	2.51930500
H	-5.52550500	-2.44066800	0.92318500
H	-4.48952100	-2.32825500	2.34554700
C	-3.40510600	0.36867100	2.07563200
C	-3.30184800	0.23636400	3.60818900
H	-2.83029900	1.26755700	1.79111000
H	-2.86213400	-0.48854400	1.64378500
H	-2.25611300	0.23400100	3.95352800
H	-3.80856300	1.05666400	4.12833200
H	-3.75855800	-0.69462200	3.96305900
C	-5.56176100	1.97279500	1.46358500

C	-5.95728200	2.54805500	2.83589300
H	-6.45304000	2.02583900	0.81809700
H	-4.84777100	2.67702300	0.99829000
H	-6.42977400	3.53792200	2.75191900
H	-6.66865200	1.89386700	3.35583300
H	-5.08953400	2.66587400	3.49668800

19-ts

Zero-point correction= 0.866588 (Hartree/Particle)

Thermal correction to Energy= 0.915087

Thermal correction to Enthalpy= 0.916031

Thermal correction to Gibbs Free Energy= 0.785300

E(Solv)= -2327.64485253

Pd	-0.31993800	0.23566600	0.42359000
P	-2.09011000	1.86633600	0.27414400
P	-1.43595300	-1.94256800	0.41017300
C	-3.85382500	1.18066500	0.11641600
C	-4.23526200	0.21972600	-0.99235400
C	-5.00090000	0.71047900	-2.06437400
C	-5.48818500	-0.11061700	-3.07726400
C	-5.24771400	-1.48063800	-3.01225800
C	-4.53028500	-1.99125400	-1.93433800
C	-3.99638100	-1.17424500	-0.92208100
C	-3.32838100	-1.85616100	0.25748700
C	-1.88006000	3.04701700	-1.24188900
C	-1.44909800	2.14099600	-2.41842900
C	-3.14355300	3.82418600	-1.66306900
C	-0.75982600	4.07555800	-0.98175000
C	-2.33433000	2.91418800	1.89462900
C	-2.91848300	1.98952600	2.98759900
C	-3.27257700	4.12740200	1.73935800
C	-0.96769100	3.40374500	2.41511000
C	-0.91552500	-3.14538900	-1.01411900
C	-0.98999900	-2.29749100	-2.30700000
C	-1.78777400	-4.40711500	-1.16007400
C	0.54602000	-3.61190100	-0.86164700
C	-1.32740500	-2.81280200	2.14023000
C	-2.32848300	-3.96299300	2.36999800
C	0.09828400	-3.34331400	2.39369700
C	-1.60667700	-1.71122400	3.18700400
H	-4.01660600	0.68535300	1.07694800
H	-4.54273400	2.03159300	0.09261700
H	-5.25679100	1.76467900	-2.08457900
H	-6.07321400	0.31446400	-3.88791000
H	-5.63736300	-2.15121200	-3.77293700
H	-4.39833600	-3.06617500	-1.86249800
H	-3.71301000	-2.87756800	0.31657600
H	-3.63709500	-1.36522900	1.18694200
H	-0.51498100	1.61491000	-2.19872600
H	-2.20957800	1.39231800	-2.66041000
H	-1.29205700	2.75992900	-3.31210000
H	-3.94208300	3.16448600	-2.00152500
H	-3.53723100	4.46666300	-0.87306000
H	-2.88633800	4.47264000	-2.51112400
H	-0.53454700	4.59287900	-1.92358300
H	-1.05853300	4.84100600	-0.25921300
H	0.16412800	3.61231800	-0.63301700
H	-2.36044400	1.05214600	3.06994900
H	-2.84808600	2.50120500	3.95602800
H	-3.97578600	1.75753200	2.82732400
H	-4.25370500	3.85780900	1.33462400
H	-3.44408300	4.57195100	2.72887400
H	-2.84189200	4.90869300	1.10752300
H	-0.43796800	4.03675300	1.70025100
H	-1.12621300	3.99636300	3.32585700
H	-0.32023700	2.56142600	2.67159700
H	-0.66877900	-2.91499700	-3.15648600
H	-1.99734500	-1.93517100	-2.52162600
H	-0.32064600	-1.43311800	-2.24788400
H	-1.66246600	-5.09120700	-0.31567100
H	-2.85251000	-4.19323400	-1.26773100
H	-1.47568500	-4.95037300	-2.06188200
H	0.86714600	-4.06421800	-1.80898900
H	1.22245500	-2.78493800	-0.64776600
H	0.66680800	-4.37154500	-0.08683100
H	-2.16031800	-4.38410500	3.37019800
H	-3.37006100	-3.62914400	2.33598000
H	-2.20679100	-4.77829600	1.65215900
H	0.86720000	-2.62510200	2.09523900
H	0.22283300	-3.53744000	3.46698800
H	0.28645200	-4.28509700	1.87347900
H	-0.88315000	-0.89351500	3.10865700
H	-2.61323400	-1.28926000	3.09419600
H	-1.52886300	-2.14228700	4.19395900
C	2.24072600	0.16772800	2.37345800
C	1.90288400	0.36993500	0.90922900
H	2.11959700	-0.87446200	2.68577700
H	3.29671400	0.42623300	2.52013600

H	1.62632200	0.79728700	3.02577300
C	1.35918500	1.60156100	0.46807100
H	1.29901600	2.42236500	1.17489700
H	1.51311700	1.91038300	-0.56255200
C	2.33860200	-0.61306400	-0.01954500
C	2.67694200	-0.44194600	-1.40349500
H	2.23908700	0.41705900	-1.91580500
H	2.61231600	-1.56768000	0.42191200
C	7.31171000	0.01512700	0.25127800
C	6.60176000	0.20349800	-0.97761200
C	7.27826700	0.59313600	-2.15341900
C	8.64649500	0.78729800	-2.08075700
C	9.35882700	0.60327900	-0.86563800
C	8.70706900	0.22108300	0.29453000
C	6.28910800	-0.36532100	1.15788600
H	6.73577600	0.73482500	-3.08508500
H	9.19373200	1.08753500	-2.97176900
H	10.43391100	0.76710100	-0.85342200
H	9.26244100	0.08300800	1.22028500
H	6.36179800	-0.61513600	2.21000600
N	5.10944200	-0.39705600	0.52854600
N	5.28298400	-0.05152600	-0.75882800
H	3.89414000	-0.21147700	-1.32203300
H	2.61408500	-1.35196600	-2.00567500

20-ts

Zero-point correction= 0.953266 (Hartree/Particle)

Thermal correction to Energy= 1.006206

Thermal correction to Enthalpy= 1.007150

Thermal correction to Gibbs Free Energy=0.869162

E(Solv)= -2394.91262419

Pd	0.03935100	0.07104200	0.11283100
P	-1.34704000	1.65018400	1.08883800
P	-1.15653700	-2.08080200	-0.08396400
C	-3.07477800	0.96590800	1.49361600
C	-3.99275900	0.38014000	0.43801100
C	-5.05400200	1.19045100	-0.00655900
C	-6.01612700	0.74200100	-0.90602700
C	-5.95191800	-0.57172100	-1.36763900
C	-4.93152700	-1.39970600	-0.91054500
C	-3.93418700	-0.95684500	-0.02210100
C	-2.96158000	-1.99971400	0.49280400
C	-1.63632800	3.22661900	0.01290200
C	-2.26475200	2.76054200	-1.31970900
C	-2.55002500	4.28348900	0.66271700
C	-0.28569600	3.88543300	-0.34305200
C	-0.81670800	2.14246200	2.88816900
C	-0.37591300	0.83779400	3.58637500
C	-1.92650100	2.78926400	3.74531700
C	0.39878400	3.08989900	2.85335100
C	-1.20217700	-2.71710500	-1.89923600
C	-1.95697500	-1.65561500	-2.73097500
C	-1.87805000	-4.08456400	-2.10431200
C	0.24471500	-2.77051300	-2.44052600
C	-0.55735400	-3.48257400	1.10935200
C	-1.55617000	-4.63950500	1.32496300
C	0.78227600	-4.06671500	0.62065000
C	-0.30479800	-2.80568600	2.47432700
H	-2.85773100	0.20759400	2.25448500
H	-3.62553300	1.75968000	2.00603400
H	-5.13051200	2.20330300	0.38155600
H	-6.81672000	1.40455000	-1.22287100
H	-6.70062300	-0.95736600	-2.05395200
H	-4.91134400	-2.43742600	-1.23532000
H	-3.41032100	-2.98323400	0.32607500
H	-2.86438200	-1.89515300	1.57997000
H	-1.66542200	1.97297400	-1.78542700
H	-3.28250200	2.38752000	-1.20507700
H	-2.29434200	3.61200800	-2.01238900
H	-3.50524800	3.87013500	1.00307300
H	-2.06866400	4.77726500	1.51203200
H	-2.77932700	5.06331400	-0.07549700
H	-0.47658400	4.71438300	-1.03725800
H	0.23546400	4.29758500	0.52204000
H	0.38591200	3.18385800	-0.84555000
H	0.47281400	0.37749200	3.07686100
H	-0.07096100	1.07038200	4.61544000
H	-1.18333500	0.10008100	3.64767000
H	-2.74678300	2.09704700	3.95831900
H	-1.49501900	3.07724400	4.71291400
H	-2.34776200	3.69204500	3.29707500
H	0.12103800	4.10701100	2.56184300
H	0.83062900	3.14950700	3.86077900
H	1.18338400	2.73036200	2.18051800
H	-1.83616100	-1.88861600	-3.79716600
H	-3.02571400	-1.62879700	-2.51429300
H	-1.55529300	-0.65160100	-2.56121400
H	-1.29906500	-4.90162100	-1.66395400

H	-2.89184800	-4.12009300	-1.68960300
H	-1.96065900	-4.29060000	-3.18004100
H	0.21086900	-2.98007600	-3.51800200
H	0.76603100	-1.81816600	-2.30232700
H	0.84657500	-3.55266800	-1.97486000
H	-1.08823800	-5.38998000	1.97582700
H	-2.47317400	-4.31346800	1.82544500
H	-1.83468600	-5.14349300	0.39637400
H	1.50969500	-3.28796300	0.37149200
H	1.21813700	-4.67876200	1.42109800
H	0.65595200	-4.71779100	-0.24937900
H	0.46373800	-2.03282900	2.40612700
H	-1.21020200	-2.35198900	2.89332600
H	0.03955800	-3.56180100	3.19226500
C	3.39641600	1.39032500	-2.75957700
C	2.08405500	1.03615100	-2.34829200
C	0.98108200	1.24202200	-3.19986300
C	1.22389000	1.79281600	-4.44675200
C	2.53332300	2.14322400	-4.86572300
C	3.62172600	1.94638900	-4.03584200
C	4.20069000	1.04700800	-1.65228500
H	-0.01996900	0.96649000	-2.88698300
H	0.39173300	1.95792100	-5.12635600
H	2.67630700	2.56819100	-5.85527400
H	4.62573600	2.20982800	-4.35737300
H	5.26964200	1.11871800	-1.52680400
N	3.44623300	0.53637600	-0.67901000
N	2.13161400	0.49901000	-1.08511900
H	1.18926100	1.16451100	-0.14857400
B	4.10180700	-0.20924100	0.67293000
C	2.96907700	-0.14607700	1.85612100
C	3.14163600	-1.12118500	3.03545700
H	1.97095100	-0.35409200	1.41820600
H	2.89362700	0.87844000	2.25902300
H	2.35747700	-0.99707000	3.79732700
H	3.10059800	-2.16345600	2.69758700
H	4.10163700	-0.98731700	3.54392200
C	4.43024500	-1.73099200	0.11571100
C	5.47537900	-2.55617600	0.88977900
H	4.78748000	-1.65867500	-0.92476300
H	3.49877100	-2.31950400	0.05167500
H	5.62804800	-3.54772800	0.43952700
H	6.45077000	-2.05408600	0.89565700
H	5.19196600	-2.71771800	1.93597300
C	5.45004800	0.68925400	0.99979900
C	6.03974400	0.58451700	2.41857100
H	5.22787600	1.75593400	0.82644300
H	6.26158300	0.44637400	0.29157400
H	6.94277600	1.20161200	2.52896100
H	5.32414800	0.92687700	3.17604600
H	6.31890400	-0.44335200	2.67677400

21

Zero-point correction=0.309166 (Hartree/Particle)
Thermal correction to Energy=0.325774
Thermal correction to Enthalpy=0.326718
Thermal correction to Gibbs Free Energy=0.265204
E(Solv)= -642.184345728

C	-1.91581900	-0.80589700	-0.37789600
C	-1.85783200	0.48073800	0.26010100
C	-3.05174700	1.14331600	0.63470200
C	-4.25908000	0.52469200	0.37197000
C	-4.31815000	-0.75079200	-0.25981200
C	-3.16481500	-1.41640500	-0.63350000
C	-0.56204400	-1.11925400	-0.58082200
H	-3.00413900	2.11702700	1.11677600
H	-5.18939300	1.01697300	0.65106900
H	-5.29017700	-1.20322600	-0.44854100
H	-3.22123600	-2.39117500	-1.11615600
H	-0.09932300	-1.98760600	-1.02424800
N	0.18465300	-0.10184700	-0.10100200
N	-0.57957300	0.89003100	0.41947200
B	1.79824500	0.03647800	-0.15565200
C	2.16121900	1.00468000	-1.44720900
C	1.75647400	2.48580500	-1.35722200
H	1.70469000	0.57339100	-2.35585500
H	3.24973600	0.95790300	-1.62652200
H	0.68646800	2.58769500	-1.14290500
H	2.28989800	2.99388700	-0.54253500
H	1.97270800	3.04465100	-2.28304800
C	2.28988600	0.68757100	1.27154200
C	2.01136200	-0.15098500	2.53057000
H	1.81514400	1.66891000	1.40941300
H	3.37390900	0.88959800	1.21484400
H	2.36157500	0.33399300	3.45660000
H	0.93420200	-0.32705600	2.64566700
H	2.49588600	-1.13647500	2.48162800
C	2.40410900	-1.48294400	-0.41178200

C	3.93630000	-1.59066300	-0.31817200
H	2.10847300	-1.85453900	-1.40955700
H	1.97195800	-2.20389000	0.30311700
H	4.30595900	-2.60849900	-0.52285200
H	4.43078000	-0.91942400	-1.03300600
H	4.29691600	-1.31099700	0.68025800

21-iso

Zero-point correction= 0.309025 (Hartree/Particle)

Thermal correction to Energy= 0.325659

Thermal correction to Enthalpy= 0.326604

Thermal correction to Gibbs Free Energy= 0.264945

E(solv)=-642.18367227

C	-2.15433300	1.10063500	-0.07905000
C	-1.18593300	0.04633700	-0.05297500
C	-1.61834700	-1.29939600	-0.08856500
C	-2.97843500	-1.55630800	-0.15859400
C	-3.93648000	-0.51227500	-0.19199700
C	-3.53100700	0.81141300	-0.15157100
C	-1.35999800	2.27152300	-0.01411800
H	-0.90553000	-2.11323400	-0.05672500
H	-3.32074500	-2.58942500	-0.18606400
H	-4.99539200	-0.75831600	-0.24694900
H	-4.26318700	1.61753900	-0.17262800
H	-1.67406600	3.30973300	-0.00836700
N	-0.06949500	1.96682300	0.04123900
N	0.06267700	0.61215400	0.01125300
B	1.55715100	-0.02250500	0.15774000
C	1.86996800	-0.18669400	1.77443300
C	0.99676900	-1.16532900	2.57848700
H	1.79439500	0.80769000	2.24633000
H	2.92387700	-0.48917600	1.90503200
H	-0.06622900	-0.89886200	2.51315500
H	1.08987000	-2.19372100	2.20188400
H	1.25677100	-1.19366600	3.64975800
C	1.66957900	-1.46929800	-0.63238000
C	1.35107600	-1.46642300	-2.13801200
H	1.07834100	-2.26685300	-0.15412700
H	2.71135500	-1.80947200	-0.50600300
H	1.50610800	-2.44867300	-2.61431800
H	0.30939400	-1.17637500	-2.32695600
H	1.98112400	-0.74406400	-2.67342400
C	2.58871200	1.08886600	-0.50227300
C	4.06598500	0.66524900	-0.58697400
H	2.53087000	2.02432100	0.07210100
H	2.25337200	1.36648900	-1.51553500
H	4.71322900	1.46236300	-0.98844000
H	4.46761700	0.39604000	0.40004200
H	4.20546500	-0.21246200	-1.23337100

22

Zero-point correction= 0.602181 (Hartree/Particle)

Thermal correction to Energy= 0.638798

Thermal correction to Enthalpy= 0.639743

Thermal correction to Gibbs Free Energy= 0.528656

E(Solv) = -2029.64698778

C	-2.27520600	-2.16919200	2.16141600
O	-1.02040000	-2.84841000	1.90432400
C	-0.30109000	-2.05245200	1.09233700
C	-2.35656000	-1.15274100	1.00549700
H	-3.06839100	-2.91598200	2.16141400
H	-2.19778600	-1.69474000	3.14543800
H	-2.73573500	-0.19018700	1.35745700
N	-0.92474000	-1.01171900	0.62743400
C	1.05113600	-2.56830900	0.78537800
C	1.25187900	-3.93797000	1.04106500
C	2.10298800	-1.81195100	0.21014500
C	2.44889300	-4.56683300	0.71071300
H	0.44990500	-4.51229100	1.48723600
C	3.29848600	-2.46754900	-0.11698900
C	3.47445100	-3.83147600	0.12221000
H	2.57230600	-5.62689100	0.90921400
H	4.10912200	-1.90282300	-0.56414600
H	4.41218200	-4.30885500	-0.14627800
P	1.99325400	0.01350300	-0.02603800
Pd	-0.19157600	0.71193100	-0.44248400
C	-3.21915300	-1.64714000	-0.15342500
C	-2.68120100	-2.17654800	-1.33167400
C	-4.61326100	-1.62173900	0.00286700
C	-3.52119600	-2.66874700	-2.33583200
H	-1.60550200	-2.20464000	-1.47357400
C	-5.45022400	-2.12166900	-0.99331900
H	-5.04778600	-1.20152000	0.90718200
C	-4.90541700	-2.64562300	-2.16925800
H	-3.08845500	-3.07728500	-3.24485200
H	-6.52735900	-2.09897100	-0.85396600
H	-5.55662200	-3.03377300	-2.94699500
C	3.27149000	0.37314300	-1.29235900

C	4.47156800	1.03215000	-0.98925900
C	3.00854200	-0.00163800	-2.62247400
C	5.39546900	1.30697700	-2.00184100
H	4.68896100	1.33171700	0.03085100
C	3.93704600	0.26651800	-3.62628200
H	2.07717800	-0.50481500	-2.87256500
C	5.13211500	0.92427300	-3.31729300
H	6.32124300	1.81979100	-1.75767300
H	3.72724800	-0.03211300	-4.64932100
H	5.85230500	1.13912300	-4.10126500
C	2.61235200	0.70527700	1.56230100
C	3.57233500	0.04310500	2.34561900
C	2.11417200	1.94506400	1.99642100
C	4.02771500	0.61696300	3.53328900
H	3.96295200	-0.92114700	2.03638900
C	2.57490000	2.51726800	3.18260800
H	1.36044500	2.45751700	1.40570300
C	3.53192700	1.85362100	3.95265300
H	4.76854300	0.09514700	4.13207100
H	2.18261800	3.47678600	3.50715700
H	3.88737000	2.29590700	4.87872000
C	-2.14982500	1.86263800	-1.05837600
C	-1.02184100	2.69383800	-1.01406400
H	-2.31589000	1.27404800	-1.96087900
H	-0.97193200	3.47416000	-0.25545000
C	0.14946900	2.40853600	-1.76186100
C	1.33444300	3.34198200	-1.73761400
H	0.01677700	1.86468800	-2.70094200
H	1.19696200	4.12737800	-2.49355400
H	1.44958000	3.83314500	-0.76562500
C	-3.32911800	2.05902500	-0.19864500
C	-4.60185200	1.72789000	-0.69681700
C	-3.23948400	2.61498300	1.09358600
C	-5.74960200	1.97282200	0.05603300
H	-4.68934000	1.28949600	-1.68716400
C	-4.38605200	2.84978000	1.84845400
H	-2.26626700	2.85692500	1.51331400
C	-5.64649700	2.53475700	1.33009000
H	-6.72452200	1.72554000	-0.35393600
H	-4.29831900	3.28029600	2.84197300
H	-6.54003600	2.72498500	1.91743100
H	2.26553800	2.82312000	-1.97697200

23-ts

Zero-point correction= 0.786891 (Hartree/Particle)
Thermal correction to Energy= 0.832513
Thermal correction to Enthalpy= 0.833457
Thermal correction to Gibbs Free Energy= 0.699443
E(Solv) = -2434.12873165

C	-2.76224700	4.00705500	0.40287600
O	-3.77589900	3.11060500	-0.11007300
C	-3.19998300	1.89801800	-0.26492400
C	-1.44264500	3.24235400	0.14271900
H	-2.84497600	4.95231300	-0.13393500
H	-2.96289500	4.16049400	1.46805500
H	-0.80283000	3.26401000	1.02827500
N	-1.92022800	1.85396100	-0.07135700
C	-4.13771700	0.84357000	-0.72063000
C	-5.36178000	1.31228400	-1.23785100
C	-3.88195800	-0.55297800	-0.71638200
C	-6.31043200	0.44171000	-1.76450000
H	-5.55807100	2.37669500	-1.23462200
C	-4.85576800	-1.40861200	-1.25392700
C	-6.05562000	-0.92711400	-1.77754900
H	-7.23989100	0.83592000	-2.16376100
H	-4.67292900	-2.47772600	-1.26130300
H	-6.78382500	-1.62154000	-2.18638700
P	-2.35732300	-1.30382500	0.01934100
Pd	-0.53701100	0.18908200	0.10580600
C	-0.65912900	3.78211900	-1.04764800
C	-0.82108200	3.28019500	-2.34446300
C	0.20398100	4.86888200	-0.84503200
C	-0.13170000	3.85288700	-3.41678000
H	-1.48037500	2.43557900	-2.51922500
C	0.88768700	5.44502500	-1.91615500
H	0.34343300	5.26426700	0.15844700
C	0.72271700	4.93627300	-3.20693800
H	-0.27008100	3.45469200	-4.41840700
H	1.54874100	6.28972500	-1.74284300
H	1.25339700	5.38416100	-4.04228900
C	-2.19329000	-2.88414600	-0.91687600
C	-2.43277700	-4.14239300	-0.34546800
C	-1.76892500	-2.81407700	-2.25674400
C	-2.25713500	-5.30559100	-1.10114700
H	-2.76156300	-4.21838900	0.68606400
C	-1.60730600	-3.97543100	-3.01089200
H	-1.57158400	-1.84567400	-2.71161700
C	-1.84910500	-5.22560700	-2.43288500

H	-2.44744200	-6.27374900	-0.64648200
H	-1.29069200	-3.90601000	-4.04798800
H	-1.71916700	-6.13092900	-3.01883900
C	-2.88478300	-1.80597500	1.71494400
C	-4.22605200	-1.89534500	2.11776000
C	-1.87530400	-2.10911200	2.64592200
C	-4.54778500	-2.28255600	3.42066300
H	-5.02430800	-1.66163700	1.42125000
C	-2.19990100	-2.50802200	3.94223800
H	-0.83256600	-2.02861800	2.35023700
C	-3.53836100	-2.59204500	4.33337400
H	-5.59034200	-2.34275900	3.71993200
H	-1.40912200	-2.74404100	4.64896500
H	-3.79250900	-2.89349300	5.34548300
C	1.40694700	1.01928600	0.47674900
C	1.48970200	-0.41768100	0.54105300
H	1.73523300	1.48917000	-0.45293800
H	1.58318800	-0.90306900	1.51188900
C	1.79201900	-1.21008900	-0.60085500
C	1.65292200	-2.70708400	-0.58843600
H	1.68815000	-0.73156800	-1.57183500
H	2.30748800	-3.18023800	-1.32590800
H	1.86949100	-3.12298900	0.40066100
C	1.56394400	1.87825600	1.67138600
C	2.17712400	3.13944100	1.54691700
C	1.12582100	1.48288400	2.95218200
C	2.35319300	3.96919100	2.65478000
H	2.52154200	3.46706000	0.56924100
C	1.30332000	2.31142400	4.05828700
H	0.62543600	0.52636100	3.07813900
C	1.91847500	3.55895400	3.91663400
H	2.83773800	4.93424700	2.53261800
H	0.95647900	1.98444800	5.03484400
H	2.05645800	4.20266100	4.78045700
H	0.62522700	-2.97980300	-0.85011500
C	4.63952900	-1.66673600	0.28258000
C	6.14596700	-1.50721900	0.15113600
C	6.73015300	-1.17562000	-1.08174600
C	5.86947900	-0.89135300	-2.30052900
C	4.43317800	-1.40207200	-2.13207000
H	6.50101000	-1.98466900	2.22295900
H	4.28327800	-1.24283800	1.22749000
C	6.95939400	-1.73072900	1.26936300
C	8.12558500	-1.07626500	-1.16669300
H	5.84442700	0.19176900	-2.49282500
H	4.40291600	-2.49538200	-2.19901300
C	8.93065900	-1.30251800	-0.05310400
C	8.34494800	-1.63127100	1.17260100
H	8.58199300	-0.81913100	-2.11992800
H	10.01039600	-1.22345000	-0.13947600
H	8.96467600	-1.80536200	2.04729100
N	3.88301600	-1.03182500	-0.81278200
H	3.92957700	-0.01769200	-0.70030800
H	4.37010300	-2.73124200	0.28482800
H	3.77782900	-0.99969600	-2.91228900
H	6.31121500	-1.34510800	-3.19606200

24

Zero-point correction= 0.789987 (Hartree/Particle)

Thermal correction to Energy= 0.835338

Thermal correction to Enthalpy= 0.836282

Thermal correction to Gibbs Free Energy= 0.703446

E(Solv)= -2434.14645737

C	-2.48361900	4.11957100	0.64880700
O	-3.57070300	3.30690000	0.14772300
C	-3.06649200	2.07664700	-0.10668400
C	-1.22066700	3.29360300	0.29636400
H	-2.53355900	5.09132600	0.15653800
H	-2.62654900	4.23830100	1.72758700
H	-0.55290800	3.21995700	1.15873200
N	-1.78565700	1.95287200	0.01332900
C	-4.07557800	1.09420800	-0.57030200
C	-5.28627900	1.64890000	-1.02942600
C	-3.89554700	-0.31335600	-0.62423000
C	-6.29735400	0.85273500	-1.55776600
H	-5.42179200	2.72179300	-0.97889600
C	-4.93175200	-1.09190000	-1.16298600
C	-6.11819200	-0.52611000	-1.63030700
H	-7.21538600	1.31171000	-1.91192000
H	-4.80946600	-2.16826600	-1.21716500
H	-6.89521100	-1.16393000	-2.04179700
P	-2.38758900	-1.17085600	0.03995100
Pd	-0.48166700	0.19490300	0.06594700
C	-0.44090500	3.86123600	-0.88282700
C	-0.70343500	3.48290300	-2.20499300
C	0.52334900	4.84989200	-0.64042400
C	-0.01514800	4.08188900	-3.26318800
H	-1.44077700	2.71280500	-2.40973900

C	1.20685500	5.45304800	-1.69706100
H	0.74298100	5.14598800	0.38269300
C	0.93975800	5.06903400	-3.01349200
H	-0.23268700	3.78074100	-4.28454800
H	1.94696500	6.22185800	-1.49222900
H	1.46907400	5.53907600	-3.83763600
C	-2.36677200	-2.73438100	-0.94424500
C	-2.61571300	-3.99670000	-0.38688800
C	-2.03047000	-2.64919300	-2.30818300
C	-2.53406300	-5.14774500	-1.17711600
H	-2.87985000	-4.08567300	0.66206000
C	-1.96383500	-3.79697400	-3.09665300
H	-1.82855500	-1.67754600	-2.75413700
C	-2.21287000	-5.05171400	-2.53114500
H	-2.73136600	-6.11875100	-0.73124400
H	-1.71740200	-3.71364000	-4.15184000
H	-2.15805600	-5.94682400	-3.14420600
C	-2.90656500	-1.69702800	1.73400600
C	-4.24554500	-1.83312400	2.13292000
C	-1.89164200	-1.97718100	2.66531200
C	-4.55895200	-2.24414200	3.43014600
H	-5.04913400	-1.61467500	1.43740300
C	-2.20695900	-2.39847800	3.95739100
H	-0.85261500	-1.85471300	2.37201100
C	-3.54256900	-2.53029200	4.34334000
H	-5.59998300	-2.33966600	3.72585700
H	-1.41101300	-2.61312500	4.66531600
H	-3.79009300	-2.84895900	5.35192100
C	1.57311700	0.76326900	0.31445200
C	1.42076200	-0.67097800	0.27775600
H	1.90371700	1.25430600	-0.60663700
H	1.52403200	-1.21678500	1.21778900
C	1.93600000	-1.43302200	-0.91177100
C	1.54955600	-2.90540000	-0.96178700
H	1.64668100	-0.93196600	-1.84063400
H	2.04010600	-3.44763200	-1.77712300
H	1.76480600	-3.41583400	-0.01743600
C	1.89095200	1.53889700	1.53712600
C	2.56763900	2.76873200	1.42544900
C	1.55204400	1.09711500	2.83292800
C	2.89568500	3.52223000	2.55357200
H	2.83616500	3.13739600	0.43810900
C	1.88305500	1.84784200	3.95928600
H	1.00522400	0.16630200	2.95736400
C	2.55750400	3.06557500	3.82852000
H	3.42318200	4.46523400	2.43466500
H	1.60749500	1.48309000	4.94545600
H	2.81336100	3.64904100	4.70812500
H	0.47182700	-2.96556100	-1.12768200
C	4.25909400	-1.95176500	0.15432400
C	5.74912100	-1.68705300	0.08446900
C	6.37031100	-1.29465100	-1.11083700
C	5.55270700	-1.03334900	-2.36272500
C	4.14661500	-1.62367700	-2.28273700
H	6.02895800	-2.17614600	2.16659600
H	3.83251100	-1.58783900	1.09152800
C	6.51643700	-1.87852200	1.24110100
C	7.75808200	-1.10280800	-1.12441200
H	5.48165800	0.04885400	-2.54703700
H	4.16260500	-2.71438700	-2.34474300
C	8.51873500	-1.30184700	0.02474800
C	7.89554900	-1.69130900	1.21373000
H	8.24317500	-0.79527700	-2.04770400
H	9.59382100	-1.15253700	-0.00501200
H	8.48090600	-1.84255900	2.11547200
N	3.51821600	-1.27120100	-0.96172400
H	3.63862000	-0.26126100	-0.81513200
H	4.03479400	-3.01948100	0.06972400
H	3.49874000	-1.23822200	-3.07402900
H	6.05122400	-1.45389100	-3.24363000

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Zero-point correction= 0.587750 (Hartree/Particle)

Thermal correction to Energy= 0.624616

Thermal correction to Enthalpy= 0.625560

Thermal correction to Gibbs Free Energy= 0.511320

E(Solv)= -2029.15848187

C	-4.75685800	0.35909700	-0.74710000
O	-4.04112900	-0.61857900	-1.53617300
C	-2.72164600	-0.48406000	-1.23310800
C	-3.66480400	0.99991500	0.15946700
H	-5.21402800	1.08027600	-1.43068900
H	-5.53840100	-0.16304600	-0.19048500
H	-3.79706800	0.69017800	1.20257000
N	-2.41428600	0.38145500	-0.33285200
C	-1.81665700	-1.33773700	-2.03603300
C	-2.24525600	-1.64311200	-3.33778600
C	-0.57313000	-1.83587300	-1.56514800

C	-1.45031500	-2.39582700	-4.19907900
H	-3.20820900	-1.27311300	-3.67144000
C	0.20339100	-2.59657800	-2.44959500
C	-0.21844600	-2.86791600	-3.75341300
H	-1.79406200	-2.60853800	-5.20722500
H	1.15623300	-2.98912100	-2.11254400
H	0.41588800	-3.45600300	-4.41130200
P	0.02062100	-1.46555200	0.16211000
Pd	-0.36901000	0.80360000	0.61248900
C	-3.66092200	2.51553300	0.10495300
C	-3.18134200	3.19683100	-1.02153200
C	-4.19847900	3.25328200	1.16475300
C	-3.23879800	4.58874900	-1.08351000
H	-2.74161500	2.63573500	-1.84177400
C	-4.26182100	4.64733900	1.10304100
H	-4.56608800	2.73463200	2.04775600
C	-3.78172100	5.31836700	-0.02206300
H	-2.85498800	5.10544500	-1.95923200
H	-4.67986800	5.20630300	1.93595100
H	-3.82457700	6.40303000	-0.07090100
C	1.68622900	-2.26400800	0.22246800
C	1.89791400	-3.62629500	0.49211200
C	2.79783300	-1.43179900	0.01355500
C	3.19357900	-4.14363200	0.53816400
H	1.05251700	-4.28332000	0.67347600
C	4.09290800	-1.95278100	0.05211400
H	2.64820800	-0.36956500	-0.15497400
C	4.29217700	-3.30949900	0.31453000
H	3.34452600	-5.19883100	0.75185100
H	4.94028900	-1.29094300	-0.10448500
H	5.29983900	-3.71518100	0.35476500
C	-1.03196800	-2.60564700	1.17669700
C	-1.66479100	-3.75054600	0.66733900
C	-1.19987200	-2.29107300	2.53591800
C	-2.44037400	-4.56331000	1.49800800
H	-1.55563100	-4.01021700	-0.38169200
C	-1.96721800	-3.10838500	3.36687400
H	-0.73166600	-1.39452000	2.93446500
C	-2.59098900	-4.24600100	2.84914500
H	-2.92556600	-5.44521900	1.08747300
H	-2.08450300	-2.85160500	4.41653400
H	-3.19459900	-4.87920100	3.49411000
C	3.48712900	1.98449100	1.10922200
C	2.23021600	2.33884200	0.75220300
H	3.62258500	1.51732700	2.08570100
H	2.05774100	2.81268500	-0.21468500
C	1.03990800	2.14798800	1.57500300
C	-0.18713500	2.80681600	1.30441700
H	1.22560000	1.78120700	2.58542200
C	4.71258000	2.13503900	0.32241600
C	5.93377700	1.68325500	0.86468700
C	4.75055600	2.70820000	-0.96691000
C	7.13132100	1.79537200	0.15974400
H	5.93396800	1.24098100	1.85873800
C	5.94622400	2.82109500	-1.67011400
H	3.83358200	3.07090700	-1.42255600
C	7.14650500	2.36574900	-1.11442800
H	8.05500500	1.43815900	0.60880100
H	5.94289700	3.26855100	-2.66122800
H	8.07774900	2.45614900	-1.66707900
H	-0.88742900	2.99558700	2.11613900
H	-0.25238100	3.51611300	0.47969100

26-ts

Zero-point correction= 0.952594 (Hartree/Particle)

Thermal correction to Energy= 1.008496

Thermal correction to Enthalpy= 1.009440

Thermal correction to Gibbs Free Energy= 0.847905

E(Solv)= -2821.34636531

C	4.50694600	3.51732300	1.52988000
O	5.27821800	2.79211100	0.54099200
C	4.47317700	1.84453300	0.01104200
C	3.06365900	2.96783200	1.36598400
H	4.93502600	3.29966600	2.51206300
H	4.59991900	4.58354400	1.31526300
H	2.42423100	3.70471000	0.86683800
N	3.24825100	1.84292400	0.41870200
C	5.12585200	0.97854900	-0.99790000
C	6.30510600	1.48692600	-1.56993900
C	4.64376600	-0.29393900	-1.40864100
C	6.99974100	0.77890800	-2.54737500
H	6.67021000	2.45328100	-1.24428300
C	5.36698900	-0.98957400	-2.38694700
C	6.52804500	-0.46415900	-2.95861300
H	7.90202600	1.20005000	-2.98012100
H	5.01748900	-1.96326000	-2.71181900
H	7.05788900	-1.03155800	-3.71835400
P	3.11072000	-1.05525600	-0.68934800

Pd	1.54788900	0.66723000	-0.30220300
C	2.41097600	2.56982300	2.67560600
C	2.74734100	1.37403800	3.32440600
C	1.49572700	3.43807200	3.28336400
C	2.17376400	1.05331200	4.55532700
H	3.44890600	0.68558200	2.86215000
C	0.92637800	3.12124300	4.51883000
H	1.22952700	4.36919800	2.78811800
C	1.26335500	1.92620100	5.15696100
H	2.44224000	0.12123800	5.04505700
H	0.22252800	3.80783600	4.98117900
H	0.82287700	1.67816400	6.11862100
C	3.71919200	-1.91037000	0.82649600
C	5.06414400	-2.25673000	1.03061100
C	2.77636800	-2.22899800	1.81882700
C	5.45514500	-2.91122800	2.20111400
H	5.80950200	-2.01742800	0.27832700
C	3.16793600	-2.89224700	2.98214500
H	1.73530700	-1.95016800	1.67825000
C	4.50912400	-3.23218400	3.17644000
H	6.49966300	-3.17134700	2.34824100
H	2.42759900	-3.13714000	3.73888700
H	4.81606400	-3.74226600	4.08516100
C	2.70090300	-2.41661500	-1.86048000
C	1.96396700	-2.08474100	-3.01059700
C	3.06258200	-3.75520700	-1.64725600
C	1.61771400	-3.06636200	-3.93857500
H	1.66596300	-1.05194800	-3.17632900
C	2.70130900	-4.73906800	-2.57140300
H	3.62744400	-4.03252500	-0.76277400
C	1.98407900	-4.39720100	-3.71890300
H	1.05866100	-2.79454600	-4.82993300
H	2.98714300	-5.77231600	-2.39479000
H	1.70985500	-5.16370800	-4.43832400
C	-0.19758300	1.92985700	-0.23252300
C	-0.53021600	0.71411400	-0.91447600
H	-0.46477800	1.98197800	0.82463300
H	-0.64859300	0.71119000	-1.99727100
C	-0.84131300	-0.48077600	-0.21185900
C	-1.31643800	-1.68847300	-0.76126400
H	-0.82605500	-0.40742400	0.87778400
C	-0.10912600	3.24764600	-0.89426100
C	-0.37488800	4.41312000	-0.15008800
C	0.24107700	3.40006700	-2.25094900
C	-0.29688500	5.67780100	-0.73354600
H	-0.65761900	4.31812300	0.89612400
C	0.31453900	4.66273600	-2.83469300
H	0.47578300	2.52263800	-2.84769100
C	0.04728200	5.80933700	-2.08022400
H	-0.51263900	6.56055800	-0.13739600
H	0.58699100	4.75408600	-3.88280200
H	0.10693000	6.79249000	-2.53800200
H	-1.18519500	-2.57973900	-0.14529700
H	-1.11999700	-1.86299300	-1.82176100
C	-6.48350200	1.03688500	-0.61098500
C	-5.96854100	-0.01664400	-1.26894200
H	-5.78697000	1.69709400	-0.09088100
H	-6.61917900	-0.69109300	-1.82354800
C	-4.49144400	-0.29179600	-1.36550900
C	-4.01715400	-0.32982700	-2.82528200
H	-3.94406500	0.50325100	-0.84636300
H	-2.96345700	-0.61371400	-2.90317200
C	-7.89202800	1.43798900	-0.50388900
C	-8.20914500	2.57413000	0.26169500
C	-8.94363600	0.74111200	-1.12912400
C	-9.52847800	3.00125200	0.40350500
H	-7.40890400	3.12659100	0.74896200
C	-10.26057400	1.16667000	-0.98810200
H	-8.73320000	-0.13675400	-1.73329800
C	-10.55917600	2.29794000	-0.22095900
H	-9.75045000	3.88195100	0.99927100
H	-11.05896500	0.61729800	-1.47890300
H	-11.58861200	2.62750100	-0.11436700
H	-4.13521800	0.66985100	-3.25301900
C	-4.30725200	-1.42578800	0.83884500
C	-3.99186500	-2.68843100	1.61463300
C	-3.88028300	-3.93398800	0.98156500
C	-3.99899300	-4.03662300	-0.52418200
C	-4.67880700	-2.81550700	-1.14327300
H	-3.94117200	-1.63326400	3.49498700
H	-3.67807000	-0.59829200	1.18762100
C	-3.85096000	-2.60143300	3.00671700
C	-3.62870800	-5.07392100	1.75752400
H	-3.00363600	-4.16434600	-0.97051800
H	-5.74915600	-2.80607300	-0.90550100
C	-3.49202000	-4.98377100	3.14001300
C	-3.60408200	-3.73993500	3.76873500
H	-3.54336200	-6.04085300	1.26692000

H	-3.30282200	-5.87814600	3.72644700
H	-3.50028700	-3.65932700	4.84681700
N	-4.06880500	-1.55711600	-0.62481500
H	-5.35074000	-1.12316100	0.99013100
H	-4.57007400	-2.82969600	-2.22899000
H	-4.57418500	-4.92758400	-0.80233700
H	-2.81453500	-1.60465200	-0.72300500
H	-4.61190300	-1.01511500	-3.43759900

27-ts

Zero-point correction= 0.951465 (Hartree/Particle)

Thermal correction to Energy= 1.007413

Thermal correction to Enthalpy= 1.008357

Thermal correction to Gibbs Free Energy= 0.851572

E(Solv)= -2821.34226348

C	4.28065800	1.95014600	-2.64550600
O	4.04839100	0.58727600	-3.06655000
C	3.09063200	0.07437800	-2.25562800
C	3.30055700	2.15160600	-1.45110000
H	5.33033500	2.04388300	-2.35763100
H	4.07316100	2.60432800	-3.49548400
H	2.54750300	2.90776000	-1.70319500
N	2.61391700	0.84213400	-1.34069000
C	2.74829600	-1.33395900	-2.55914500
C	3.76941200	-2.10086700	-3.14415000
C	1.46635700	-1.90921100	-2.35083300
C	3.55912800	-3.42706700	-3.51232400
H	4.73503800	-1.63943300	-3.31418000
C	1.27118500	-3.23428600	-2.76556600
C	2.30033900	-3.99123800	-3.33048900
H	4.36749900	-4.00232100	-3.95320400
H	0.29400100	-3.68866700	-2.66297000
H	2.10527900	-5.01514700	-3.63639900
P	0.07888100	-0.94573700	-1.56194000
Pd	0.83697800	0.24817000	0.37966900
C	4.00562900	2.57588000	-0.17502100
C	4.74829400	1.65727600	0.58040300
C	3.97059700	3.91554400	0.23006200
C	5.43476700	2.07254900	1.72211500
H	4.77550200	0.61167500	0.28580600
C	4.66172300	4.33400500	1.36960900
H	3.40205500	4.63949500	-0.35037000
C	5.39391000	3.41213300	2.11955200
H	5.99920500	1.34781800	2.30206700
H	4.62578900	5.37725000	1.67023300
H	5.93118100	3.73506400	3.00668700
C	-1.38295700	-2.08168000	-1.65003400
C	-2.53036000	-1.73674200	-2.38101200
C	-1.38964100	-3.29219500	-0.93309300
C	-3.64770800	-2.57542700	-2.39154000
H	-2.56011700	-0.81338900	-2.94773500
C	-2.49993100	-4.13492200	-0.95678600
H	-0.51074500	-3.59799800	-0.37589500
C	-3.63739100	-3.77572700	-1.68346200
H	-4.52728000	-2.28483600	-2.95813200
H	-2.47578900	-5.07228200	-0.40759100
H	-4.50751800	-4.42494400	-1.69416600
C	-0.31735800	0.31591000	-2.85401600
C	-0.03732500	0.10348600	-4.21310900
C	-0.96971500	1.49725900	-2.46971800
C	-0.39324900	1.06110700	-5.16474300
H	0.45444300	-0.80920300	-4.53483100
C	-1.33661700	2.44686900	-3.42550800
H	-1.19401300	1.67270500	-1.42185000
C	-1.04384800	2.23366100	-4.77405200
H	-0.16783800	0.88576000	-6.21293400
H	-1.85285300	3.35089600	-3.11392500
H	-1.32450500	2.97424100	-5.51763800
C	-3.65337000	-1.81465400	2.36991400
C	-2.52278200	-1.08986400	2.35531600
H	-3.76109700	-2.57571700	3.14530000
H	-2.34715300	-0.33862300	1.58689500
C	-1.48464000	-1.16745100	3.44513000
C	-1.53524000	0.10651700	4.30666900
H	-1.72235200	-2.01916900	4.10179900
H	-0.91312500	0.03954100	5.20332500
H	-1.23825200	0.99356300	3.74016000
C	-4.80154200	-1.70047100	1.45900000
C	-5.75067600	-2.73755100	1.42933100
C	-5.01169200	-0.58136400	0.63206900
C	-6.85929400	-2.67442700	0.58622700
H	-5.61350200	-3.60189300	2.07521000
C	-6.12005200	-0.51613900	-0.20817900
H	-4.32025800	0.25585500	0.66520900
C	-7.04669000	-1.56331000	-0.23813300
H	-7.58097300	-3.48655500	0.58082100
H	-6.27084300	0.36167200	-0.83063400
H	-7.91594200	-1.50481600	-0.88716000

H	-2.56818000	0.25163000	4.63437900
C	0.96439500	-1.24143800	3.88032700
C	2.33142800	-1.71783800	3.43748800
C	2.47941100	-2.67180300	2.42381400
C	1.26161500	-3.16370100	1.67514900
C	-0.04827900	-2.85693200	2.39801800
H	3.34573600	-0.49329800	4.89546600
H	1.01231400	-0.18213500	4.13027600
C	3.46412000	-1.23159900	4.10501600
C	3.76289500	-3.12629400	2.09272400
H	1.24755300	-2.69962000	0.68091000
H	-0.15918600	-3.51268200	3.27554700
C	4.88619400	-2.64489000	2.76126000
C	4.73617300	-1.69185600	3.77362300
H	3.87676600	-3.87087000	1.30786900
H	5.87353600	-3.01544900	2.50090800
H	5.60527100	-1.31495000	4.30511700
N	-0.10903900	-1.44756300	2.87292000
H	0.11617100	-0.58492600	1.67966600
H	0.66765200	-1.77315900	4.79999500
H	-0.90753200	-3.02298700	1.74719400
H	1.32216300	-4.24746600	1.51364000
C	-1.54481200	3.68421900	0.45207000
C	-0.90367200	2.79085700	1.24387200
H	-0.96412900	4.15550800	-0.34213500
H	-1.42813600	2.31709100	2.06965000
C	0.49803800	2.45954000	1.07539800
C	1.28257800	1.76015400	1.98042000
H	1.00003800	2.96544800	0.25134500
C	-2.93845200	4.11643700	0.53336700
C	-3.37854300	5.14322300	-0.32460100
C	-3.87350900	3.55103700	1.42506800
C	-4.69685900	5.59318300	-0.29376300
H	-2.67041100	5.59667500	-1.01467700
C	-5.19018300	3.99882100	1.45406900
H	-3.57044800	2.75512600	2.09932500
C	-5.60840200	5.02214900	0.59599600
H	-5.01172100	6.38977600	-0.96174100
H	-5.89552900	3.55024500	2.14794200
H	-6.63692100	5.37002500	0.62329400
H	2.36471300	1.82546600	1.93678800
H	0.85671800	1.46582300	2.93335900

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Zero-point correction= 0.598740 (Hartree/Particle)
Thermal correction to Energy=0.635753
Thermal correction to Enthalpy= 0.636697
Thermal correction to Gibbs Free Energy= 0.522630
E(Solv) =-2029.61102079

C	0.98111300	-3.35239600	2.25932600
O	2.24622900	-2.76112800	1.87278500
C	1.99259900	-1.85402900	0.91351000
C	-0.01687300	-2.83519800	1.18667000
H	1.10086600	-4.43628500	2.25897600
H	0.74897600	-3.00256400	3.26883500
H	-0.87570100	-2.35788100	1.66855800
N	0.77289400	-1.78704600	0.48407900
C	3.18469900	-1.10430100	0.45745400
C	4.41465600	-1.77439700	0.55255700
C	3.14748600	0.21925900	-0.04759800
C	5.59501300	-1.17010800	0.12366500
H	4.43769200	-2.77930400	0.95780600
C	4.34625000	0.81232600	-0.46211600
C	5.56038100	0.12472300	-0.38680300
H	6.53334300	-1.71161700	0.19189800
H	4.33556700	1.82537300	-0.84829400
H	6.47284900	0.60837600	-0.72240700
P	1.57227600	1.17577000	-0.13614900
Pd	-0.06473900	-0.24876100	-0.87502800
C	-0.51459800	-3.93119800	0.25814600
C	0.28980700	-4.43864700	-0.77194800
C	-1.77299800	-4.50463400	0.48262800
C	-0.16265400	-5.49358900	-1.56635000
H	1.26874400	-4.00614600	-0.96105300
C	-2.22453500	-5.56262400	-0.30916500
H	-2.40321600	-4.12696600	1.28573100
C	-1.42052600	-6.05739600	-1.33737400
H	0.46860900	-5.87676200	-2.36304600
H	-3.20252600	-5.99687700	-0.12322100
H	-1.77034900	-6.87851700	-1.95596700
C	1.95688700	2.66703000	-1.12648300
C	2.36193800	3.86603400	-0.51941100
C	1.86616400	2.59676800	-2.52638100
C	2.67192600	4.97751500	-1.30591900
H	2.42865900	3.93865700	0.56148400
C	2.18708600	3.70682100	-3.30632400
H	1.53700400	1.67782600	-3.00361500
C	2.58770600	4.89901900	-2.69701100

H	2.97597100	5.90449600	-0.82863900
H	2.11387000	3.64421600	-4.38810700
H	2.82729800	5.76613700	-3.30554400
C	1.25103100	1.74994700	1.57578200
C	2.27064800	1.84488200	2.53618800
C	-0.05903800	2.12706100	1.91820300
C	1.98138200	2.31410400	3.81925700
H	3.28762300	1.55673700	2.28803100
C	-0.33940500	2.60138200	3.19934100
H	-0.85583700	2.04848500	1.18312900
C	0.67934800	2.69340800	4.15134100
H	2.77535900	2.38431500	4.55708300
H	-1.35355300	2.89473300	3.45465100
H	0.45840300	3.05852800	5.15011200
H	-0.52119900	0.92608900	-1.76463300
C	-4.12660500	0.03296500	-0.13156600
C	-3.23717300	-0.09344900	-1.14710300
H	-4.08935000	-0.71559700	0.66141000
H	-3.22560700	0.61576700	-1.97159800
C	-2.28925700	-1.18547600	-1.20827400
C	-1.44155100	-1.45915500	-2.26277000
H	-2.34549300	-1.91434500	-0.40133900
C	-5.15778600	1.05114700	0.03716700
C	-5.99831000	0.97770700	1.16541800
C	-5.35692000	2.10737500	-0.87626600
C	-7.00087400	1.92094500	1.37731300
H	-5.86071300	0.16732700	1.87760500
C	-6.35751400	3.04883000	-0.66357000
H	-4.72858100	2.19129700	-1.75796200
C	-7.18351500	2.96011700	0.46294500
H	-7.63988900	1.84448000	2.25217900
H	-6.49871500	3.85488700	-1.37780600
H	-7.96529600	3.69680600	0.62338400
H	-0.92447700	-2.41222200	-2.31077100
H	-1.49247200	-0.88127100	-3.18102900

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Zero-point correction= 0.597488 (Hartree/Particle)

Thermal correction to Energy= 0.633958

Thermal correction to Enthalpy= 0.634903

Thermal correction to Gibbs Free Energy= 0.522858

E(Solv)= -2029.60512671

C	1.65035900	1.76842600	2.51088500
O	0.26295600	2.18088200	2.59993700
C	-0.36949600	1.66954500	1.52941700
C	1.79818200	1.35536200	1.02997700
H	2.27298200	2.61290800	2.80481700
H	1.78993000	0.93383000	3.20539300
H	2.36147100	0.42212200	0.94095400
N	0.38761400	1.10956300	0.63550800
C	-1.82955500	1.91426100	1.51817100
C	-2.26948900	3.02339000	2.26189900
C	-2.77672600	1.13629300	0.80659200
C	-3.61368600	3.38782400	2.28276600
H	-1.54454100	3.60802500	2.81507800
C	-4.12434600	1.51631700	0.84760000
C	-4.54392800	2.63497000	1.57087900
H	-3.92682100	4.25660900	2.85331700
H	-4.85952600	0.92946300	0.30804300
H	-5.59503200	2.90766000	1.57831100
P	-2.28630800	-0.38178400	-0.11447700
Pd	-0.19725200	-0.08184300	-1.08341700
C	2.46981200	2.43048500	0.18079500
C	1.75182300	3.31711100	-0.62957600
C	3.86442800	2.56731600	0.26519500
C	2.41673700	4.31514400	-1.34916400
H	0.67272100	3.22843100	-0.70760100
C	4.52655600	3.56724800	-0.44682800
H	4.43599400	1.88922300	0.89634200
C	3.80281800	4.44325500	-1.26059700
H	1.84594100	4.99583000	-1.97459800
H	5.60579800	3.66214900	-0.36772000
H	4.31694900	5.22068600	-1.81788600
C	-3.70003600	-0.75131200	-1.22157900
C	-4.70700400	-1.66174700	-0.86662100
C	-3.77093700	-0.09320900	-2.46107400
C	-5.76826400	-1.90729600	-1.74110000
H	-4.66320500	-2.18328800	0.08429500
C	-4.83783700	-0.33407900	-3.32532000
H	-2.98989600	0.60592400	-2.74989800
C	-5.83654600	-1.24408700	-2.96727200
H	-6.53977000	-2.61895800	-1.46192800
H	-4.88545600	0.18076000	-4.28049600
H	-6.66237300	-1.43870000	-3.64526900
C	-2.25694800	-1.71319500	1.14968400
C	-2.92208600	-1.59926500	2.38069300
C	-1.55081000	-2.89290100	0.85671700
C	-2.88171000	-2.65014100	3.29952300

H	-3.47179700	-0.69607100	2.62628700
C	-1.52056800	-3.94215300	1.77452100
H	-1.02658700	-2.98864300	-0.09055400
C	-2.18376900	-3.82101900	2.99831200
H	-3.39815900	-2.55209500	4.24999200
H	-0.97540400	-4.85105500	1.53688800
H	-2.15482000	-4.63619800	3.71540400
H	-0.65877900	-0.89443200	-2.36005500
C	3.86445200	-0.85841100	-1.01601700
C	2.66032900	-1.18127200	-1.54883000
H	4.18239800	0.18088800	-1.09377800
H	2.31864900	-2.21555300	-1.54288200
C	1.79356700	-0.21949600	-2.20902100
C	0.77981400	-0.62170000	-3.10469800
H	2.12441600	0.81651500	-2.24222100
C	4.82391300	-1.75169700	-0.37044500
C	6.08924900	-1.23974300	-0.02152700
C	4.54883700	-3.10289000	-0.07538600
C	7.04750700	-2.04422600	0.59112900
H	6.32121100	-0.20151000	-0.24774100
C	5.50517400	-3.90510500	0.53749000
H	3.58031000	-3.52799500	-0.32291500
C	6.75866600	-3.38064100	0.87284000
H	8.01872000	-1.63006700	0.84598800
H	5.27595900	-4.94411900	0.75651300
H	7.50273400	-4.01137600	1.35040100
H	0.40634300	0.09064400	-3.83505300
H	0.74002400	-1.66225600	-3.42130900

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Zero-point correction= 0.072584 (Hartree/Particle)
Thermal correction to Energy= 0.076262
Thermal correction to Enthalpy= 0.077206
Thermal correction to Gibbs Free Energy= 0.046350
E(Solv)= -226.290238920

C	-1.09736900	-0.36702400	-0.00013100
C	-0.68448900	0.98352300	0.00003000
C	0.69087500	0.91869300	0.00001500
N	1.00481500	-0.39775600	0.00005000
H	1.92334000	-0.81383600	0.00012000
H	-2.10307100	-0.76357000	-0.00022400
H	-1.29867600	1.87032100	0.00004700
H	1.45258400	1.68385000	0.00003800
N	-0.06599800	-1.20051800	0.00002700

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Zero-point correction= 0.242891 (Hartree/Particle)
Thermal correction to Energy= 0.256024
Thermal correction to Enthalpy= 0.256968
Thermal correction to Gibbs Free Energy=0.200742
E(Solv)= -613.524318877

C	3.83431000	-1.43233200	-0.65043800
C	2.53695300	-0.93298800	-0.72021700
C	2.18055000	0.24829100	-0.04241400
C	3.17666900	0.90935300	0.69781300
C	4.47685700	0.41051800	0.76860700
C	4.81145600	-0.76455200	0.09479700
H	4.08690300	-2.34554900	-1.18282600
H	1.79658000	-1.46278200	-1.31239600
H	2.92233600	1.82581100	1.22572400
H	5.22730500	0.94053600	1.34906200
H	5.82350900	-1.15663200	0.14533900
C	0.82527000	0.82209200	-0.07044900
H	0.73489700	1.78077100	0.43774500
C	-0.26790400	0.29413900	-0.64132600
H	-0.21283200	-0.66980000	-1.14513800
C	-1.63978700	0.92471500	-0.67751500
C	-1.77589600	2.27864900	0.02868900
H	-1.52099400	2.20183500	1.09107000
H	-1.12292800	3.02528100	-0.43525200
H	-1.93086900	1.05437400	-1.72741900
C	-4.54819600	-0.94213600	0.00902000
C	-3.77490600	-1.45220800	1.07440400
C	-2.54644100	-0.83379300	0.93241700
N	-2.63485000	-0.02953100	-0.16261700
H	-5.57336600	-1.17180100	-0.25243600
H	-4.06240900	-2.17120700	1.82797300
H	-1.63191100	-0.90672500	1.50290500
N	-3.85938400	-0.07709300	-0.73617600
H	-2.81020300	2.62377000	-0.05311900

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Zero-point correction= 0.080563 (Hartree/Particle)
Thermal correction to Energy= 0.086904
Thermal correction to Enthalpy= 0.087849
Thermal correction to Gibbs Free Energy= 0.047779
E(Solv)= -687.146831365

C	-1.25418700	1.15572400	-0.00018800

C	-2.48350500	0.46421100	0.00072000
C	-2.13479700	-0.87455500	0.00045000
N	-0.78036100	-0.91872500	-0.00081700
H	-1.07099800	2.22146300	-0.00039700
H	-3.47992800	0.88003200	0.00132600
H	-2.73118800	-1.77538700	0.00067200
N	-0.22479600	0.30943100	-0.00095900
H	-0.17432100	-1.72710300	0.00013700
H	1.52704600	0.28832300	-0.00115500
Cl	2.83531900	-0.00556200	0.00035100

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Zero-point correction= 1.026275 (Hartree/Particle)

Thermal correction to Energy= 1.085781

Thermal correction to Enthalpy= 1.086726

Thermal correction to Gibbs Free Energy=0.926251

E(Solv)= -2906.62424475

Pd	-1.35775700	0.03411200	0.23353200
P	-2.94980200	1.56597200	1.17118100
P	-2.65650100	-1.92484600	-0.44679700
C	-4.75401000	0.97579400	1.14327600
C	-5.45726100	0.57009700	-0.13940900
C	-6.37194900	1.47185500	-0.71018700
C	-7.17207800	1.14273300	-1.80097100
C	-7.10806100	-0.14663000	-2.32183000
C	-6.23408700	-1.06553100	-1.74756800
C	-5.37456000	-0.73541800	-0.68534600
C	-4.52055700	-1.83867700	-0.08967400
C	-2.99147900	3.29794800	0.31315700
C	-2.95029100	3.00903300	-1.20534100
C	-4.23235200	4.16217900	0.61562500
C	-1.74472300	4.12680500	0.68498000
C	-2.73681900	1.77816000	3.09112600
C	-3.10670500	0.43683600	3.76579700
C	-3.60108300	2.89050400	3.71691200
C	-1.25637200	2.04835000	3.42933100
C	-2.53468800	-2.25627600	-2.34418400
C	-2.65611300	-0.87124500	-3.02091000
C	-3.60648900	-3.19166800	-2.93693900
C	-1.15071900	-2.83868800	-2.68745000
C	-2.21734000	-3.53231400	0.53844300
C	-2.82658100	-4.83320500	-0.01752900
C	-0.68281800	-3.67274800	0.59727500
C	-2.71090200	-3.34598000	1.99141900
H	-4.74326200	0.11472100	1.81574100
H	-5.35971700	1.74048800	1.64063700
H	-6.49283900	2.45106600	-0.25936500
H	-7.86224200	1.87532500	-2.20972900
H	-7.74973300	-0.44756800	-3.14510600
H	-6.24340600	-2.08734900	-2.11223700
H	-4.96087300	-2.80391500	-0.36127600
H	-4.56800600	-1.77807100	1.00142600
H	-2.04955000	2.45328100	-1.48326100
H	-3.81886200	2.43391900	-1.53969000
H	-2.94739200	3.96060000	-1.75377300
H	-5.16036100	3.69391200	0.28835200
H	-4.33004600	4.41436700	1.67311700
H	-4.14094100	5.10685400	0.06336200
H	-1.71380100	5.01755300	0.04379400
H	-1.77429600	4.47855600	1.72061800
H	-0.81371200	3.57992700	0.53040100
H	-2.60410400	-0.40980500	3.28708500
H	-2.77796700	0.46601000	4.81236800
H	-4.18426000	0.24691100	3.77558900
H	-4.66412600	2.79422300	3.47255200
H	-3.51525200	2.83361400	4.81025300
H	-3.26781500	3.88917700	3.42169800
H	-0.86994400	2.95953900	2.96786800
H	-1.15655200	2.16361500	4.51664100
H	-0.62214000	1.21308600	3.12251000
H	-2.56850300	-0.99282200	-4.10901900
H	-3.61731700	-0.39175500	-2.81468300
H	-1.86072100	-0.19533900	-2.68939600
H	-3.61857600	-4.17879900	-2.47041500
H	-4.60795500	-2.76744900	-2.87509000
H	-3.38833700	-3.33907700	-4.00314200
H	-1.00881900	-2.79507200	-3.77548100
H	-0.33799000	-2.27865500	-2.22272100
H	-1.05869500	-3.88868500	-2.39351900
H	-2.61261400	-5.65429700	0.67979600
H	-3.91532200	-4.78017000	-0.12708100
H	-2.39617400	-5.11281800	-0.98284300
H	-0.22407000	-2.78820000	1.04629000
H	-0.42527500	-4.54206900	1.21698400
H	-0.22948600	-3.82182500	-0.38399700
H	-2.37550500	-2.39346300	2.41505600
H	-3.80004200	-3.40581700	2.08176200
H	-2.29194800	-4.14725800	2.61331600

C	1.64994600	-0.55380800	1.52996900
C	1.00123100	0.03115200	0.29494400
H	1.53767300	-1.64174100	1.58629100
H	2.72562000	-0.32632800	1.49400600
H	1.22621000	-0.11959200	2.44139100
C	0.35553400	1.29888400	0.35891500
H	0.48152100	1.88428800	1.26364500
H	0.30502100	1.89613700	-0.55286900
C	1.21946700	-0.55095000	-0.97548300
C	2.07768100	-1.64685700	-1.26851200
H	2.27195400	-2.35486700	-0.46108100
H	1.91791800	-2.13401700	-2.23272200
H	0.84467200	0.01900100	-1.82686100
P	5.30037300	-0.13606100	-0.55362100
O	4.60186600	0.34102300	0.68532000
O	4.45392800	-0.59577100	-1.75555400
H	3.22322200	-1.09013600	-1.45564700
O	6.37213800	0.97750700	-1.10407900
O	6.33581600	-1.36031600	-0.26456000
C	5.89800200	2.31327600	-1.29928100
H	5.44413900	2.68126900	-0.36991600
H	5.12353300	2.31641000	-2.07998900
C	7.07555700	3.18602100	-1.71557000
H	7.84458600	3.13474400	-0.93292700
H	7.52418600	2.76204600	-2.62382100
C	6.67418300	4.64604800	-1.96072400
H	6.21609700	5.05713600	-1.04968900
H	5.89650000	4.68564600	-2.73698700
C	7.85491100	5.52892000	-2.37927600
H	7.54082100	6.56566700	-2.54849600
H	8.63474200	5.53778900	-1.60778200
H	8.31281200	5.16281900	-3.30645200
C	7.21738200	-1.25892600	0.86120700
H	7.94537800	-0.45624800	0.68055700
H	6.63929200	-0.99685800	1.75611900
C	7.92545400	-2.59635800	1.03717700
H	8.45321600	-2.84150200	0.10581800
H	7.16854700	-3.37892500	1.18292900
C	8.91038100	-2.59350700	2.21319100
H	9.65683800	-1.80055400	2.06267300
H	8.37494800	-2.33508400	3.13799200
C	9.62585200	-3.93617300	2.39772300
H	10.19841800	-4.20536400	1.50155000
H	10.32325500	-3.90632400	3.24318600
H	8.90794900	-4.74434400	2.58508600

34-ts

Zero-point correction= 1.026397 (Hartree/Particle)

Thermal correction to Energy= 1.085948

Thermal correction to Enthalpy= 1.086892

Thermal correction to Gibbs Free Energy=0.927931

E(Solv)= -2906.61889013

Pd	-1.27489100	0.52403300	0.68596300
P	-1.43029200	1.38341100	-1.53667800
P	-3.39571700	-0.60678000	1.14336400
C	-3.02151400	0.89924600	-2.45731900
C	-3.45365700	-0.54831700	-2.61365500
C	-3.24316300	-1.17409000	-3.85451400
C	-3.71577400	-2.45085800	-4.14466700
C	-4.47157300	-3.12586000	-3.19030700
C	-4.72422200	-2.50835400	-1.96870700
C	-4.21124200	-1.24252500	-1.63662400
C	-4.61976000	-0.63506100	-0.30746100
C	0.00663000	0.83151900	-2.70841600
C	0.26188600	-0.66188100	-2.39951400
C	-0.29493200	0.97587600	-4.21493600
C	1.30225100	1.61646600	-2.41402300
C	-1.61917300	3.31756700	-1.60400200
C	-2.99341600	3.69907200	-1.01044800
C	-1.52371600	3.92477400	-3.01781000
C	-0.55332300	3.97473700	-0.70264300
C	-3.18580200	-2.46292300	1.63791900
C	-2.14098700	-3.04080800	0.65480900
C	-4.45829400	-3.33037500	1.57156700
C	-2.61354500	-2.56782600	3.06531400
C	-4.48620200	0.29490300	2.47027700
C	-5.69687700	-0.50459100	2.98796400
C	-3.58718800	0.68601500	3.66086600
C	-5.01129500	1.61045400	1.85388500
H	-3.80083700	1.43458300	-1.90960000
H	-2.98071200	1.35604800	-3.45170600
H	-2.72511700	-0.62729700	-4.63454400
H	-3.52266600	-2.89346600	-5.11779800
H	-4.88563100	-4.10821100	-3.39953600
H	-5.37025500	-3.01259500	-1.25757200
H	-5.54376000	-1.11710700	0.02973900
H	-4.86327300	0.42029900	-0.45776300
H	0.64637700	-0.80269600	-1.38701200

H	-0.63825600	-1.27153900	-2.52905800
H	1.02696000	-1.04008300	-3.08977600
H	-1.10052700	0.32019400	-4.54465000
H	-0.53859000	1.99749800	-4.51321700
H	0.60277000	0.67991200	-4.77299700
H	2.12286300	1.14455200	-2.96787000
H	1.23892600	2.65784500	-2.74565000
H	1.58773900	1.58838500	-1.36315800
H	-3.16343100	3.21261700	-0.04544300
H	-3.01784400	4.78360200	-0.84270600
H	-3.82831500	3.46091300	-1.67654900
H	-2.23168800	3.47389500	-3.72125900
H	-1.76341700	4.99525200	-2.96115800
H	-0.51871400	3.84237300	-3.43925300
H	0.46834200	3.72666600	-0.99607400
H	-0.66096800	5.06610200	-0.76332600
H	-0.68903100	3.68126700	0.34173500
H	-1.95643100	-4.09408400	0.90707200
H	-2.48415400	-3.00323400	-0.38272700
H	-1.18956600	-2.50670800	0.72158400
H	-5.24663500	-2.98962800	2.24514600
H	-4.87034200	-3.39055500	0.56430200
H	-4.19655000	-4.35465200	1.86917300
H	-2.29189100	-3.60254400	3.24225600
H	-1.74322100	-1.92347100	3.20585100
H	-3.35761600	-2.32547500	3.83036600
H	-6.30524300	0.14506300	3.63186500
H	-6.34725600	-0.85749800	2.18029300
H	-5.39951500	-1.36583500	3.59192300
H	-2.76758500	1.33208000	3.33627100
H	-4.18490100	1.23768500	4.39921900
H	-3.15356800	-0.17862700	4.16817200
H	-4.20683700	2.19206200	1.39397600
H	-5.79562200	1.44667800	1.10843200
H	-5.44857200	2.22616000	2.65056500
C	0.00705200	1.72167800	3.45241700
C	0.32816400	0.71983800	2.35367100
H	-0.61229400	1.28368800	4.24233700
H	0.93591700	2.07402200	3.92217200
H	-0.51428200	2.60184300	3.06136500
C	0.72770900	1.18413100	1.06860300
H	0.87875100	2.25436400	0.95495800
H	1.41080700	0.57472000	0.47961300
C	0.48261400	-0.64503400	2.71610300
C	1.14660700	-1.68640100	2.02286600
H	0.17633400	-0.87506400	3.73950700
P	4.21922500	-0.63119400	0.83903200
O	3.24198900	-0.49542800	-0.29480200
O	3.73058400	-1.28906900	2.14879800
H	2.43729100	-1.46706600	2.20283200
O	5.58671200	-1.39669200	0.37001000
O	4.86719700	0.78640200	1.30102600
C	5.45378700	-2.69239700	-0.22833100
H	4.81831800	-2.61949000	-1.12061800
H	4.96567600	-3.37316600	0.48301700
C	6.84412500	-3.20095400	-0.58657700
H	7.31798600	-2.48023500	-1.26675100
H	7.45623800	-3.22150100	0.32476600
C	6.81729200	-4.59195200	-1.23281200
H	6.19235100	-4.56342500	-2.13688000
H	6.33158800	-5.30285300	-0.54927500
C	8.21368300	-5.10879900	-1.59552700
H	8.16597700	-6.10326600	-2.05434900
H	8.71216900	-4.43693500	-2.30514100
H	8.85161900	-5.18132900	-0.70613200
C	5.43783100	1.64522900	0.30363800
H	6.34463000	1.17615500	-0.10021300
H	4.72498500	1.77328800	-0.52098500
C	5.76617800	2.98276800	0.95435400
H	6.43968500	2.80518300	1.80317300
H	4.84329500	3.40858700	1.37125200
C	6.40642700	3.97478000	-0.02514500
H	7.32367400	3.53553800	-0.44239000
H	5.73100400	4.13498600	-0.87791600
C	6.73781700	5.32390300	0.62191500
H	7.43901300	5.20022400	1.45627600
H	7.19423800	6.01255500	-0.09864600
H	5.83513000	5.80494600	1.01858200
H	1.18273900	-1.63170300	0.93450800
H	0.96017300	-2.69297500	2.40068800

35-ts

Zero-point correction= 1.025876 (Hartree/Particle)

Thermal correction to Energy= 1.085704

Thermal correction to Enthalpy= 1.086648

Thermal correction to Gibbs Free Energy=0.926168

E(Solv)= -2906.60991603

Pd	-1.15091100	0.17145100	0.53162300

P	-2.19064800	2.04091200	-0.71769300
P	-2.92519100	-1.19809400	1.30922000
C	-4.07310800	1.98532500	-0.91135800
C	-4.72954400	0.75043200	-1.49883800
C	-5.24317700	0.83819900	-2.80435100
C	-5.92942300	-0.20890100	-3.41249000
C	-6.15289400	-1.37903700	-2.69167000
C	-5.69037700	-1.46742700	-1.38162200
C	-4.96368400	-0.43685500	-0.76058500
C	-4.62249400	-0.57968100	0.71323100
C	-1.49684700	2.08406700	-2.52373200
C	-1.49306900	0.61733400	-3.01482300
C	-2.31526300	2.93049700	-3.51965300
C	-0.04091000	2.59809300	-2.54465900
C	-1.97673900	3.77899700	0.11027000
C	-2.93045400	3.86080500	1.32313200
C	-2.27159600	4.98119900	-0.80715900
C	-0.53670500	3.89140100	0.65557800
C	-2.88849400	-3.06507800	0.82538300
C	-2.52791200	-3.09956900	-0.67814800
C	-4.19806500	-3.84889600	1.04620500
C	-1.76804100	-3.78002600	1.60465000
C	-3.18072700	-1.01009800	3.22439700
C	-4.22051900	-1.96382900	3.84259300
C	-1.82609900	-1.20939700	3.93160900
C	-3.62122100	0.44241200	3.51410600
H	-4.44252200	2.13764300	0.10679000
H	-4.39079000	2.86243300	-1.48544300
H	-5.12713500	1.76982800	-3.34922800
H	-6.30611000	-0.09763700	-4.42530200
H	-6.70692700	-2.20491500	-3.12884200
H	-5.92778700	-2.35850200	-0.81080200
H	-5.38428900	-1.21086700	1.18368800
H	-4.70866200	0.40081700	1.18621700
H	-0.87503500	-0.01956500	-2.37404600
H	-2.49810500	0.18792000	-3.05026400
H	-1.07483000	0.58071000	-4.02948500
H	-3.33661600	2.56580800	-3.63491000
H	-2.35529800	3.98757300	-3.25060800
H	-1.83955100	2.86410500	-4.50697000
H	0.35430600	2.47639000	-3.56123700
H	0.03231200	3.66110300	-2.29822000
H	0.62957300	2.04346800	-1.88279700
H	-2.84721300	2.98336400	1.97198700
H	-2.66275700	4.73894700	1.92450700
H	-3.97803600	3.98032700	1.02946400
H	-3.26607300	4.92782600	-1.26352600
H	-2.23853600	5.90248700	-0.21011300
H	-1.53153100	5.08907600	-1.60412400
H	0.22637400	3.80050000	-0.12073400
H	-0.40795800	4.87301400	1.13050300
H	-0.33944100	3.12564200	1.41157800
H	-2.45639100	-4.14648400	-1.00276200
H	-3.28181600	-2.60939100	-1.29972500
H	-1.56179800	-2.62426100	-0.86452700
H	-4.45851400	-3.95077900	2.10110100
H	-5.05354100	-3.41208100	0.52923900
H	-4.06645300	-4.86272500	0.64553100
H	-1.62230300	-4.78057400	1.17661600
H	-0.81759100	-3.24949600	1.52843000
H	-2.01850500	-3.91401800	2.66143000
H	-4.39157300	-1.67337100	4.88787700
H	-5.18993600	-1.92613600	3.33454600
H	-3.87539500	-3.00104100	3.85152500
H	-1.09255100	-0.47874000	3.58270100
H	-1.96161900	-1.06877600	5.01238900
H	-1.40548500	-2.20498000	3.77931300
H	-2.96630700	1.16595800	3.01857400
H	-4.65603900	0.64292500	3.22006800
H	-3.55459800	0.62263400	4.59464000
C	1.32223300	-1.32921500	2.31207700
C	0.89099600	-0.80892600	0.96243000
H	0.89000800	-2.30262100	2.55930800
H	2.41842000	-1.42039700	2.27289700
H	1.07142900	-0.62476700	3.10943100
C	1.15022700	0.60251300	0.70743900
H	1.19861000	1.23082900	1.59844100
H	0.51916900	1.07426200	-0.10085400
C	1.03354500	-1.70479700	-0.19679600
C	1.39827800	-2.99796400	-0.16391500
H	1.62155600	-3.52029600	0.76088300
H	1.52299200	-3.56307100	-1.08275300
H	0.89241800	-1.23858200	-1.17105500
P	4.51546900	-0.01156800	-0.13311900
O	4.28657100	-0.66528800	1.19908700
O	3.41195200	0.88861200	-0.70740100
H	2.17595600	0.72594400	0.07883800
O	5.93508400	0.82020000	-0.14578000

O	4.85605800	-1.08347500	-1.31694600
C	6.17313400	1.73431600	0.92697000
H	6.06617200	1.21190900	1.88649500
H	5.42554600	2.54111800	0.89625600
C	7.57643300	2.30743400	0.76984100
H	8.29614800	1.47756500	0.77123800
H	7.65320600	2.78638500	-0.21552500
C	7.93445900	3.31288400	1.87148800
H	7.84323700	2.82697800	2.85343500
H	7.20257100	4.13347700	1.86920000
C	9.34570300	3.89079400	1.71916200
H	9.57520000	4.60600200	2.51790400
H	10.10313700	3.09794200	1.75300800
H	9.45783400	4.41269000	0.76073100
C	5.80118700	-2.12288200	-1.04072400
H	6.80846700	-1.68917800	-0.97210000
H	5.56534600	-2.58584800	-0.07435900
C	5.73343000	-3.14661800	-2.16742300
H	5.92530500	-2.63643300	-3.12096400
H	4.70875800	-3.53916100	-2.22349700
C	6.72747700	-4.29979100	-1.98044800
H	7.74770600	-3.89536200	-1.91671700
H	6.53652100	-4.79446800	-1.01733900
C	6.66184800	-5.33677900	-3.10698500
H	6.88275100	-4.87891600	-4.07913500
H	7.38226600	-6.14795600	-2.94856800
H	5.66290200	-5.78571600	-3.17380000

36-ts

Zero-point correction= 1.025311 (Hartree/Particle)

Thermal correction to Energy= 1.084917

Thermal correction to Enthalpy= 1.085862

Thermal correction to Gibbs Free Energy= 0.926916

E(Solv) = -2906.58650282

P	-2.13873700	-0.69985300	0.63639200
P	-2.40055000	1.25794100	-0.70421600
P	2.60633000	2.27194000	-1.49344100
C	-0.88978100	2.42027500	-0.63599200
C	-0.23757800	2.76985200	0.69351100
C	-0.89531600	3.62948900	1.58865300
C	-0.36443300	3.97907500	2.82811500
C	0.87468500	3.46570900	3.20449900
C	1.57182800	2.66310400	2.30543700
C	1.06495400	2.32379800	1.03648100
C	1.97203200	1.50991300	0.13428300
C	-3.93362100	2.39158300	-0.36078400
C	-4.16775000	2.41106500	1.16771300
C	-3.77091800	3.84026300	-0.86843700
C	-5.21093200	1.79638400	-0.99122300
C	-2.39001600	0.77586100	-2.58164300
C	-0.98921200	0.22681700	-2.93575100
C	-2.69968200	1.93556100	-3.54857500
C	-3.39002200	-0.37978500	-2.80453200
C	3.67645600	0.77166000	-2.09836000
C	2.66896600	-0.19528200	-2.76236200
C	4.44749600	-0.00649100	-1.01319900
C	4.67005600	1.22321000	-3.18638800
C	3.75065700	3.73461600	-0.96902700
C	4.91365200	3.39068100	-0.02382400
C	4.30051100	4.40334600	-2.24960100
C	2.83874100	4.78354400	-0.29055100
H	-0.15276200	1.93018500	-1.26811000
H	-1.16762400	3.33982600	-1.16310000
H	-1.85069300	4.05221200	1.30266600
H	-0.91552700	4.64441300	3.48732900
H	1.30698200	3.70625800	4.17215700
H	2.56030600	2.30050200	2.57893800
H	1.45210400	0.59856500	-0.18011500
H	2.82793500	1.18309500	0.73237900
H	-4.52143100	1.43961000	1.51384100
H	-3.27485300	2.66041900	1.74293600
H	-4.94138700	3.15533900	1.40167800
H	-2.97064100	4.38395000	-0.35971300
H	-3.57994400	3.89351900	-1.94293600
H	-4.70309100	4.38729900	-0.67437300
H	-6.07575000	2.36616300	-0.62472600
H	-5.21950100	1.86657600	-2.08166800
H	-5.36319700	0.75387200	-0.69907800
H	-0.62674400	-0.49720100	-2.20171300
H	-1.05217300	-0.27640300	-3.90985000
H	-0.24323500	1.02029700	-3.03742500
H	-2.02073400	2.78331900	-3.40605800
H	-2.56072100	1.58230100	-4.57928700
H	-3.72755200	2.29888000	-3.46923600
H	-4.42345500	-0.11252300	-2.57785800
H	-3.35022200	-0.68594700	-3.85854800
H	-3.12070100	-1.24648300	-2.19245900
H	3.20680000	-1.07241200	-3.14860100

H	1.91312700	-0.56281900	-2.06221800
H	2.15410300	0.27936500	-3.60470700
H	5.13126800	0.62968000	-0.44310900
H	3.77673000	-0.51161400	-0.31204800
H	5.05259200	-0.78904200	-1.49268100
H	5.07255400	0.33781000	-3.69735900
H	4.19403800	1.85380200	-3.94600600
H	5.52230700	1.76852000	-2.76939900
H	5.42986500	4.31056300	0.28690000
H	4.56854800	2.88869300	0.88697300
H	5.65839900	2.74860500	-0.50488700
H	3.49403900	4.63924200	-2.95350900
H	4.79381900	5.34768400	-1.98086600
H	5.03639800	3.79000800	-2.77249100
H	1.96339800	5.01645200	-0.90816000
H	2.48473700	4.46403000	0.69063900
H	3.40477900	5.71548300	-0.15354800
C	-4.96348300	-2.80672500	0.10000600
C	-5.04505400	-1.62978100	1.04596500
H	-4.17038600	-2.66546400	-0.64277500
H	-4.73190100	-3.73551500	0.63734400
H	-5.91150300	-2.95691000	-0.42551300
C	-6.21894900	-1.01120800	1.27047300
H	-7.13151300	-1.31676500	0.76497600
H	-6.30735700	-0.18727400	1.97411600
C	-3.81851100	-1.19805900	1.76247900
C	-2.79908200	-2.16907500	2.17401000
H	-4.00768100	-0.39395400	2.47415000
P	0.55417900	-2.37996300	0.49999100
O	0.01758500	-1.07475700	-0.06203900
O	-0.40761200	-3.10205800	1.46849700
H	-1.51972600	-2.42664000	1.58809000
O	0.96423800	-3.32548500	-0.73426800
O	1.99065900	-2.20036300	1.23424300
C	1.42428400	-4.67520600	-0.49674800
H	0.68519500	-5.19959400	0.11988200
H	2.37137700	-4.63308000	0.05433000
C	1.60453700	-5.35766900	-1.84457000
H	0.64544700	-5.34378900	-2.37884700
H	2.30976000	-4.76966400	-2.44639900
C	2.10790300	-6.80081100	-1.70536700
H	1.40204700	-7.37692300	-1.09057400
H	3.06203400	-6.80442500	-1.15960900
C	2.29219600	-7.49777400	-3.05762600
H	2.65209300	-8.52494100	-2.93014400
H	1.34714900	-7.54100100	-3.61252600
H	3.01869300	-6.96389500	-3.68222500
C	2.03420400	-1.67304500	2.57967800
H	1.67268600	-0.63717700	2.57039800
H	1.36812300	-2.26728600	3.21536600
C	3.47207300	-1.74349800	3.07358200
H	4.11355400	-1.17262200	2.38917500
H	3.81127400	-2.78677600	3.02610100
C	3.62334800	-1.20673100	4.50355200
H	3.26786500	-0.16729900	4.54326200
H	2.97098000	-1.77771400	5.17901300
C	5.06711900	-1.27209000	5.01292700
H	5.73878600	-0.68244300	4.37710100
H	5.14676600	-0.88298500	6.03422200
H	5.43831400	-2.30412800	5.01864600
H	-2.41556100	-2.01685800	3.18529600
H	-3.05401300	-3.21662900	1.99519900

37-ts

Zero-point correction= 1.024445 (Hartree/Particle)

Thermal correction to Energy= 1.084477

Thermal correction to Enthalpy= 1.085422

Thermal correction to Gibbs Free Energy= 0.923955

E(Solv) = -2906.58726636

Pd	1.47773900	1.58210800	0.18616400
P	3.40886200	0.25177800	0.03891500
P	0.23778300	-3.31330000	-0.90015500
C	3.01065500	-1.52196800	0.59242600
C	2.01222600	-1.64788000	1.72783600
C	2.49079100	-1.75448700	3.04381300
C	1.63590200	-1.80187300	4.14323300
C	0.25954300	-1.72454900	3.93535800
C	-0.23219900	-1.66792200	2.63312400
C	0.61206500	-1.67556400	1.50884100
C	-0.03141900	-1.72889900	0.13707600
C	4.77109500	0.87066500	1.25885400
C	4.04186000	1.37864100	2.52479100
C	5.79347200	-0.20701900	1.67221500
C	5.53563400	2.06611100	0.65383100
C	4.11836100	-0.03695000	-1.72777400
C	2.96082300	-0.61766100	-2.56959100
C	5.30966800	-1.01272200	-1.76678600
C	4.52153600	1.29858600	-2.38761900

C	-1.01399200	-3.00776800	-2.34056800
C	-0.74925300	-1.58760700	-2.89007400
C	-2.50836900	-3.11150600	-1.98876400
C	-0.67266500	-4.00412500	-3.47170500
C	-0.38463100	-4.77650000	0.19460000
C	-1.65079700	-4.53214400	1.03588300
C	-0.60563900	-6.01166200	-0.70349300
C	0.78835600	-5.11049400	1.14686600
H	2.62729600	-2.03310600	-0.29337400
H	3.94695700	-2.02137800	0.85857700
H	3.56374200	-1.80543000	3.20953400
H	2.04291600	-1.88677700	5.14712800
H	-0.42841300	-1.72495600	4.77639100
H	-1.30479800	-1.61609800	2.47122200
H	0.37772700	-0.93665900	-0.50130600
H	-1.09481700	-1.49615900	0.23544400
H	3.39107700	2.22788700	2.29475500
H	3.42688400	0.60948300	2.99714800
H	4.79121000	1.70981400	3.25676600
H	5.33725900	-1.02067000	2.24206100
H	6.31896800	-0.64376300	0.81894000
H	6.54969400	0.25334500	2.32152400
H	6.10150900	2.56255400	1.45297000
H	6.25730400	1.75501100	-0.10628500
H	4.86420000	2.80910100	0.21149100
H	2.08817900	0.04379600	-2.55343400
H	3.29354000	-0.70581900	-3.61189100
H	2.64387300	-1.61364800	-2.24771100
H	5.08055800	-1.97497100	-1.29700100
H	5.57344400	-1.21628800	-2.81305900
H	6.20025500	-0.59613100	-1.28653000
H	5.43476600	1.72201500	-1.96684900
H	4.71068300	1.11872200	-3.45404800
H	3.73092400	2.05031300	-2.31096000
H	-1.30126200	-1.46391900	-3.83195400
H	-1.09190200	-0.80501900	-2.20792500
H	0.31087800	-1.42791700	-3.11444200
H	-2.79971800	-4.12475700	-1.69702200
H	-2.79068000	-2.41941700	-1.18878100
H	-3.10833000	-2.84730200	-2.87162300
H	-1.29077700	-3.78222900	-4.35256500
H	0.37827800	-3.92096400	-3.77080500
H	-0.86059300	-5.04435800	-3.19490100
H	-1.89390000	-5.44335500	1.60151100
H	-1.50440500	-3.73161300	1.76394900
H	-2.52183600	-4.28423400	0.42535600
H	0.25146100	-6.20061100	-1.36032800
H	-0.73747800	-6.89914800	-0.06952600
H	-1.50170600	-5.92226300	-1.32450100
H	1.70317600	-5.33945200	0.58862700
H	1.00810300	-4.29496600	1.84049000
H	0.52966500	-5.99477700	1.74604900
C	0.86036100	3.61290500	-2.57934600
C	1.87114800	4.04593700	-1.54289200
H	0.91001900	2.52594600	-2.72748100
H	-0.17140800	3.82695800	-2.27981500
H	1.05555600	4.09843500	-3.54043900
C	2.94512400	4.79188600	-1.86675700
H	3.11844600	5.13013400	-2.88475300
H	3.67365600	5.10070100	-1.12065700
C	1.67185600	3.65913600	-0.12990300
C	0.34596300	3.51616500	0.45877000
H	2.46844100	4.00023600	0.53187600
P	-2.54810000	1.85823100	-0.27808500
O	-2.38961600	3.02892300	-1.19192400
O	-1.32961900	1.36457900	0.54209000
H	-0.28145500	2.33514600	0.47566300
O	-3.75597500	2.17402200	0.77779300
O	-3.05632800	0.50805200	-1.06134500
C	-4.00746200	1.27675200	1.86933500
H	-3.09916600	1.18023800	2.47638700
H	-4.26073100	0.28202400	1.47671800
C	-5.15932300	1.83694700	2.69383000
H	-4.89137300	2.84745200	3.02964900
H	-6.03960800	1.94599000	2.04627500
C	-5.50380000	0.95583500	3.90171500
H	-4.61497000	0.84649000	4.53948800
H	-5.75738800	-0.05667000	3.55611100
C	-6.66260800	1.51322500	4.73536500
H	-6.88771500	0.86582300	5.59076300
H	-6.42555900	2.51101300	5.12434400
H	-7.57555100	1.60181200	4.13384800
C	-3.96631900	0.64986300	-2.17185200
H	-3.74988100	1.58725000	-2.69505700
H	-3.73671400	-0.18314700	-2.84544800
C	-5.42813100	0.59180200	-1.73424400
H	-5.62775900	1.42243900	-1.04633500
H	-5.59249200	-0.33684800	-1.16981100

C	-6.39423200	0.65480600	-2.92513700
H	-6.21397500	1.57954700	-3.49100500
H	-6.17920000	-0.17314100	-3.61636300
C	-7.86640900	0.59568400	-2.50346000
H	-8.12018000	1.43107600	-1.83967200
H	-8.53356100	0.64445500	-3.37185500
H	-8.08701900	-0.33408500	-1.96447000
H	0.28220000	3.80886300	1.50837100
H	-0.48356400	3.90186000	-0.14283100

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Zero-point correction= 0.835230 (Hartree/Particle)

Thermal correction to Energy= 0.882485

Thermal correction to Enthalpy= 0.883430

Thermal correction to Gibbs Free Energy= 0.754457

E(Solv)=-2014.87744868

Pd	-2.77280400	-0.44123900	-0.76551600
P	-1.04554300	0.94961900	0.20187700
P	4.13260900	0.13455800	-0.55181000
C	0.64787700	0.16439000	-0.12222200
C	1.00086900	-1.15001400	0.55677900
C	0.07213600	-2.20373600	0.55485200
C	0.34814700	-3.43410900	1.14746600
C	1.57673200	-3.63091100	1.77619000
C	2.51803800	-2.60458800	1.76524000
C	2.27455800	-1.36847800	1.14049500
C	3.39133200	-0.33913200	1.14034000
C	-1.04890800	1.34394400	2.08513200
C	-1.50290700	0.05970200	2.81475000
C	0.33012600	1.75045000	2.63946900
C	-2.07692900	2.44945500	2.39799900
C	-0.87258000	2.56697600	-0.83657700
C	-0.47632900	2.14268200	-2.27092200
C	0.16648200	3.57885800	-0.31960800
C	-2.25482700	3.24831300	-0.93219800
C	5.07460600	-1.45409400	-1.10566100
C	3.99330500	-2.35197600	-1.75434600
C	5.78747800	-2.25423400	-0.00068300
C	6.09392500	-1.09144200	-2.20460700
C	5.39472000	1.49517000	-0.00803800
C	6.59379500	1.03370900	0.83841700
C	5.90065000	2.19738000	-1.28844800
C	4.60346900	2.55147000	0.79796000
H	0.66607200	0.00577900	-1.20561700
H	1.41509900	0.91500000	0.07099000
H	-0.90390600	-2.04421400	0.09677600
H	-0.39858200	-4.22327200	1.12759100
H	1.80475600	-4.57328200	2.26692400
H	3.47530800	-2.76023100	2.25634100
H	4.17843700	-0.66858900	1.82759900
H	3.01735300	0.60934900	1.53791900
H	-2.49728100	-0.25668900	2.48997100
H	-0.81444500	-0.77350300	2.65406100
H	-1.54306700	0.25979700	3.89428700
H	1.05218300	0.93389500	2.55043500
H	0.74441300	2.63671800	2.15237400
H	0.23237300	1.97941300	3.70925300
H	-2.19012300	2.53131200	3.48705700
H	-1.76577600	3.43110600	2.02956900
H	-3.06383800	2.22044800	1.98168600
H	-1.13175400	1.35097500	-2.65454500
H	-0.58140600	3.00828700	-2.93774900
H	0.56191400	1.80466300	-2.33949100
H	1.16393900	3.13843100	-0.21427200
H	0.25306300	4.40472500	-1.03856000
H	-0.11920300	4.01725600	0.64111900
H	-2.62020200	3.60743100	0.03275800
H	-2.18082800	4.11758600	-1.59961300
H	-3.00136600	2.56309900	-1.34479900
H	4.46374400	-3.26417600	-2.14694700
H	3.22343300	-2.65772700	-1.04051400
H	3.50009700	-1.84243200	-2.58947700
H	6.55688400	-1.67141800	0.51226900
H	5.08516700	-2.62898500	0.74808000
H	6.28088800	-3.13045600	-0.44457000
H	6.45752500	-2.01305500	-2.67891600
H	5.64705500	-0.47170500	-2.99055900
H	6.96793500	-0.56644300	-1.80682400
H	7.17565300	1.90671800	1.16707700
H	6.28107800	0.49423900	1.73954600
H	7.27331400	0.38828800	0.27400700
H	5.06637000	2.57360900	-1.89097600
H	6.53049300	3.05469700	-1.01365200
H	6.50136000	1.54065900	-1.92173900
H	3.67832100	2.84821400	0.28807300
H	4.34774100	2.20719900	1.80490200
H	5.21738600	3.45463400	0.91226800
B	-4.54097600	-0.23422000	0.12659100

C	-5.42183900	1.03428100	-0.26502000
C	-6.92771200	1.01043200	0.07149500
H	-5.28754600	1.29856100	-1.32124500
H	-4.96010200	1.86985400	0.29124900
H	-7.39530500	1.98308400	-0.12742100
H	-7.45951400	0.26562800	-0.53168700
H	-7.10730700	0.76897900	1.12566600
C	-4.92579600	-1.21780000	1.32012600
C	-6.01678100	-2.25298500	0.95215500
H	-5.29869000	-0.61300300	2.16520300
H	-4.05237100	-1.76548600	1.69320600
H	-6.25402100	-2.89006100	1.81307000
H	-6.94674400	-1.77283100	0.63132600
H	-5.68338900	-2.90653800	0.13950100
C	-3.86057700	-1.76770900	-1.98066800
C	-5.09323700	-1.35225800	-2.79071600
H	-4.05542700	-2.71304700	-1.45832300
H	-3.02747700	-1.97287600	-2.68003000
H	-5.36436000	-2.10794000	-3.54472900
H	-5.97566800	-1.21217500	-2.15269500
H	-4.93076400	-0.40649300	-3.32230500

39-ts

Zero-point correction= 0.830785 (Hartree/Particle)

Thermal correction to Energy= 0.877146

Thermal correction to Enthalpy= 0.878091

Thermal correction to Gibbs Free Energy= 0.751576

E(Solv) = -2014.83434712

Pd	-3.33339800	0.01388900	0.54823100
P	4.77040400	-0.51017800	0.38814700
P	-1.41422100	1.16076400	-0.20918300
C	3.16555700	0.49166000	0.58940700
C	2.11702600	-0.13991900	1.49462000
C	2.53645600	-0.55818200	2.77265400
C	1.66931600	-1.15988800	3.67733500
C	0.33742900	-1.36669700	3.31404100
C	-0.10329500	-0.93851400	2.06683900
C	0.75324900	-0.30409300	1.14773800
C	0.17466800	0.13382100	-0.18970000
C	4.23852000	-1.94798300	-0.78335400
C	3.61397200	-3.01424500	0.14840900
C	3.21590900	-1.59460400	-1.87812700
C	5.48528400	-2.57648800	-1.43733400
C	5.86227900	0.76003500	-0.57323300
C	5.90208000	2.05058200	0.27874100
C	5.41690400	1.12632300	-1.99959200
C	7.30301200	0.20143200	-0.60524800
C	-1.51214200	1.62217700	-2.08836000
C	-1.27740300	0.33182000	-2.90634900
C	-0.49246500	2.66416800	-2.58870000
C	-2.93650000	2.14068200	-2.38081500
C	-0.95870100	2.74643600	0.81319000
C	0.45867400	3.28808800	0.52933100
C	-2.00797800	3.84173500	0.53602000
C	-1.01454200	2.41712200	2.32204800
H	3.49333700	1.42756600	1.05452400
H	2.76047600	0.76194100	-0.38778500
H	3.57953500	-0.42067500	3.04388900
H	2.03285300	-1.47261900	4.65263000
H	-0.35608700	-1.84768800	3.99883700
H	-1.14680600	-1.07237300	1.79336400
H	-0.08752700	-0.75570600	-0.77165600
H	0.91377300	0.68279100	-0.77602700
H	4.32287300	-3.33822300	0.91799700
H	2.71510200	-2.64874600	0.65296000
H	3.33067500	-3.89575300	-0.44353200
H	2.26955500	-1.24904500	-1.45234500
H	3.58148900	-0.82793100	-2.56684500
H	2.99131800	-2.49085600	-2.47354700
H	5.20512400	-3.52535400	-1.91467200
H	5.91635500	-1.93833300	-2.21504400
H	6.26632900	-2.79749000	-0.70077700
H	6.09818100	1.83795100	1.33681700
H	6.71139400	2.69891000	-0.08241700
H	4.97417100	2.62714900	0.21019700
H	4.38642800	1.49868600	-2.02784100
H	6.06129100	1.92266500	-2.39896500
H	5.49071000	0.27767000	-2.68639500
H	7.39192000	-0.70566900	-1.20750600
H	7.97902300	0.95117900	-1.03895600
H	7.66127400	-0.02894900	0.40425200
H	-1.56956400	0.51444400	-3.94859300
H	-0.22385200	0.03471300	-2.91136600
H	-1.86979900	-0.50981000	-2.54078700
H	-0.66884200	3.66011200	-2.17505600
H	0.54317700	2.37758500	-2.37664100
H	-0.58580000	2.74784600	-3.67981900
H	-3.04408900	2.31643400	-3.45984700

H	-3.69530400	1.41710100	-2.07458100
H	-3.14624900	3.08473000	-1.87084300
H	0.63080900	4.16455900	1.16809400
H	1.22834900	2.55360900	0.78184900
H	0.60930800	3.60722700	-0.50199600
H	-3.02541800	3.46891000	0.69791900
H	-1.84552200	4.67695900	1.22985600
H	-1.94118800	4.24613600	-0.47812600
H	-1.99019400	2.02113100	2.61326500
H	-0.24834500	1.69822900	2.61917100
H	-0.84016400	3.34547400	2.88260300
B	-3.62884600	-1.50484300	-0.91062000
C	-3.01621800	-2.97513100	-0.94462600
C	-1.93085700	-3.39716200	0.05341000
H	-2.66773000	-3.17977900	-1.97316400
H	-3.88044700	-3.65458000	-0.83146800
H	-1.65886900	-4.45501100	-0.06025200
H	-1.01493700	-2.80919900	-0.07042800
H	-2.26470600	-3.25082400	1.08752800
C	-4.97379400	-1.21926300	1.25246400
C	-4.87301500	-0.09986900	2.13310400
H	-4.62754500	-2.18773200	1.60331500
H	-5.80927100	-1.25359000	0.55809500
H	-5.61737200	0.68871700	2.07359300
H	-4.45659900	-0.24328200	3.12586800
H	-3.57383300	1.13444800	1.77754300
C	-4.68300600	-1.17579700	-2.08191600
C	-5.64993600	-2.30905800	-2.49171300
H	-4.08709200	-0.90627700	-2.97081000
H	-5.27195400	-0.27564900	-1.85716000
H	-5.11178000	-3.19307600	-2.85102500
H	-6.27395800	-2.63020900	-1.64742300
H	-6.32908700	-1.98902700	-3.29213500

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E(Solv)=-1936.26758189

Zero-point correction= 0.779561 (Hartree/Particle)

Thermal correction to Energy= 0.822835

Thermal correction to Enthalpy= 0.823779

Thermal correction to Gibbs Free Energy= 0.706959

Pd	0.39091900	-0.97360600	-0.16611000
P	1.60515800	0.92631000	0.40322900
P	-1.96807800	-0.57679500	0.39039200
C	0.48808000	2.33604300	1.04509300
C	-0.67266600	2.89567400	0.24204700
C	-0.45548800	4.10235800	-0.44774400
C	-1.46604100	4.77388000	-1.12967500
C	-2.75957600	4.25772500	-1.10209900
C	-3.00325900	3.08195900	-0.39805400
C	-1.98855400	2.36787100	0.26383400
C	-2.39498800	1.14467600	1.06456400
C	2.64631200	1.73822800	-1.00995900
C	1.66964900	1.91892400	-2.19581400
C	3.29867500	3.08946400	-0.66317800
C	3.75132700	0.77211100	-1.48514600
C	2.68004100	0.71236300	2.01004400
C	1.81912200	-0.11559000	2.98961300
C	3.09135300	2.01814800	2.72199000
C	3.95398900	-0.10056800	1.70628400
C	-3.07942900	-0.79473200	-1.17287600
C	-2.34687900	-0.05204100	-2.31545900
C	-4.51625700	-0.24862300	-1.07180900
C	-3.14194100	-2.28864300	-1.55348400
C	-2.63968500	-1.68739200	1.82933800
C	-4.17032400	-1.72257400	1.99236600
C	-2.11256100	-3.12411100	1.62016400
C	-2.02606200	-1.16966000	3.15017600
H	0.10988600	1.92809700	1.98863500
H	1.13468800	3.17534400	1.31690800
H	0.53991800	4.53751300	-0.43088000
H	-1.24750800	5.70163400	-1.65131500
H	-3.57602700	4.77373500	-1.59980000
H	-4.02323600	2.71447200	-0.33438300
H	-3.46829000	1.20298000	1.27900900
H	-1.88620500	1.17113300	2.03270700
H	1.22190200	0.96242100	-2.48290000
H	0.86057300	2.61843300	-1.97985700
H	2.22638300	2.30577900	-3.06031100
H	2.58770300	3.82556100	-0.27685900
H	4.10378600	2.97898200	0.06966600
H	3.74655600	3.51785000	-1.57017500
H	4.14985700	1.13576000	-2.44186400
H	4.58917500	0.71219300	-0.78777200
H	3.36394600	-0.23602700	-1.64811900
H	1.52099300	-1.07122400	2.54741700
H	2.39965100	-0.31946900	3.89974100
H	0.91159900	0.41490700	3.29759700
H	2.23247900	2.57869800	3.10320300

H	3.71769000	1.76589200	3.58852700
H	3.67692200	2.68432400	2.08312300
H	4.71731600	0.50424400	1.20940000
H	4.38819400	-0.45265400	2.65168000
H	3.74618700	-0.97749900	1.08746000
H	-2.90545500	-0.19083300	-3.25168600
H	-2.26809100	1.02237400	-2.12909500
H	-1.33519000	-0.44611800	-2.45849000
H	-5.10617700	-0.74154000	-0.29626300
H	-4.53709300	0.82682500	-0.88433500
H	-5.02998000	-0.41599200	-2.02854200
H	-3.58004600	-2.38252700	-2.55627300
H	-2.14682000	-2.74484900	-1.58045400
H	-3.77177400	-2.86730400	-0.87077900
H	-4.42561200	-2.27819300	2.90546000
H	-4.60483600	-0.72145100	2.09093600
H	-4.66440800	-2.23061100	1.15945100
H	-1.02044000	-3.13984000	1.55114800
H	-2.41241500	-3.74688600	2.47426700
H	-2.50874600	-3.59278900	0.71660600
H	-0.94363600	-1.02937500	3.06884200
H	-2.47773500	-0.22991500	3.48406600
H	-2.20499700	-1.91033300	3.94065900
B	1.69996700	-2.43411700	-1.20474900
C	2.85001900	-3.30106800	-0.51927300
C	2.59475300	-3.86310800	0.88696800
H	3.77266200	-2.69511200	-0.51465700
H	3.09269100	-4.13765500	-1.19886400
H	3.44658800	-4.44271400	1.26705200
H	2.39218200	-3.05948900	1.60472900
H	1.71856400	-4.52393900	0.89123300
H	0.48769800	-2.65286000	-0.76964400
C	1.81341700	-2.21177000	-2.78843100
C	1.25171900	-3.43750400	-3.54997300
H	2.86242200	-2.07090500	-3.09279200
H	1.26599500	-1.32325300	-3.13102800
H	1.78488400	-4.35817400	-3.28284800
H	0.19067700	-3.59668800	-3.31934900
H	1.33815900	-3.31144400	-4.63674000

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Zero-point correction= 0.492654 (Hartree/Particle)

Thermal correction to Energy= 0.523047

Thermal correction to Enthalpy= 0.523991

Thermal correction to Gibbs Free Energy= 0.427738

E(Solv) = -1759.16502557

C	-3.06292700	2.69480400	-0.56810800
O	-1.71319100	3.22778000	-0.53333200
C	-0.86104700	2.19956700	-0.67633500
C	-2.87597500	1.20781300	-0.96610000
H	-3.49213200	2.81655700	0.42945600
H	-3.63583700	3.27743700	-1.29091900
H	-3.16662900	1.05130600	-2.01118100
N	-1.39746300	1.04227100	-0.89945000
C	0.56950700	2.56640800	-0.59776100
C	0.87712100	3.91385200	-0.84995700
C	1.61492900	1.65918800	-0.28483600
C	2.19327300	4.36969200	-0.81928900
H	0.07328700	4.60284000	-1.07959500
C	2.92910400	2.14251700	-0.24926500
C	3.22232300	3.48197600	-0.51833200
H	2.40722800	5.41291100	-1.02943300
H	3.74025400	1.46352500	-0.01042500
H	4.25293000	3.82280600	-0.48884400
P	1.30012900	-0.11683400	0.11714200
Pd	-0.46680400	-0.85073300	-1.20434300
C	-3.64714600	0.23409600	-0.09799600
C	-3.27765500	0.00058600	1.23441300
C	-4.77690800	-0.41165500	-0.61471100
C	-4.02272100	-0.87036800	2.03003800
H	-2.40286500	0.49227100	1.65197600
C	-5.52677000	-1.27882600	0.18326300
H	-5.07660200	-0.23312000	-1.64525000
C	-5.14892000	-1.51165500	1.50684300
H	-3.72524000	-1.04438600	3.06022500
H	-6.40367200	-1.76940100	-0.22904300
H	-5.73077500	-2.18543200	2.12893700
C	0.94074200	-0.14876600	1.91645200
C	1.34993600	0.87669600	2.78393900
C	0.24967400	-1.25593800	2.43817500
C	1.07365000	0.79134500	4.14994500
H	1.88367800	1.74024000	2.39958300
C	-0.01523500	-1.34078000	3.80503600
H	-0.08120600	-2.05053000	1.77500100
C	0.39434800	-0.31603600	4.66196600
H	1.39246400	1.59016700	4.81314600
H	-0.54384300	-2.20402100	4.19898400
H	0.18347000	-0.37985500	5.72547100

C	2.92200600	-0.94377000	-0.10288800
C	3.37587200	-1.18571400	-1.41203200
C	3.70843300	-1.35178200	0.98414000
C	4.60056200	-1.81500000	-1.62692600
H	2.77299900	-0.87630900	-2.26274900
C	4.93077200	-1.99209300	0.76240600
H	3.37291300	-1.17400700	2.00068300
C	5.37848000	-2.22255700	-0.53861400
H	4.94540800	-1.99285600	-2.64140100
H	5.53146800	-2.30822800	1.61019400
H	6.32897900	-2.72023900	-0.70674200
C	-1.97680900	-1.97716100	-2.46311300
H	-2.58351600	-2.35455300	-1.64260400
C	-0.68423400	-2.46124100	-2.68619200
C	0.10348800	-2.87966600	-1.57796900
H	-0.19726700	-2.25700000	-3.63837800
H	-2.51398700	-1.47976700	-3.26511500
H	1.15323800	-3.11284400	-1.72862900
H	-0.37313300	-3.41261900	-0.75501500

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Zero-point correction= 0.677584 (Hartree/Particle)
Thermal correction to Energy= 0.716921
Thermal correction to Enthalpy= 0.717865
Thermal correction to Gibbs Free Energy= 0.598111
SCF Done: E(RB3LYP) = -2163.64578385

C	-4.84360600	-1.54162100	-1.27620200
O	-4.76902600	-0.10192800	-1.42753400
C	-3.47828700	0.25593600	-1.26115800
C	-3.36181700	-1.99756100	-1.25488500
H	-5.36414300	-1.75191000	-0.33775700
H	-5.41827600	-1.94071200	-2.11341800
H	-3.07770900	-2.42652800	-2.22305200
N	-2.63158400	-0.71082700	-1.12530100
C	-3.22843000	1.71395300	-1.31443900
C	-4.20645700	2.48159700	-1.96922400
C	-2.08927800	2.35738800	-0.76060500
C	-4.06716000	3.86039700	-2.10981200
H	-5.07755200	1.98368600	-2.37785500
C	-1.97771800	3.74586900	-0.90714800
C	-2.94766800	4.49435100	-1.57902000
H	-4.83079600	4.42963100	-2.63077100
H	-1.11679700	4.25633100	-0.48989100
H	-2.82374800	5.56876400	-1.67892500
P	-0.77749800	1.41778900	0.15643100
Pd	-0.47054100	-0.62665400	-0.98113800
C	-3.04139700	-3.00604700	-0.17030500
C	-3.03752800	-2.63869400	1.18258200
C	-2.79010700	-4.33984100	-0.51282600
C	-2.78308700	-3.58943200	2.17124800
H	-3.22310800	-1.60617300	1.46574800
C	-2.54086000	-5.29411300	0.47658400
H	-2.79441900	-4.63648400	-1.55953800
C	-2.53560900	-4.91994200	1.82137000
H	-2.78383100	-3.29100700	3.21601800
H	-2.35553000	-6.32713200	0.19588600
H	-2.34624000	-5.66085400	2.59297100
C	-1.46013500	1.28101500	1.86303100
C	-2.42729900	2.16125600	2.37418600
C	-0.97560700	0.25101000	2.68651600
C	-2.89319500	2.01606600	3.68281100
H	-2.81948800	2.96119900	1.75362500
C	-1.43561400	0.11373700	3.99666600
H	-0.24203600	-0.44856400	2.29443300
C	-2.39694600	0.99554100	4.49639700
H	-3.64307900	2.70247400	4.06573200
H	-1.04910800	-0.68457000	4.62433700
H	-2.76036100	0.88578700	5.51415600
C	0.61748800	2.61131800	0.29866100
C	1.51647000	2.69536300	-0.77887600
C	0.83145900	3.41474200	1.42892500
C	2.59617300	3.57662700	-0.73355300
H	1.36433700	2.06924600	-1.65513100
C	1.92156500	4.28744700	1.47618900
H	0.15141000	3.36111100	2.27323000
C	2.80210300	4.37258500	0.39661500
H	3.28018600	3.63705900	-1.57542000
H	2.07874700	4.90254500	2.35779500
H	3.64725800	5.05385100	0.43590100
C	0.29015000	-2.34075300	-1.98312800
H	0.09821000	-3.20719200	-1.35001500
C	1.37956500	-1.46633900	-1.68566000
C	2.02550800	-1.44011600	-0.41606200
H	1.79749200	-0.84336400	-2.47467200
H	-0.01781000	-2.45988000	-3.01940200
H	2.59057900	-0.55816900	-0.13677700
H	1.59378000	-2.00369000	0.40514900
C	4.68549100	-2.09968400	-1.40057700

C	5.49646900	-1.00069300	-0.74458200
C	5.54421700	-0.86582500	0.65164800
C	4.71759300	-1.76719900	1.55038100
C	4.21295400	-3.01630500	0.82701500
H	6.20934800	-0.24797000	-2.63482600
H	5.34850700	-2.91618800	-1.72697100
C	6.24745000	-0.13659800	-1.55318700
C	6.34739300	0.13855400	1.21000800
H	5.30696400	-2.07967000	2.42007600
H	3.42690700	-3.51456600	1.40303700
C	7.09451200	0.99213600	0.40301400
C	7.04482800	0.85419400	-0.98737900
H	6.38743600	0.24464900	2.29174900
H	7.71658000	1.75940400	0.85460000
H	7.62490800	1.51456900	-1.62521300
N	3.65519400	-2.64427100	-0.49317000
H	3.22373800	-3.45726300	-0.93234700
H	4.17613100	-1.72766300	-2.29666700
H	5.03218800	-3.73637900	0.68673300
H	3.86214200	-1.20592800	1.95161800

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Zero-point correction= 0.680545 (Hartree/Particle)

Thermal correction to Energy= 0.719663

Thermal correction to Enthalpy= 0.720607

Thermal correction to Gibbs Free Energy= 0.601907

C	-4.65339800	-2.12793600	-1.10293300
O	-4.81403600	-0.69462500	-1.22933100
C	-3.58310900	-0.14153500	-1.12169100
C	-3.11904100	-2.34339100	-1.17409300
H	-5.07799500	-2.42964900	-0.14097700
H	-5.20628300	-2.60484900	-1.91397500
H	-2.82699700	-2.70788800	-2.16630100
N	-2.59064800	-0.96330700	-1.05214300
C	-3.56570600	1.33865800	-1.15745400
C	-4.69658100	1.95176500	-1.72381300
C	-2.50089200	2.14615400	-0.67364100
C	-4.78408700	3.33630300	-1.84556900
H	-5.50783800	1.32776400	-2.07883700
C	-2.61849200	3.53658800	-0.80045200
C	-3.73937900	4.13177300	-1.38446400
H	-5.66369100	3.78417300	-2.29777100
H	-1.81860800	4.17160400	-0.43614400
H	-3.79060100	5.21342500	-1.47040500
P	-0.99197800	1.41221300	0.12900500
Pd	-0.43175300	-0.55597200	-1.03218300
C	-2.58401900	-3.30725100	-0.13411400
C	-2.54249700	-2.95919900	1.22311600
C	-2.16812800	-4.58711400	-0.51901900
C	-2.09224400	-3.87533900	2.17393800
H	-2.85130400	-1.96612000	1.53753300
C	-1.72195800	-5.50779500	0.43242400
H	-2.19810800	-4.86821900	-1.56958700
C	-1.68251400	-5.15310600	1.78198400
H	-2.06787200	-3.59216400	3.22281500
H	-1.41216200	-6.50101000	0.11893600
H	-1.34246600	-5.86929700	2.52497000
C	-1.53116400	1.18686900	1.88143000
C	-2.55458400	1.94172200	2.47701100
C	-0.87493000	0.21145300	2.65032100
C	-2.90596600	1.72960300	3.81195800
H	-3.08141600	2.69587400	1.90025500
C	-1.22103400	0.00653400	3.98673300
H	-0.09882200	-0.39486500	2.19043600
C	-2.23879900	0.76494100	4.56972100
H	-3.70134800	2.31940100	4.25901600
H	-0.70258500	-0.74969000	4.57022600
H	-2.51411600	0.60203800	5.60791000
C	0.19410100	2.82446100	0.19243200
C	0.96150000	3.07563500	-0.95865200
C	0.38504900	3.63130700	1.32408300
C	1.88280700	4.12204300	-0.98341100
H	0.82925400	2.44753600	-1.83669000
C	1.32084300	4.66914200	1.30203200
H	-0.19474000	3.45332400	2.22425800
C	2.06706400	4.91955100	0.14967200
H	2.45992400	4.31297400	-1.88424900
H	1.46053700	5.28477900	2.18638700
H	2.78948000	5.73081600	0.13381500
C	0.67769900	-2.03874000	-2.06006500
H	0.63092700	-2.99557400	-1.53552500
C	1.53796100	-0.99242300	-1.58202500
C	2.44861300	-1.24378500	-0.42169000
H	1.90294700	-0.25312300	-2.29673800
H	0.43290900	-2.09749300	-3.11898700
H	2.86333500	-0.33542200	0.01814600
H	1.96620900	-1.84373000	0.35312200
C	4.70453100	-1.33643100	-1.64705300

C	5.58001300	-0.48574900	-0.75363000
C	5.74302000	-0.77798200	0.60918400
C	4.95548100	-1.89551400	1.26742500
C	4.34345200	-2.86432300	0.26045300
H	6.14643100	0.80727800	-2.38476100
H	5.29493800	-2.07748100	-2.19943900
C	6.27917800	0.58384000	-1.32865500
C	6.61200700	0.01206400	1.37321600
H	5.59959600	-2.47461900	1.93890700
H	3.58686400	-3.50701100	0.71730600
C	7.31262800	1.06822000	0.79676500
C	7.14576900	1.35644800	-0.56078400
H	6.73880400	-0.20811600	2.43046600
H	7.98642500	1.66586600	1.40322300
H	7.68521900	2.18094100	-1.01666800
N	3.67712800	-2.11098100	-0.86382800
H	3.25743700	-2.79255300	-1.50620200
H	4.16103900	-0.73421500	-2.37870400
H	5.10850000	-3.49814800	-0.19898500
H	4.16424900	-1.47278500	1.90087200

44

Zero-point correction= 0.259826 (Hartree/Particle)
Thermal correction to Energy= 0.271248
Thermal correction to Enthalpy= 0.272192
Thermal correction to Gibbs Free Energy= 0.222073
E(Solv) = -521.702205814

C	-4.03361600	-1.30416800	-0.71079400
C	-3.46397800	-0.12005300	-0.47322600
H	-4.00080300	-2.11811500	0.01034900
H	-3.55211000	0.68076900	-1.20458600
C	-2.77348000	0.20556300	0.81679700
H	-2.88216700	-0.60317900	1.54425500
C	-0.51628300	-0.81282900	0.25325300
C	0.96748100	-0.55381600	0.11146200
C	1.47390200	0.73893300	-0.09134300
C	0.55689600	1.94858400	-0.08386100
C	-0.91181600	1.57953200	-0.26272000
H	1.44018500	-2.65118400	0.31018500
H	-0.72206400	-1.57265400	1.01318900
C	1.83749300	-1.65181400	0.14879000
C	2.85482800	0.90805300	-0.25547300
H	0.67989900	2.51466900	0.85135100
H	-1.12648500	1.22765500	-1.27422200
C	3.71663400	-0.18525600	-0.22641200
C	3.20675500	-1.47095600	-0.02367300
H	3.25415200	1.90755300	-0.40822600
H	4.78360800	-0.03620900	-0.35999000
H	3.87354800	-2.32693000	0.00518300
N	-1.26429600	0.43450400	0.66638200
H	-0.98260900	-1.13987300	-0.68148200
H	-1.57756300	2.41354200	-0.02678700
H	0.82638400	2.64275900	-0.88785700
H	-4.57581300	-1.49507400	-1.63195100
H	-3.15817900	1.12980300	1.26117300
H	-0.91880900	0.69431200	1.59793900

45-ts

Zero-point correction= 0.843033 (Hartree/Particle)
Thermal correction to Energy= 0.892898
Thermal correction to Enthalpy= 0.893842
Thermal correction to Gibbs Free Energy= 0.747414
E(Solv) = -2550.86641313

C	4.50694600	3.51732300	1.52988000
O	5.27821800	2.79211100	0.54099200
C	4.47317700	1.84453300	0.01104200
C	3.06365900	2.96783200	1.36598400
H	4.93502600	3.29966600	2.51206300
H	4.59991900	4.58354400	1.31526300
H	2.42423100	3.70471000	0.86683800
N	3.24825100	1.84292400	0.41870200
C	5.12585200	0.97854900	-0.99790000
C	6.30510600	1.48692600	-1.56993900
C	4.64376600	-0.29393900	-1.40864100
C	6.99974100	0.77890800	-2.54737500
H	6.67021000	2.45328100	-1.24428300
C	5.36698900	-0.98957400	-2.38694700
C	6.52804500	-0.46415900	-2.95861300
H	7.90202600	1.20005000	-2.98012100
H	5.01748900	-1.96326000	-2.71181900
H	7.05788900	-1.03155800	-3.71835400
P	3.11072000	-1.05525600	-0.68934800
Pd	1.54788900	0.66723000	-0.30220300
C	2.41097600	2.56982300	2.67560600
C	2.74734100	1.37403800	3.32440600
C	1.49572700	3.43807200	3.28336400
C	2.17376400	1.05331200	4.55532700
H	3.44890600	0.68558200	2.86215000

C	0.92637800	3.12124300	4.51883000
H	1.22952700	4.36919800	2.78811800
C	1.26335500	1.92620100	5.15696100
H	2.44224000	0.12123800	5.04505700
H	0.22252800	3.80783600	4.98117900
H	0.82287700	1.67816400	6.11862100
C	3.71919200	-1.91037000	0.82649600
C	5.06414400	-2.25673000	1.03061100
C	2.77636800	-2.22899800	1.81882700
C	5.45514500	-2.91122800	2.20111400
H	5.80950200	-2.01742800	0.27832700
C	3.16793600	-2.89224700	2.98214500
H	1.73530700	-1.95016800	1.67825000
C	4.50912400	-3.23218400	3.17644000
H	6.49966300	-3.17134700	2.34824100
H	2.42759900	-3.13714000	3.73888700
H	4.81606400	-3.74226600	4.08516100
C	2.70090300	-2.41661500	-1.86048000
C	1.96396700	-2.08474100	-3.01059700
C	3.06258200	-3.75520700	-1.64725600
C	1.61771400	-3.06636200	-3.93857500
H	1.66596300	-1.05194800	-3.17632900
C	2.70130900	-4.73906800	-2.57140300
H	3.62744400	-4.03252500	-0.76277400
C	1.98407900	-4.39720100	-3.71890300
H	1.05866100	-2.79454600	-4.82993300
H	2.98714300	-5.77231600	-2.39479000
H	1.70985500	-5.16370800	-4.43832400
C	-0.19758300	1.92985700	-0.23252300
C	-0.53021600	0.71411400	-0.91447600
H	-0.46477800	1.98197800	0.82463300
H	-0.64859300	0.71119000	-1.99727100
C	-0.84131300	-0.48077600	-0.21185900
C	-1.31643800	-1.68847300	-0.76126400
H	-0.82605500	-0.40742400	0.87778400
C	-0.10912600	3.24764600	-0.89426100
C	-0.37488800	4.41312000	-0.15008800
C	0.24107700	3.40006700	-2.25094900
C	-0.29688500	5.67780100	-0.73354600
H	-0.65761900	4.31812300	0.89612400
C	0.31453900	4.66273600	-2.83469300
H	0.47578300	2.52263800	-2.84769100
C	0.04728200	5.80933700	-2.08022400
H	-0.51263900	6.56055800	-0.13739600
H	0.58699100	4.75408600	-3.88280200
H	0.10693000	6.79249000	-2.53800200
H	-1.18519500	-2.57973900	-0.14529700
H	-1.11999700	-1.86299300	-1.82176100
C	-6.48350200	1.03688500	-0.61098500
C	-5.96854100	-0.01664400	-1.26894200
H	-5.83622584	1.70935200	-0.08780079
H	-6.61917900	-0.69109300	-1.82354800
C	-4.49144400	-0.29179600	-1.36550900
H	-3.95935761	0.54067852	-0.95469243
C	-4.30725200	-1.42578800	0.83884500
C	-3.99186500	-2.68843100	1.61463300
C	-3.88028300	-3.93398800	0.98156500
C	-3.99899300	-4.03662300	-0.52418200
C	-4.67880700	-2.81550700	-1.14327300
H	-3.94117200	-1.63326400	3.49498700
H	-3.67807000	-0.59829200	1.18762100
C	-3.85096000	-2.60143300	3.00671700
C	-3.62870800	-5.07392100	1.75752400
H	-3.00363600	-4.16434600	-0.97051800
H	-5.74915600	-2.80607300	-0.90550100
C	-3.49202000	-4.98377100	3.14001300
C	-3.60408200	-3.73993500	3.76873500
H	-3.54336200	-6.04085300	1.26692000
H	-3.30282200	-5.87814600	3.72644700
H	-3.50028700	-3.65932700	4.84681700
N	-4.06880500	-1.55711600	-0.62481500
H	-5.35074000	-1.12316100	0.99013100
H	-4.57007400	-2.82969600	-2.22899000
H	-4.57418500	-4.92758400	-0.80233700
H	-2.78415493	-1.60580338	-0.72538329
H	-7.54056408	1.20277537	-0.61059264
H	-4.22770819	-0.39354298	-2.39749300

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Zero-point correction= 0.244126 (Hartree/Particle)
Thermal correction to Energy= 0.255547
Thermal correction to Enthalpy= 0.256491
Thermal correction to Gibbs Free Energy= 0.206354
E(Solv) = -521.239340703

C	-4.16303100	-1.29354500	-0.55062800
C	-3.46541700	-0.15935300	-0.47161100
H	-4.23170900	-1.97932300	0.29251400
H	-3.42467600	0.50022300	-1.33936700

C	-2.70844300	0.29895500	0.75767200
H	-2.86694400	-0.42512700	1.56793300
C	-0.55564500	-0.74805200	0.28174800
C	0.94029000	-0.54228600	0.13263200
C	1.48412300	0.74073400	-0.03357000
C	0.58029100	1.95633900	-0.01095400
C	-0.87733700	1.58024300	-0.28808700
H	1.36444800	-2.64998900	0.25064500
H	-0.74758100	-1.46890900	1.08831800
C	1.79022100	-1.65632100	0.12281300
C	2.86861800	0.87801900	-0.20534200
H	0.63432300	2.43493500	0.97658700
H	-0.99673300	1.32223700	-1.35869200
C	3.70857300	-0.23307900	-0.21090200
C	3.16504900	-1.51006700	-0.04556800
H	3.28803200	1.87363800	-0.33716700
H	4.77948200	-0.10584700	-0.34591400
H	3.80935600	-2.38531800	-0.04694400
N	-1.26325700	0.48794800	0.60135100
H	-0.94300200	-1.21730000	-0.64497800
H	-1.52943800	2.43859900	-0.08825900
H	0.92372100	2.69801500	-0.74388000
H	-4.70043200	-1.57970300	-1.45130000
H	-3.11980600	1.25870900	1.10182800

47-ts

Zero-point correction=0.783267 (Hartree/Particle)

Thermal correction to Energy= 0.828328

Thermal correction to Enthalpy=0.829273

Thermal correction to Gibbs Free Energy= 0.699822

E(Solv)= -2434.11589350

C	-3.96346400	1.38038500	2.07438400
O	-2.78209000	1.84264300	2.77357200
C	-1.71355400	1.31772700	2.13494200
C	-3.41895200	0.31289000	1.08069200
H	-4.65877700	0.97886300	2.81304700
H	-4.41063500	2.24332500	1.57364000
H	-3.72689100	0.54839200	0.05737700
N	-1.94763800	0.48600500	1.17753700
C	-0.40554800	1.75373000	2.67705800
C	-0.35155600	2.00898000	4.05590000
C	0.75342800	1.93929300	1.88131000
C	0.83810900	2.40296300	4.66562000
H	-1.25231200	1.89197400	4.64809800
C	1.93410500	2.35014800	2.51251800
C	1.98353000	2.57065000	3.89145900
H	0.86301000	2.58380000	5.73584500
H	2.82811300	2.50938800	1.92010100
H	2.91580700	2.88606100	4.35093800
P	0.71677500	1.63959100	0.05325100
Pd	-0.29169400	-0.47175600	-0.30282700
C	-3.87523600	-1.09753200	1.41752400
C	-3.34930000	-1.78950000	2.51706300
C	-4.90131900	-1.69385900	0.67291900
C	-3.83508300	-3.05268400	2.85837600
H	-2.55640000	-1.34012100	3.10915100
C	-5.38792700	-2.95916500	1.01107600
H	-5.33436800	-1.15823200	-0.16918200
C	-4.85362600	-3.64269100	2.10466000
H	-3.42217000	-3.57500300	3.71711100
H	-6.18600500	-3.40562900	0.42468500
H	-5.23321900	-4.62422300	2.37348100
C	2.38851500	2.12384900	-0.53965700
C	2.67037400	3.41932800	-1.00332500
C	3.41408400	1.16490400	-0.52821800
C	3.95432900	3.74612200	-1.44262400
H	1.89079800	4.17323400	-1.02737200
C	4.70005700	1.50023400	-0.95362000
H	3.21248200	0.15545300	-0.18144900
C	4.97122100	2.79018000	-1.41518400
H	4.15801500	4.74996600	-1.80441200
H	5.48303300	0.74889000	-0.92715000
H	5.97013200	3.04840200	-1.75526800
C	-0.39868100	2.96490000	-0.57834300
C	-0.60450700	4.16965600	0.11359300
C	-1.04716500	2.76411100	-1.80734600
C	-1.44230500	5.15276700	-0.41716400
H	-0.11206900	4.34562100	1.06527200
C	-1.88009500	3.75098300	-2.33664000
H	-0.90699300	1.83383000	-2.35053300
C	-2.08076000	4.94571300	-1.64202900
H	-1.59283900	6.08110200	0.12667300
H	-2.37586100	3.57979300	-3.28789200
H	-2.73183200	5.71244600	-2.05228600
C	-0.74179200	-1.77591000	-2.07613000
C	-0.97722000	-2.50552900	-0.90952200
H	0.21699700	-1.87247600	-2.57580300
H	-2.00131100	-2.65629000	-0.57744300

C	0.01712400	-3.49495100	-0.30017100
C	-0.43083200	-3.86125800	1.12041600
H	0.00569900	-4.42268600	-0.89245400
H	0.19476300	-4.63570400	1.57052000
H	-0.45398600	-2.98686700	1.77748400
C	-1.75458500	-1.09582300	-2.90956600
C	-1.32101700	-0.40938200	-4.06018800
C	-3.13461200	-1.13000300	-2.63454100
C	-2.22934900	0.23240500	-4.90007000
H	-0.25911200	-0.38446400	-4.29489400
C	-4.04180100	-0.48768700	-3.47444600
H	-3.50310000	-1.67622000	-1.77240300
C	-3.59506300	0.19898500	-4.60758500
H	-1.87276200	0.74893800	-5.78664900
H	-5.10501200	-0.53544900	-3.25487500
H	-4.30723400	0.68961500	-5.26463500
H	-1.45095000	-4.25316700	1.06827100
C	2.27437600	-3.12691100	0.79749600
C	3.70525500	-2.66078200	0.59954000
C	4.25697400	-2.48694100	-0.67764600
C	3.38327300	-2.65326700	-1.90151600
C	2.13975900	-3.48009900	-1.59150400
H	4.07935200	-2.61399800	2.72312900
H	1.81849300	-2.58195400	1.62754100
C	4.50945100	-2.47584100	1.73320900
C	5.61199600	-2.14653000	-0.79645300
H	3.08100900	-1.66747100	-2.28325500
H	2.42011300	-4.52622500	-1.38783400
C	6.40913000	-1.97257900	0.33302500
C	5.85288900	-2.13281200	1.60579900
H	6.04331000	-2.02790900	-1.78800900
H	7.45988500	-1.72008900	0.22322600
H	6.46523000	-1.99759300	2.49243500
N	1.42595000	-2.94248500	-0.40252800
H	1.04109200	-1.43682500	-0.50052700
H	2.28782700	-4.19238500	1.07404300
H	1.45639600	-3.48998000	-2.44175100
H	3.94133000	-3.14202900	-2.70886000

48-ts

Zero-point correction= 0.596390 (Hartree/Particle)

Thermal correction to Energy= 0.632628

Thermal correction to Enthalpy= 0.633572

Thermal correction to Gibbs Free Energy=0.519804

E(Solv)= -2046.37642331

C	1.21412100	4.33335400	-0.04732000
O	2.18647500	3.56368200	0.69840400
C	1.69578500	2.29469700	0.77998600
C	0.16333500	3.28034600	-0.51447200
H	0.78618800	5.08443600	0.62329300
H	1.73504900	4.83066700	-0.86864500
H	0.24591500	3.10614400	-1.59428500
N	0.59566000	2.04657900	0.17039100
C	2.49522200	1.37426200	1.62158400
C	3.18075800	1.95465500	2.69994000
C	2.57919500	-0.02604700	1.40171100
C	3.91264900	1.17431100	3.59236100
H	3.12313300	3.02870500	2.83678800
C	3.32421100	-0.78764700	2.31241400
C	3.97669900	-0.20314300	3.40063200
H	4.42462400	1.64222500	4.42827200
H	3.40291300	-1.85914200	2.16783400
H	4.54024900	-0.82887400	4.08754500
P	1.71554400	-0.83716400	-0.03776400
Pd	-0.45055500	-0.17303400	-0.19363400
C	-1.26499700	3.68588600	-0.20320100
C	-1.77908400	3.58638900	1.09565400
C	-2.06909400	4.23005700	-1.21026300
C	-3.07270000	4.02365100	1.37926600
H	-1.17181000	3.14386800	1.88044400
C	-3.36299500	4.67286000	-0.92796400
H	-1.68314700	4.30282500	-2.22503800
C	-3.86788200	4.57101800	0.36895700
H	-3.46287700	3.93197100	2.38953800
H	-3.97634000	5.09026400	-1.72214100
H	-4.87633000	4.90968600	0.59084000
C	2.10934200	-2.63145700	0.17209700
C	3.33288100	-3.20652900	-0.20791000
C	1.11538800	-3.45379800	0.72505400
C	3.55844500	-4.57234300	-0.02833700
H	4.10856400	-2.59058700	-0.65327800
C	1.34641400	-4.81756400	0.91334400
H	0.15473000	-3.01783900	0.98672000
C	2.56764100	-5.37937400	0.53607300
H	4.50732600	-5.00619700	-0.33317600
H	0.56641300	-5.44169500	1.34119400
H	2.74414300	-6.44319100	0.67191800
C	2.78159400	-0.33403200	-1.46639400

C	4.10942600	0.10106200	-1.33360700
C	2.21721900	-0.40072500	-2.75142800
C	4.85606100	0.45594700	-2.46004000
H	4.56438300	0.16795700	-0.34966300
C	2.96700300	-0.05465400	-3.87595100
H	1.18283600	-0.71688200	-2.86021700
C	4.28813300	0.37637900	-3.73266000
H	5.88219600	0.79413800	-2.34061500
H	2.51615200	-0.11354400	-4.86317500
H	4.87014000	0.65319300	-4.60778300
C	-3.44761700	-0.27015100	0.67879000
C	-4.36007300	-1.48338200	0.52742400
C	-4.53937500	-2.09313900	-0.72647700
C	-3.78494400	-1.58248200	-1.94020100
C	-3.21760700	-0.17115200	-1.70829900
H	-4.92102900	-1.49854300	2.60515200
H	-2.86537500	-0.36273900	1.60200800
C	-5.06002400	-1.97693100	1.63637500
C	-5.41564500	-3.18248300	-0.83421300
H	-2.94873400	-2.26229600	-2.16334200
H	-4.04775700	0.55890400	-1.74243200
C	-6.10509300	-3.66994700	0.27434700
C	-5.92493600	-3.06344000	1.52058600
H	-5.55672200	-3.65103800	-1.80688700
H	-6.77992200	-4.51570700	0.16784000
H	-6.45367500	-3.43640200	2.39444200
N	-2.54034800	-0.02505700	-0.42986000
H	-1.55690100	-1.29434800	-0.42128300
H	-4.08758600	0.62460000	0.81450900
H	-2.52978200	0.09499800	-2.51753900
H	-4.44031200	-1.59536000	-2.82329300

49

Zero-point correction= 0.599046 (Hartree/Particle)

Thermal correction to Energy= 0.634786

Thermal correction to Enthalpy= 0.635730

Thermal correction to Gibbs Free Energy= 0.525400

E(Solv)=-2046.40272

C	-0.61481500	-3.95377100	1.42394500
O	0.54399800	-3.93817900	0.54962000
C	0.64481500	-2.66659100	0.08062800
C	-1.37735500	-2.66002700	1.05140300
H	-1.17098000	-4.87137000	1.22853900
H	-0.24951600	-3.94988800	2.45670400
H	-1.70758200	-2.09658300	1.92520100
N	-0.32672000	-1.87060600	0.36333600
C	1.81745400	-2.42199700	-0.79253500
C	2.32525400	-3.55349200	-1.45604800
C	2.39696400	-1.15053200	-1.03875000
C	3.35724500	-3.44466700	-2.38371200
H	1.88552900	-4.52152800	-1.24719700
C	3.43042700	-1.06785600	-1.98331900
C	3.90547900	-2.19393100	-2.65715800
H	3.72200400	-4.33234000	-2.89237200
H	3.87711600	-0.10232800	-2.19395300
H	4.70549300	-2.08911000	-3.38488900
P	1.86628600	0.36500400	-0.10197600
Pd	-0.34838400	0.36463900	0.48048700
C	-2.58397400	-2.91447700	0.16143200
C	-2.44334700	-3.31038900	-1.17493900
C	-3.87012600	-2.82253700	0.70627200
C	-3.56612000	-3.61150500	-1.94809100
H	-1.45482000	-3.37552600	-1.62161000
C	-4.99361800	-3.12843700	-0.06275800
H	-3.98976800	-2.48993500	1.73389000
C	-4.84459600	-3.52439200	-1.39355100
H	-3.44096100	-3.91209700	-2.98512600
H	-5.98509800	-3.04698800	0.37474300
H	-5.71862600	-3.75655400	-1.99615200
C	2.46692400	1.76274500	-1.14232300
C	3.76800900	2.28226900	-1.05796300
C	1.55814600	2.33822300	-2.04464500
C	4.15636000	3.34691300	-1.87403600
H	4.47598300	1.86387600	-0.34837700
C	1.95187900	3.39619200	-2.86453200
H	0.53636800	1.97019400	-2.08124600
C	3.25121700	3.90170400	-2.78110300
H	5.16449900	3.74538600	-1.79580400
H	1.23760300	3.83556600	-3.55537300
H	3.55392200	4.73318400	-3.41203200
C	2.99847800	0.36512500	1.35844400
C	4.18426200	-0.38227800	1.42726000
C	2.63324000	1.16381800	2.45654200
C	4.99017800	-0.32696400	2.56726200
H	4.48242700	-1.01200500	0.59478000
C	3.44538300	1.22365600	3.58875000
H	1.70505300	1.72700000	2.41978600
C	4.62478300	0.47706900	3.64780400

H	5.90383600	-0.91425500	2.60813500
H	3.15049700	1.84619000	4.42922900
H	5.25257900	0.51764600	4.53393700
C	-3.28595700	0.61950100	0.12236200
C	-3.56710300	2.08889700	-0.17114100
C	-3.28540000	3.06751800	0.79764600
C	-2.63241900	2.67593000	2.10964800
C	-2.63174100	1.14970200	2.33166400
H	-4.36492500	1.71158900	-2.13322300
H	-2.99468300	0.10886200	-0.80318300
C	-4.14727600	2.47440700	-1.38638200
C	-3.59491300	4.40652600	0.52267900
H	-1.59296400	3.03317300	2.10942800
H	-3.64858300	0.85772800	2.66496100
C	-4.17258600	4.78278300	-0.68920700
C	-4.44944300	3.80936400	-1.65281100
H	-3.37764100	5.16359400	1.27486600
H	-4.40558800	5.82749700	-0.88098800
H	-4.89590100	4.08957600	-2.60415700
N	-2.29806100	0.35028800	1.16067300
H	-0.34108500	1.91110400	0.62624300
H	-4.24882400	0.15537800	0.42473300
H	-1.94809900	0.90158200	3.15333200
H	-3.13863700	3.17959400	2.94692600

50-ts

Zero-point correction= 0.766073 (Hartree/Particle)

Thermal correction to Energy= 0.812246

Thermal correction to Enthalpy= 0.813190

Thermal correction to Gibbs Free Energy= 0.675025

E(Solv)=-2433.5813

C	-1.84096600	4.34138700	0.06624200
O	-2.99312100	3.65943200	-0.47934900
C	-2.66570700	2.34378100	-0.58371100
C	-0.70191900	3.29619300	-0.05462300
H	-1.67581800	5.24813000	-0.51766500
H	-2.06776000	4.60264900	1.10509000
H	-0.16310200	3.20146000	0.89140200
N	-1.44189300	2.03995800	-0.30856500
C	-3.76629000	1.49031000	-1.09475000
C	-4.80027900	2.18546700	-1.75481300
C	-3.83167400	0.07353800	-1.01162000
C	-5.86598600	1.51740600	-2.34726100
H	-4.74875500	3.26539600	-1.80983100
C	-4.91916400	-0.57293000	-1.62032100
C	-5.92494600	0.12728100	-2.28466300
H	-6.64020400	2.08310600	-2.85743100
H	-4.97945800	-1.65487200	-1.57263800
H	-6.74739500	-0.41361900	-2.74453500
P	-2.58058000	-0.96574300	-0.10303300
Pd	-0.52582500	0.09849400	0.21056600
C	0.29903600	3.61624700	-1.15686300
C	0.16240200	3.12144300	-2.45882600
C	1.36275900	4.48324800	-0.86946600
C	1.07206600	3.48718700	-3.45387900
H	-0.64513100	2.43435000	-2.69157000
C	2.26792600	4.85360600	-1.86433700
H	1.48972800	4.85849900	0.14334600
C	2.12516500	4.35486100	-3.16126300
H	0.95759600	3.08920300	-4.45867500
H	3.08959900	5.52312200	-1.62437800
H	2.83383100	4.63554200	-3.93551100
C	-2.63191100	-2.55375000	-1.04257500
C	-3.41473200	-3.65601700	-0.66701500
C	-1.81415900	-2.65777900	-2.18038900
C	-3.38670000	-4.83241000	-1.42029300
H	-4.04362700	-3.60022200	0.21639600
C	-1.79775900	-3.82836700	-2.93809300
H	-1.17858700	-1.82169400	-2.46162900
C	-2.58344100	-4.91979400	-2.55820900
H	-3.99406500	-5.68039500	-1.11493400
H	-1.16020700	-3.89370800	-3.81560300
H	-2.56137200	-5.83642300	-3.14123600
C	-3.44054200	-1.35904200	1.48608400
C	-4.73571800	-0.93164300	1.81212700
C	-2.71170300	-2.09551000	2.43837900
C	-5.28971900	-1.23611100	3.05911200
H	-5.31906500	-0.36040600	1.09754600
C	-3.27286900	-2.41212400	3.67400200
H	-1.70029500	-2.41895700	2.20611700
C	-4.56385200	-1.97848200	3.99017800
H	-6.29297600	-0.89282800	3.29776100
H	-2.69843400	-2.98855000	4.39424600
H	-4.99749500	-2.21550200	4.95789400
C	1.50950300	0.48499200	0.90363900
C	1.21995100	-0.90600400	1.06022500
H	2.08545700	0.76222500	0.02026300
H	1.02573800	-1.30469000	2.05540600

C	1.34928500	-1.83747900	0.00498000
C	1.20105800	-3.27756600	0.14014000
H	1.65634900	-1.45507900	-0.96466500
H	0.71452700	-3.59701500	1.06752000
C	1.65780300	1.41107100	2.04085100
C	2.53666500	2.50817400	1.93455900
C	0.95483200	1.25450500	3.25501800
C	2.70928500	3.40419800	2.99007300
H	3.09659900	2.64544300	1.01301100
C	1.13086900	2.14756300	4.30922700
H	0.25298200	0.43203400	3.36335000
C	2.00793800	3.23014000	4.18499000
H	3.40315900	4.23438900	2.88136800
H	0.57721400	2.00034500	5.23337800
H	2.14344400	3.92498800	5.00933200
H	0.74647900	-3.76174900	-0.72997700
C	4.90521900	-3.16203600	-0.95674700
C	6.05829000	-2.15528600	-0.95149600
C	6.29665300	-1.37222500	0.19117400
C	5.38749100	-1.49779200	1.39878700
C	4.54023400	-2.78948600	1.33341300
H	6.70945100	-2.63033300	-2.94616300
H	5.36725300	-4.17151400	-0.84109400
C	6.89858900	-2.02051000	-2.06350800
C	7.37531000	-0.47655500	0.18918100
H	5.98205900	-1.46689700	2.32391200
H	3.77597800	-2.75932500	2.12452800
C	8.20679300	-0.34613100	-0.92244900
C	7.96591400	-1.12311600	-2.05867200
H	7.56286700	0.12506100	1.07740700
H	9.03828600	0.35450900	-0.90240700
H	8.60516600	-1.02942400	-2.93367400
N	3.89923100	-2.92188700	0.04782000
H	2.34064000	-3.57299900	0.13694500
H	4.43739000	-3.16381700	-1.95311900
H	5.20988100	-3.64793900	1.56616700
H	4.70633700	-0.63576800	1.43456900

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Zero-point correction= 0.697609 (Hartree/Particle)

Thermal correction to Energy= 0.742485

Thermal correction to Enthalpy= 0.743429

Thermal correction to Gibbs Free Energy= 0.618208

E(Solv) = -3085.09196565

Pd	0.52161700	-2.13492000	0.07650300
P	-1.53101000	-0.98191300	-0.28361900
P	1.90261500	-0.22350400	0.04315700
C	-2.53372600	-2.00100000	-1.46810400
C	-3.83963200	-2.42842800	-1.19203400
C	-4.51770100	-3.26699200	-2.08319300
C	-3.90734400	-3.68308300	-3.26508900
C	-2.60390000	-3.26495700	-3.55109300
C	-1.92135400	-2.44335400	-2.65605500
C	-2.69187700	-0.64207700	1.10197200
C	-3.83534800	0.15477400	0.90990500
C	-4.73146000	0.36049900	1.95699800
C	-4.48996100	-0.21820000	3.20725700
C	-3.35038700	-0.99673400	3.40502200
C	-2.44803900	-1.21326400	2.35851700
C	2.20619600	0.56296400	-1.59475500
C	2.63137600	1.89385500	-1.72807700
C	2.92704700	2.42056400	-2.98574300
C	2.80732100	1.62275900	-4.12598000
C	2.38564300	0.29764800	-4.00482300
C	2.08428200	-0.22754400	-2.74688900
C	3.61757200	-0.48281900	0.69952200
C	3.79096200	-1.33925000	1.80279600
C	5.06863900	-1.57953300	2.31117600
C	6.18872900	-0.98853500	1.72316300
C	6.02490900	-0.14936800	0.62065700
C	4.74953600	0.10433100	0.11120600
H	-4.33264000	-2.11550800	-0.27859600
H	-5.52732400	-3.59215300	-1.84654800
H	-4.43700700	-4.33287200	-3.95639000
H	-2.11542700	-3.58735200	-4.46700300
H	-0.90044300	-2.14131300	-2.87558400
H	-4.02674200	0.61112000	-0.05793200
H	-5.61383100	0.97563800	1.80016400
H	-5.18745500	-0.05306200	4.02457000
H	-3.14851100	-1.43722500	4.37744300
H	-1.54555200	-1.79782000	2.53089400
H	2.72594400	2.52283200	-0.84817100
H	3.24282000	3.45627600	-3.07413600
H	3.03774200	2.03455300	-5.10490900
H	2.28746900	-0.32705600	-4.88879300
H	1.74558100	-1.25585500	-2.64931600
H	2.92472200	-1.81113500	2.26582700
H	5.18230500	-2.23860300	3.16775600

H	7.18251400	-1.18414900	2.11778300
H	6.88969700	0.31130600	0.14998800
H	4.64882200	0.75383100	-0.75054400
C	2.08296000	-3.70853900	-0.15907000
H	2.25451000	-3.90146400	0.89580500
C	0.89314200	-4.15147700	-0.77428000
C	-0.28922600	-4.21360900	-0.00922500
H	0.83134200	-4.19414300	-1.86064100
C	-1.37439400	0.66755800	-1.14197800
C	-1.96722600	0.83591800	-2.42650800
C	-0.65966700	1.72601200	-0.57197900
C	-1.83903100	2.00453200	-3.13387800
C	-0.51329800	2.95861800	-1.30801500
C	-1.10312800	3.09191400	-2.60642100
C	1.11262800	1.04578600	1.14695300
C	1.65205500	1.18221400	2.45640700
C	-0.08424600	1.69431800	0.82107500
C	1.02494500	1.93438900	3.41632100
C	-0.76679800	2.46560700	1.82996600
C	-0.20060500	2.58485200	3.14097700
H	-2.30833800	2.10632200	-4.10967600
H	-2.54221500	0.02601800	-2.85687500
H	2.57484600	0.67568700	2.70686500
H	1.46156900	2.02437300	4.40776900
C	-0.86893500	3.35455700	4.13121000
C	-2.00219200	3.13190800	1.58158000
H	-0.41934800	3.42915400	5.11838300
C	-2.05740500	3.98677900	3.85190500
H	-2.56143600	4.57204600	4.61618900
C	-2.62821200	3.86772200	2.56237100
H	-3.57248100	4.35957200	2.34473500
H	-2.46137400	3.04919400	0.60396000
C	0.21247600	4.07469100	-0.79748200
C	-0.95076200	4.30398800	-3.33243000
C	0.34589400	5.23669800	-1.52478600
H	-1.40944700	4.37989400	-4.31549600
C	-0.24127000	5.35821000	-2.80683900
H	0.66784700	4.00620300	0.18311700
H	0.90462200	6.07027600	-1.10771200
H	-0.13179200	6.28187400	-3.36857900
Cl	0.72329900	-2.62561200	2.85267400
H	2.95887200	-3.49923800	-0.76688900
H	-1.23799800	-4.39054500	-0.50637600
H	-0.24154300	-4.41317200	1.05786400

52-ts

Zero-point correction= 0.768958 (Hartree/Particle)
Thermal correction to Energy= 0.817946
Thermal correction to Enthalpy= 0.818890
Thermal correction to Gibbs Free Energy= 0.681021
E(Solv) = -3311.36988456

Pd	-1.03644900	0.62914600	-1.20243700
P	0.61369800	1.93673000	-0.11688400
P	0.10163200	-1.44181900	-0.98584900
C	0.75425800	3.59934100	-0.92071700
C	0.85256100	4.80394100	-0.20997700
C	0.91291700	6.02515700	-0.88737100
C	0.88377000	6.06160500	-2.28128800
C	0.78008900	4.86801000	-3.00085600
C	0.70392400	3.65061300	-2.32554700
C	0.28598500	2.27528700	1.66018400
C	1.25293100	2.86822800	2.49283200
C	0.96577000	3.11688800	3.83411000
C	-0.28044200	2.76181300	4.36284600
C	-1.23492600	2.15277900	3.54931500
C	-0.95457500	1.91114100	2.20159200
C	1.63221100	-1.72127200	-1.98464200
C	2.49159000	-2.80862700	-1.76419800
C	3.58317900	-3.02837200	-2.60257400
C	3.82601000	-2.17051700	-3.67880600
C	2.97335400	-1.09134700	-3.91202700
C	1.88201200	-0.86898400	-3.06925200
C	-0.75410400	-3.06170900	-1.26925500
C	-1.63303300	-3.13509600	-2.36086400
C	-2.24962300	-4.33923400	-2.70407500
C	-2.00313700	-5.48933500	-1.95272600
C	-1.12926100	-5.42965200	-0.86552900
C	-0.50351200	-4.22805300	-0.52928900
H	0.87008500	4.79623000	0.87419600
H	0.98095600	6.94898800	-0.31899600
H	0.93111600	7.01266500	-2.80482100
H	0.74384000	4.88565800	-4.08697600
H	0.59128900	2.72801900	-2.88999800
H	2.23257000	3.12331400	2.09648100
H	1.71746200	3.57877700	4.46949600
H	-0.49616800	2.94808400	5.41183100
H	-2.19664200	1.83569600	3.94130700
H	-1.70520800	1.40257700	1.60378200

H	2.30836300	-3.48896100	-0.93788000
H	4.24541800	-3.86930100	-2.41569000
H	4.67600100	-2.34574200	-4.33290500
H	3.15483500	-0.42195400	-4.74883400
H	1.21517700	-0.02934700	-3.24825600
H	-1.82937100	-2.24121000	-2.94731700
H	-2.92707100	-4.37600900	-3.55311400
H	-2.49033800	-6.42570600	-2.21068000
H	-0.93211500	-6.32048900	-0.27498500
H	0.16892900	-4.19926100	0.32204900
C	-2.59001500	2.07832500	-1.38944800
H	-2.95137700	2.28571700	-0.38352800
C	-3.05641900	0.91430000	-2.06555100
H	-3.04684600	0.88460800	-3.15387700
C	-3.60744700	-0.19089800	-1.36581000
C	2.35650100	1.27103500	-0.14090400
C	2.68353000	0.05117700	0.46656500
C	3.36064400	1.99488800	-0.84214000
C	4.03110000	-0.44515000	0.37890900
C	4.64943300	1.53007400	-0.93610600
H	3.10831800	2.94207600	-1.30396000
C	5.02253800	0.30410000	-0.33573200
C	0.56083700	-1.42644600	0.80410900
C	-0.36794800	-1.93151600	1.70216200
C	1.69806700	-0.70584500	1.31355000
C	-0.19657700	-1.84216700	3.10594100
C	1.89583200	-0.66005000	2.68344900
C	0.98851900	-1.22713200	3.61139900
H	2.76605200	-0.13437400	3.06828900
H	-3.53638000	-0.23960300	-0.28018300
H	-1.28101500	-2.39433100	1.34197300
C	1.19242100	-1.16937000	5.01599900
C	-1.16457000	-2.34210000	4.01828800
H	2.09767000	-0.70365600	5.39822600
C	0.25011200	-1.68563800	5.87722700
H	0.41029000	-1.63604200	6.95112100
C	-0.94199500	-2.26687900	5.37474500
H	-1.68830300	-2.64350700	6.06860600
H	-2.09026400	-2.75265800	3.62647500
H	5.40070000	2.10754100	-1.46994800
C	4.43149200	-1.68076900	0.96610000
C	6.35185600	-0.19067800	-0.42283900
H	3.69759900	-2.26938000	1.50393300
H	7.08880200	0.39671400	-0.96558500
C	5.72726800	-2.13569800	0.86265900
C	6.70241200	-1.38392000	0.16435600
H	6.00402000	-3.08146200	1.32102000
H	7.72224700	-1.75226600	0.09306600
C	-7.44889400	0.34371600	0.03252000
C	-7.83598000	0.41645300	-1.30132500
C	-6.65435500	0.18947200	-2.02579000
N	-5.63338800	-0.01166000	-1.18556200
H	-8.01030100	0.45276000	0.94929100
H	-8.82610600	0.60474000	-1.68975600
H	-6.49355100	0.16141600	-3.09515500
N	-6.12747400	0.08834600	0.05901800
H	-5.46541800	-0.01758200	0.87961300
Cl	-3.96020000	-0.21538800	2.16311000
H	-2.32927900	2.95868100	-1.97217000
H	-3.69767900	-1.14232900	-1.87545700

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Zero-point correction= 0.769109 (Hartree/Particle)
Thermal correction to Energy= 0.818739
Thermal correction to Enthalpy= 0.819684
Thermal correction to Gibbs Free Energy= 0.679806
E(Solv) = -3311.38810101

Pd	-1.15227100	0.21688300	-1.05650700
P	0.36311700	1.91818400	-0.35139800
P	0.27784900	-1.63855600	-0.74864000
C	0.28167200	3.40183300	-1.46061000
C	0.41746400	4.72264700	-1.00814000
C	0.31964000	5.79271600	-1.90111300
C	0.09220000	5.56004600	-3.25824000
C	-0.04815400	4.24916200	-3.72037500
C	0.03557500	3.18135000	-2.82670500
C	0.09818500	2.61864000	1.33387400
C	1.11303800	3.28069100	2.04685000
C	0.85061700	3.82306100	3.30525300
C	-0.42543400	3.71021000	3.86664500
C	-1.43721000	3.05137700	3.16781200
C	-1.17577000	2.50518700	1.90897600
C	1.75824100	-1.81616900	-1.84656000
C	2.85554000	-2.63610800	-1.54302200
C	3.89661100	-2.79418800	-2.45665900
C	3.85195800	-2.14210200	-3.69181200
C	2.76473200	-1.32642200	-4.00604900
C	1.72545900	-1.16318200	-3.08721600
C	-0.36783600	-3.38144200	-0.82279800

C	-1.46916500	-3.61208100	-1.66061400
C	-1.96803700	-4.90312300	-1.85218100
C	-1.37871200	-5.98425600	-1.19652000
C	-0.28287300	-5.76848200	-0.35685800
C	0.22281200	-4.48066400	-0.17726500
H	0.59052600	4.92049200	0.04461000
H	0.41928900	6.81008500	-1.53168000
H	0.01522500	6.39452800	-3.95028300
H	-0.23719800	4.05834000	-4.77369700
H	-0.10474600	2.16359700	-3.18292700
H	2.10932700	3.36739100	1.62114800
H	1.64290000	4.33338300	3.84781300
H	-0.62549800	4.13230000	4.84829700
H	-2.43498200	2.94570600	3.58337700
H	-1.97600600	1.98725200	1.39054000
H	2.90669400	-3.14668700	-0.58623100
H	4.74567700	-3.42281900	-2.20222800
H	4.66369400	-2.26834000	-4.40342200
H	2.72442500	-0.81382800	-4.96369500
H	0.87942400	-0.52336300	-3.32585200
H	-1.92600900	-2.76632300	-2.16807400
H	-2.81707800	-5.06294100	-2.51222400
H	-1.76837800	-6.98890700	-1.33747800
H	0.18290600	-6.60572200	0.15657400
H	1.07357700	-4.33283500	0.48075900
C	-3.00274300	1.23818100	-1.42465600
H	-3.36255500	1.73792200	-0.52647800
C	-3.22208100	-0.14960600	-1.59698900
H	-3.29304000	-0.55408800	-2.60789700
C	-3.95325500	-0.94785000	-0.54368700
C	2.17525800	1.47385300	-0.36185100
C	2.66419900	0.39070100	0.37754200
C	3.06626500	2.20951100	-1.19339700
C	4.06132300	0.04813900	0.29855600
C	4.39753700	1.88818200	-1.28696900
H	2.68628600	3.05062700	-1.76103200
C	4.93363300	0.80496200	-0.55083900
C	0.88007000	-1.42179900	0.98914500
C	0.20178300	-2.08752200	1.99891900
C	1.81892500	-0.38819900	1.35207800
C	0.40640700	-1.81322400	3.37456700
C	2.02300000	-0.11706700	2.69381600
C	1.34261600	-0.79755000	3.73378500
H	2.73761800	0.65493800	2.96661600
H	-3.73772200	-0.58065200	0.46231400
H	-0.53341800	-2.84517500	1.74601800
C	1.55797900	-0.50928200	5.10765200
C	-0.28808700	-2.50700700	4.40210300
H	2.26896400	0.26823100	5.37604100
C	0.87221800	-1.19931800	6.08243500
H	1.03944700	-0.97064300	7.13144600
C	-0.05979200	-2.20658700	5.72635000
H	-0.59778300	-2.73899900	6.50590800
H	-1.00595900	-3.27542800	4.12524400
H	5.05725200	2.47085800	-1.92594000
C	4.63046200	-1.03878400	1.02537100
C	6.31013000	0.46197400	-0.63451100
H	3.99490400	-1.63022700	1.67375000
H	6.95217100	1.05384200	-1.28281200
C	5.96844900	-1.34921800	0.92163500
C	6.82279900	-0.59181400	0.08524800
H	6.37256600	-2.18339300	1.48928800
H	7.87738500	-0.84438800	0.01504900
C	-7.42164300	0.00403500	-0.39580000
C	-7.55269300	-1.00664600	-1.35286300
C	-6.27045800	-1.52635900	-1.50613100
N	-5.44137900	-0.85918100	-0.68055500
H	-8.15333500	0.66591400	0.04419400
H	-8.45186500	-1.32296800	-1.85917800
H	-5.89402400	-2.31629800	-2.13955700
N	-6.14204000	0.07693700	-0.01657700
H	-5.64113000	0.69999900	0.79857400
Cl	-4.81439000	1.55383900	2.06647300
H	-2.89644700	1.88082600	-2.29695100
H	-3.72165300	-2.01525200	-0.58922900

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Zero-point correction= 0.697245 (Hartree/Particle)

Thermal correction to Energy= 0.742266

Thermal correction to Enthalpy= 0.743210

Thermal correction to Gibbs Free Energy= 0.613327

E(Solv) = -3085.06730844

Pd	1.80179200	0.89040600	-0.33438800
P	1.11880400	-1.37945200	-0.20282900
P	-0.31829600	1.88011300	0.07287200
C	2.22791400	-2.60199800	-1.05920000
C	2.38277100	-3.94043000	-0.66686800
C	3.25893300	-4.78593000	-1.35112900

C	3.98878400	-4.31227600	-2.44247200
C	3.84518300	-2.98235400	-2.84309000
C	2.98015600	-2.13413200	-2.15067400
C	0.91447800	-2.12269400	1.47176200
C	0.13117500	-3.25798500	1.73151000
C	0.07432200	-3.80229900	3.01508400
C	0.80079000	-3.22054200	4.05647100
C	1.57868300	-2.08766300	3.81178300
C	1.63153400	-1.54041700	2.52862700
C	-1.32248300	2.33244000	-1.40565000
C	-2.70144500	2.58982700	-1.35322300
C	-3.39326400	2.98182400	-2.49992200
C	-2.71695900	3.11954800	-3.71417500
C	-1.34718200	2.85901000	-3.77940000
C	-0.65470200	2.46514800	-2.63302000
C	-0.18689500	3.48267500	1.00126800
C	0.83441900	3.58864900	1.96206700
C	1.01147000	4.76237400	2.69427800
C	0.18273400	5.86289600	2.46223800
C	-0.82353900	5.77674600	1.49963300
C	-1.01106300	4.59536000	0.77730700
H	1.83195300	-4.32740400	0.18341800
H	3.37117500	-5.81726700	-1.02667100
H	4.67181200	-4.97182900	-2.97106700
H	4.41681700	-2.59943300	-3.68431200
H	2.88881300	-1.09312300	-2.44779500
H	-0.44580500	-3.71235000	0.93173600
H	-0.54532200	-4.67487500	3.20266500
H	0.75467700	-3.64528400	5.05573700
H	2.14079600	-1.62585300	4.61918600
H	2.22670600	-0.65101600	2.33776000
H	-3.23729300	2.47888400	-0.41489100
H	-4.46182600	3.17199600	-2.44624200
H	-3.25791400	3.42233600	-4.60680500
H	-0.81681100	2.95705100	-4.72292100
H	0.40976100	2.25102700	-2.68247000
H	1.49865700	2.74381200	2.12523800
H	1.80545000	4.82196900	3.43402800
H	0.32699300	6.78325800	3.02179000
H	-1.46731800	6.63090600	1.30602800
H	-1.79683300	4.55033000	0.03092300
C	-0.51830100	-1.57395700	-1.08176000
C	-0.48985100	-2.17397100	-2.37453300
C	-1.71049900	-0.99566200	-0.62366100
C	-1.59347600	-2.19918300	-3.18857400
C	-2.88016000	-1.01963300	-1.46962300
C	-2.81526800	-1.62283100	-2.76773100
C	-1.44689200	0.84703400	1.14473900
C	-1.74098500	1.32090400	2.45639700
C	-1.88672800	-0.42790200	0.76412900
C	-2.43788800	0.56264000	3.36263800
C	-2.62986300	-1.23135800	1.70506500
C	-2.89788900	-0.73095000	3.02054400
H	-1.53996300	-2.67165900	-4.16672600
H	0.42881400	-2.62777100	-2.72569900
H	-1.40862200	2.30962700	2.74765100
H	-2.65034400	0.95491200	4.35454500
C	-3.62518300	-1.52618700	3.94699300
C	-3.12442900	-2.53006800	1.38455800
H	-3.81333700	-1.12238600	4.93905500
C	-4.08487800	-2.77478200	3.59997300
H	-4.64320200	-3.37379400	4.31423700
C	-3.82925700	-3.27734300	2.30191200
H	-4.19472800	-4.26267300	2.02478300
H	-2.94295400	-2.93637000	0.39682300
C	-4.13106400	-0.46671400	-1.06629900
C	-3.96935400	-1.64844600	-3.59646100
C	-5.23442700	-0.50911500	-1.88927300
H	-3.89153900	-2.11194800	-4.57714600
C	-5.15848600	-1.10535300	-3.17022900
H	-4.21496800	-0.00557200	-0.08976000
H	-6.17383200	-0.08023200	-1.55044400
H	-6.03662100	-1.13295700	-3.80961000
Cl	6.56783600	1.22959900	0.08907500
C	3.90597200	1.22853600	-0.79613300
C	3.23374400	2.46294400	-0.66262400
C	4.78142900	0.67080700	0.27069600
H	4.12648600	0.86299500	-1.79846400
H	3.35573800	3.05627100	0.24278800
H	2.97871400	3.04287300	-1.54750800
H	4.85141500	-0.41609000	0.24462800
H	4.49871500	1.00674700	1.26873900