Electronic Supplementary Information

for

A Combined Experimental and Computational Study reveals a Crossover between Conventional Cross-Coupling and Carbene Insertion Pathways in a Pd Catalyzed C(sp^2)-H Insertion

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1. Computational Details

For modelling the electronic structure and thermochemistry of the mechanistic cycle, Gaussian16 software was used.[1] All geometry optimizations were performed with the hybrid functional B3LYP with Grimme's dispersion GD3, while using the standard split valence Pople's basis set 6-31G(d,p) for all atoms except for Pd.[2] For Pd, LANL2DZ basis was used with an effective core potential (ECP).[3] The use of the B3LYP functional with standard split valence Pople's basis set has been shown to give reliable geometries for stationary point calculations on metallocarbene systems.[4] The frequency analysis on these stationary points was carried out to verify their nature (minima/saddle point) and obtain thermal corrections to the electronic energy.[5] For the TSs (transition states), IRC (Intrinsic Reaction Coordinate) calculations were done to link the TS with its corresponding minima.[6] Single point calculations were performed on the optimized structures using the triple zeta basis set 6-311+G(d,p) for all the atoms except for Pd for which LANL2DZ was used. All these single points were computed using B3LYP functional with Grimme's dispersion GD3, using an SMD (solvation model density) solvation model to simulate the solvation effects of DCM (dichloromethane).[7-8] The thermal corrections obtained from the geometry optimizations were added to the single-point electronic energies to give the thermochemical values (in this case, the Free Energies). Single points of key TSs and intermediates were also done at different functionals and basis sets to check if the trend is same including high-level *ab initio* DLPNO-CCSD(T) (domain based local

pair natural orbital coupled cluster method with single-, double- and perturbative triple excitations) calculations using the ORCA 5.0.4 software, wB97XD and M06 using Gaussian 16 software.[1,9-10] SambVca 2.1 was used for calculating percentage free volume (%V_f) for generating steric maps in key intermediates.[11] COPASI software was used to perform microkinetic modelling.[12]

2. Experimental Details

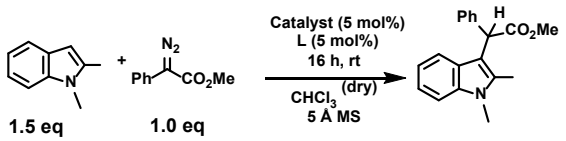
NMR spectra were recorded on a Bruker Ultrashield spectrometer at 400 MHz (for ^{1}H NMR). Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as internal standard [$CDCl_3$: δ 7.26 for ^{1}H NMR]. For ^{1}H NMR, data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, dd = double doublet, ddd = doublet of doublet of doublets, t = triplet, q = quartet, quint = quintet, sept = septet, m = multiplet), coupling constants (Hz) and integration. All spectra were processed with MestReNova x64 software package. High resolution mass spectrometry was performed on a Waters XEVO G3 QTof instrument. UV-Vis measurements were done on Shimadzu UV 2600i spectrophotometer with 1 cm pathlength cuvette of 1 mL size.

Unless stated otherwise, all reactions were carried out with distilled and dried solvents under an atmosphere of nitrogen or argon in oven (120 °C) dried glassware with standard vacuum-line techniques. Organic solvents used for carrying out reactions were dried using standard methods. $Pd(PhCN)_2Cl_2$], [$Pd(OAc)_2$], [$PdbpyCl_2$], [$Pd_2(dba)_3$], [$Pd(OH)_2$], 2,2'-bipyridine, $Sc(OTf)_3$ were purchased from Sigma-Aldrich, $NaBAr^F$ and D_2O were purchased from TCI, 1,2-dimethyl-1*H*-indole and diphenylphosphate were acquired from BLD Pharma and were used as received. 1,2-dimethyl-1*H*-indole-3-*d* and methyl-α-diazo-α-phenylacetate were synthesized from commercially available reagents according to standard protocols.[13] All work up and purification were carried out with reagent grade solvents in air. Thin-layer chromatography (TLC) was performed using Merck silica gel 60 F254 precoated plates (0.25 mm). Column chromatography was performed using silica gel (100-200 mesh). NMR yields

were determined by using mesitylene as the internal standard. Unless otherwise noted, all reported yields of the indole-alkylation reactions correspond to NMR yields.

3. Active Catalytic Species A

Table S1 Formation of Indole Alkylated Product in Different Conditions



S.No.	Catalyst	Additive	Ligand (L)	Yield (%)[b]
1[a]	$[Pd(PhCN)_2Cl_2]$	$NaBAr^F$	bpy	87
2[a]	$[PdbpyCl_2]$	$NaBAr^F$	-	49
3	$[PdbpyCl_2]$	-	-	35
4[a]	$[Pd(OAc)_2]$	$NaBAr^F$	bpy	83
5	$[Pd(OAc)_2]$	-	bpy	0
6[a,c]	$[Pd(OAc)_2]$	$Sc(OTf)_3$	-	80
7[a]	$[Pd_2(dba)_3]$	$NaBAr^F$	bpy	27
8	$[Pd(OH)_2]$	-	bpy	0

[a]12 mol% additive is used. [b]NMR yield is measured from the crude mixture using mesitylene as an internal standard. [c]Molecular-sieves are not added.

Apart from literature precedence and DFT calculations, the choice of the active catalytic species, **A** is also based on experimental observations, where the carbene insertion reactions were shown to proceed with a much lower yield in the absence of $NaBAr^F$.[14] Apart from the yield, in a few reported cases, the *ee* also reduces drastically.[15] In Zhou's procedure for preparation of indole alkylated product (Table S1, entry 1), the use of $NaBAr^F$ is more than twice the amount of the Pd catalyst indirectly suggests the abstraction of both chloride ions resulting in a dicationic Pd complex to which the chiral ligand can subsequently coordinate.[14a]

To further confirm we carried out the full reaction, *i.e.*, C3–H insertion of 1,2-dimethyl-1*H*-indole using methyl-α-diazo-α-phenylacetate as the carbene precursor using [Pd(bpy)Cl_2] catalyst (with and without $NaBAr^F$), which resulted in a much lower yield, ruling out the substitution of PhCN ligand with bpy ligand in the actual reaction with [Pd$(PhCN)_2Cl_2$] catalyst. It also suggests that the presence of PhCN ligand is important in active catalytic species. (Table 1, entries 2 & 3)

We also carried out the reaction with [Pd$(OAc)_2$] catalyst with and without $NaBAr^F$ and found no product formation in its absence. However, upon addition of $NaBAr^F$ a substantial yield of 83% is obtained (Table 1, entries 4 and 5). These findings highlight the importance of $NaBAr^F$ in removing the acetate groups and generating an active catalytic species like **A**. Additionally, we conducted the reaction using the Lewis acid Sc$(OTf)_3$ instead of $NaBAr^F$ with the [Pd$(OAc)_2$] catalyst, achieving an 80% yield. (Table 1, entry 6). Sc$(OTf)_3$ may act as an acetate scavenger, generating a species like **A**. Another possibility is a synergistic effect between Pd(II) and Sc(III) in activating the C–H bond of indole and facilitating CMD as observed in literature where reaction proceeds by heterobimetallic Pd(II)/Sc(III)-catalyzed oxidative coupling of an indole with an olefin.[16] However, this represents a different mechanism that would not occur under our actual reaction conditions. We found reduced yield (Table S1, entry 7) on employing [$Pd_2(dba)_3$] using standard condition from Zhou's procedure, precluding the possibility of Pd(0) acting as an active catalyst.

We explored the potential for hydrolysis of Pd(II) species, which is commonly observed in Au catalysis leading to the formation of a Au-OH species.[17] Prior studies have indicated a low dissociation constant for the hydrolysis of Pd complexes.[18] Furthermore, it is also known that ligands like acetonitrile or benzonitrile coordinate with the available free sites on these dicationic palladium complexes and stabilize them to prevent the formation of μ-OH dimer that is known to be catalytically inactive.[19] On performing the reaction with [Pd$(OH)_2$] (supported

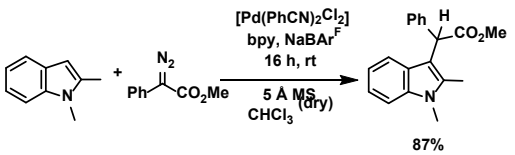
on carbon), we did not observe any alkylated indole product, (Table 1, entry 8) which further precludes the possibility of reaction being catalysed by a Pd–OH species.

To address the possibility of a C–H activation process, one of the most found mechanisms in Pd catalyzed C-H activation is the CMD in the presence of a base (either external or ligated to the metal centre). In the absence of any external base or any such species (Pd–OH/Pd–Cl) that can abstract this proton under the reaction conditions (Table 1, entry 1), CMD is ruled out.

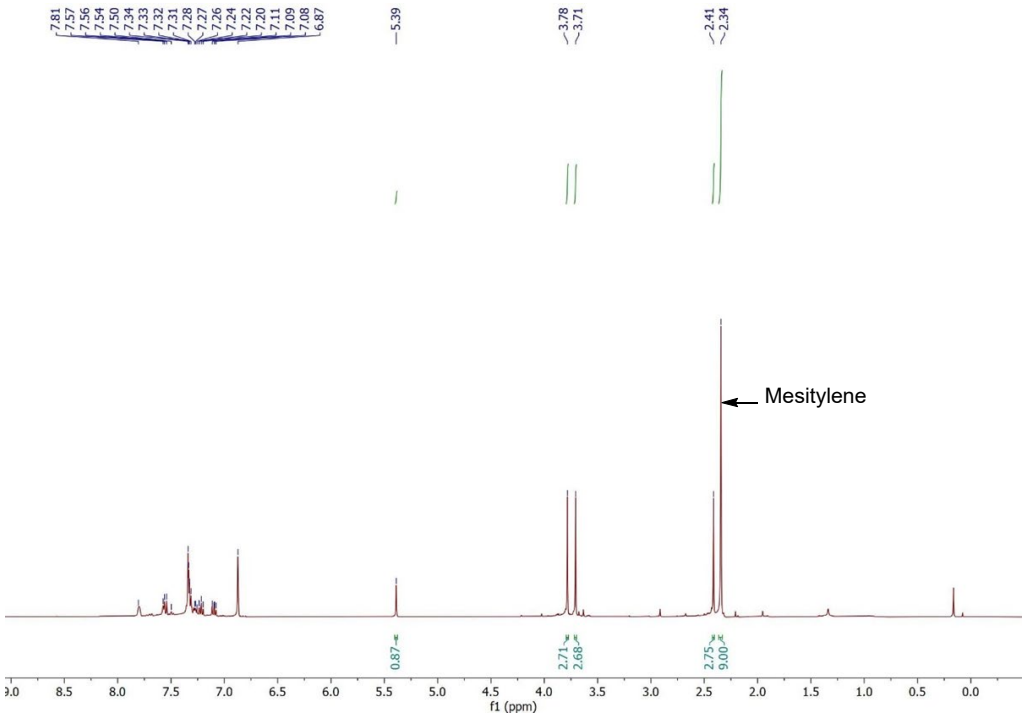
3.1. Procedure with respective NMRs for formation of Indole Alkylated Product in Different conditions

Entry 1

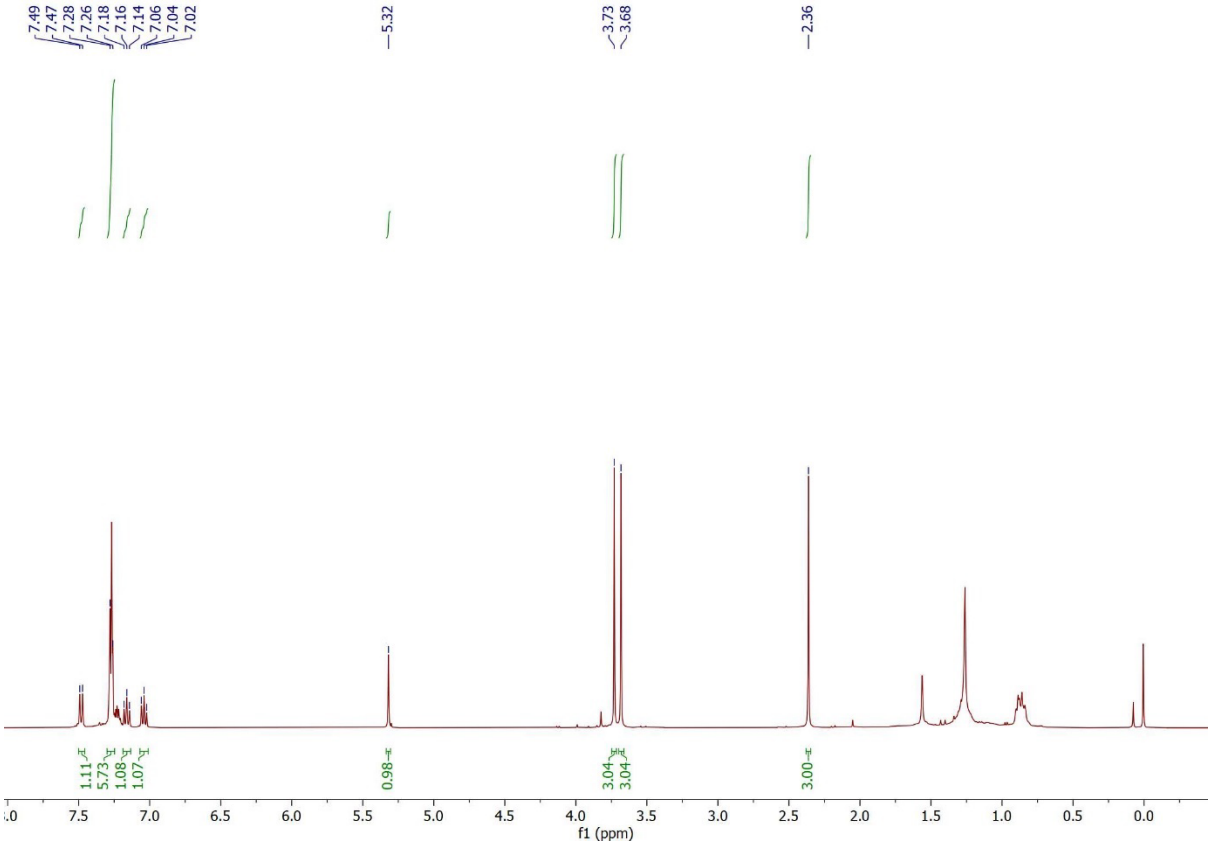
Procedure: Used the following procedure by Zhou *et al* - powdered $[Pd(PhCN)_2Cl_2]$ (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.024 mmol, 12.0 mol%), and 200 mg 5 Å molecular sieves were introduced into an oven-dried Schlenk tube under argon.[14a] After chloroform (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under argon for 1 h. 1,2-dimethyl-1*H*-indole (43.6 mg, 0.30 mmol) and methyl-α-diazo-α-phenylacetate (35.4 mg, 0.20 mmol) was then introduced in one portion. The resulting mixture was stirred at 30°C under argon till 16 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. 28 μL mesitylene was added as an internal standard. The crude reaction mixture was then subjected to ^{1}H NMR for analysis. For purification, after filtering and removing solvent under vacuum, the pure product was isolated by flash chromatography (petroleum ether/ethyl acetate=30:1, v/v).

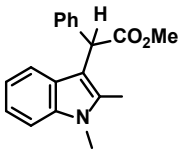


^{1}H NMR (400 MHz, $CDCl_3$) for crude reaction mixture:



^{1}H NMR (400 MHz, $CDCl_3$) for pure indole alkylated product (methyl 2-(1,2-dimethyl-1H-indol-3-yl)-2-phenylacetate):

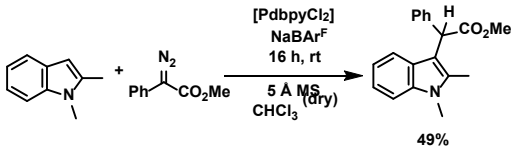




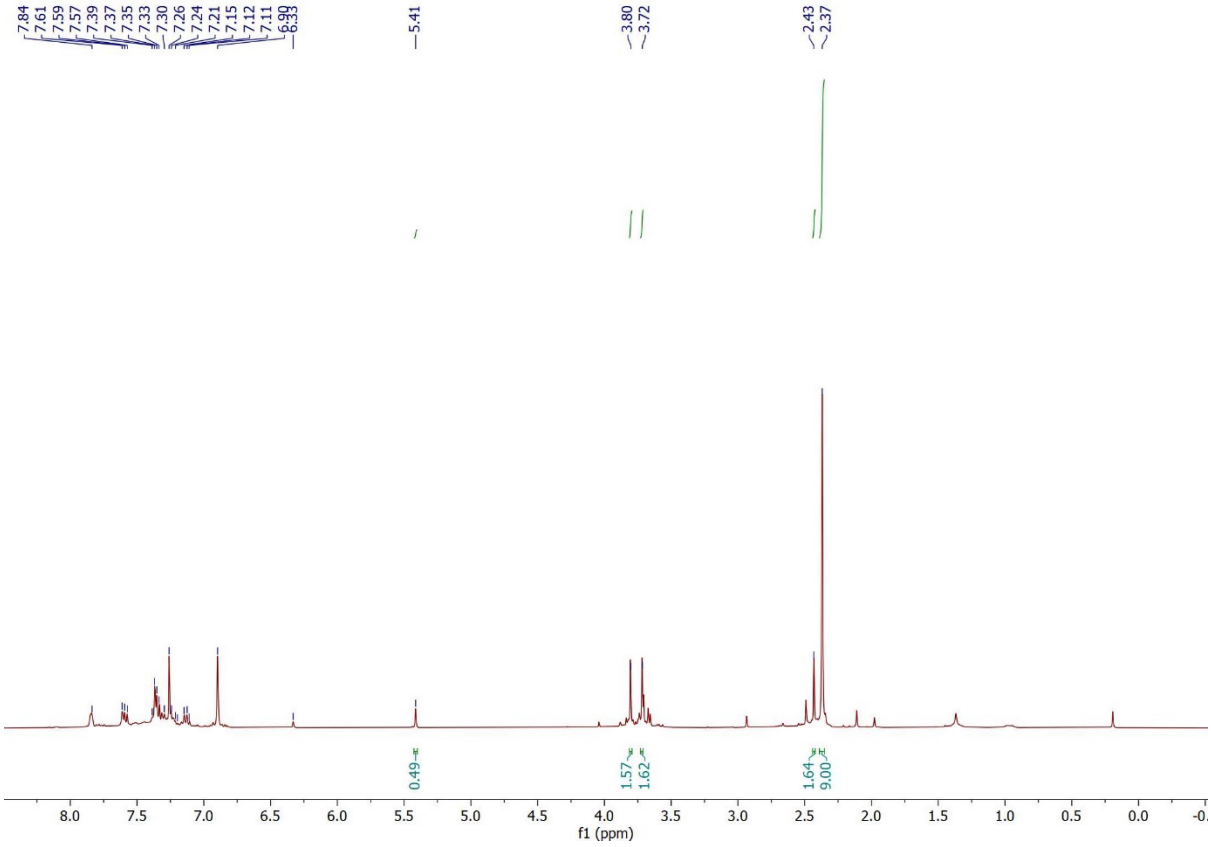
^{1}H NMR (400 MHz, $CDCl_3$): δ 2.36 (s, 3H), 3.68 (s, 3H), 3.73 (s, 3H), 5.32 (s, 1H), 7.02-7.06 (m, 1H), 7.14-7.18 (m, 1H), 7.26-7.28 (m, 6H), 7.47-7.49 (m, 1H)

Entry 2

Procedure: Powdered [$PdbpyCl_2$] (3.3 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.4 mg, 0.024 mmol, 12.0 mol%), and 200 mg 5 Å molecular sieves were taken as catalytic mixture and procedure given in entry 1 (standard procedure by Zhou[14a]) was followed.

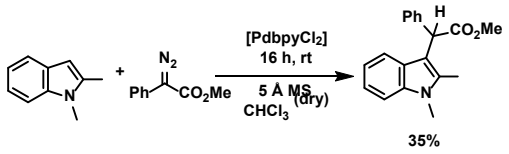


^{1}H NMR (400 MHz, $CDCl_3$):

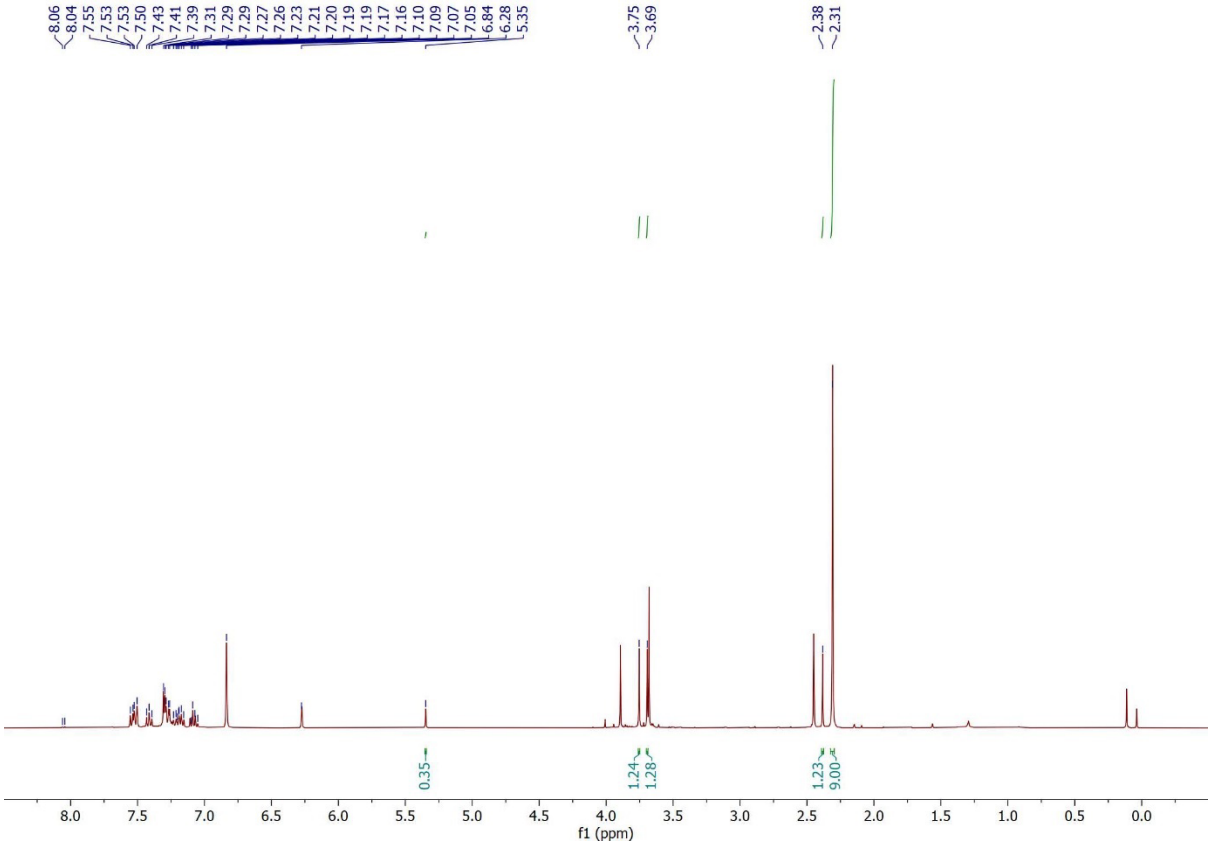


Entry 3

Procedure: Powdered [$PdbpyCl_2$] (3.3 mg, 0.01 mmol, 5.0 mol%), 200 mg 5 Å molecular sieves were taken as catalytic mixture and procedure given in entry 1 was followed.

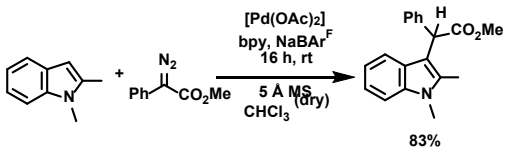


^{1}H NMR (400 MHz, $CDCl_3$):

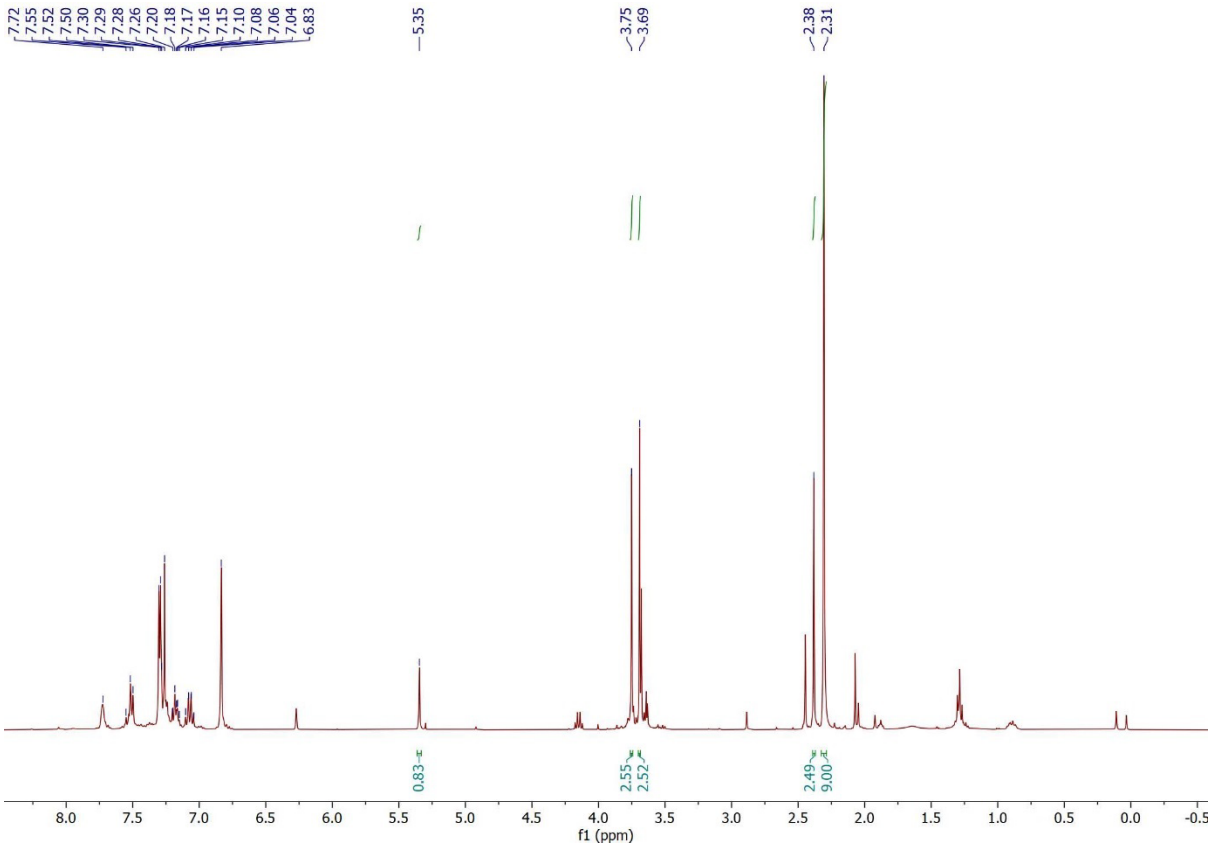


Entry 4

Procedure: Powdered [$Pd(OAc)_2$] (2.3 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.024 mmol, 12.0 mol%), and 200 mg 5 Å molecular sieves were taken as catalytic mixture and procedure given in entry 1 was followed.

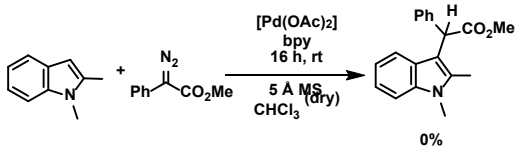


^{1}H NMR (400 MHz, $CDCl_3$):

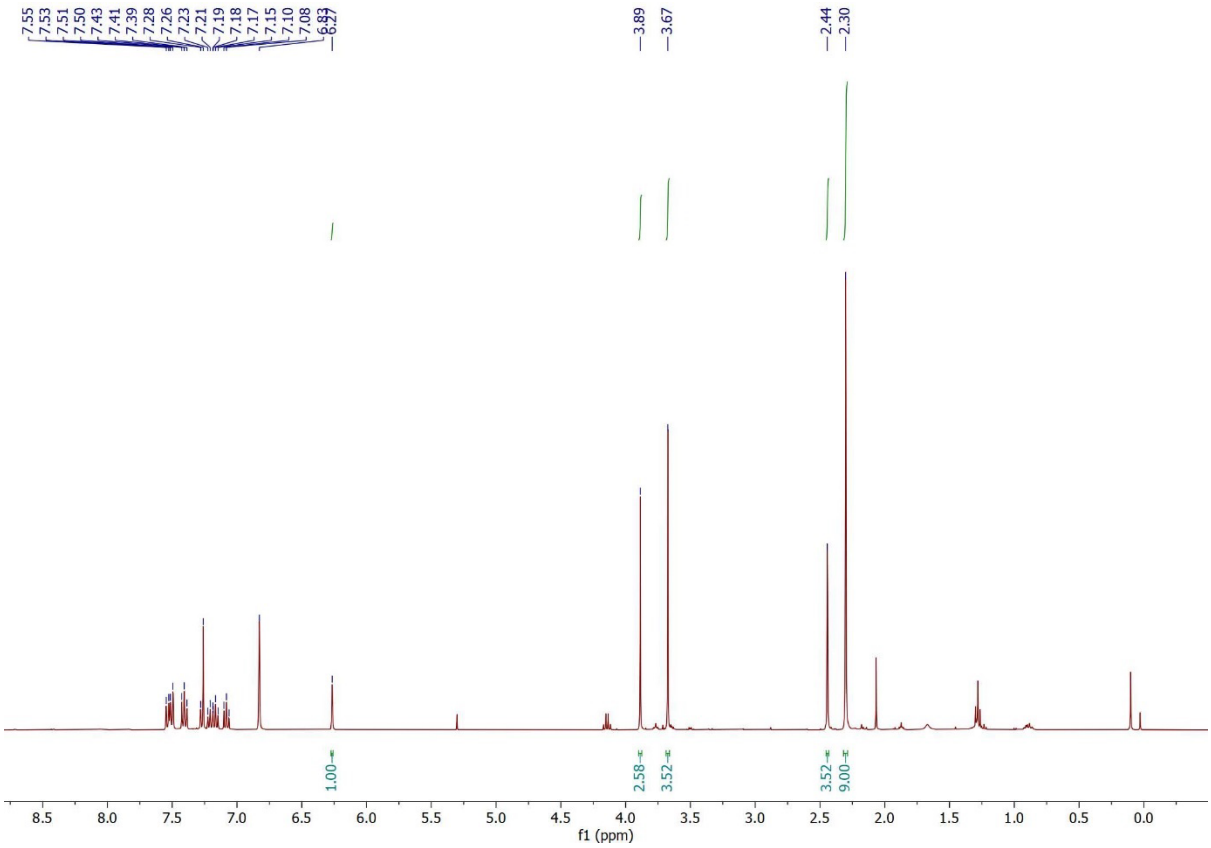


Entry 5

Procedure: Powdered [$Pd(OAc)_2$] (2.3 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), and 200 mg 5 Å molecular sieves were taken as catalytic mixture and procedure given in entry 1 was followed.

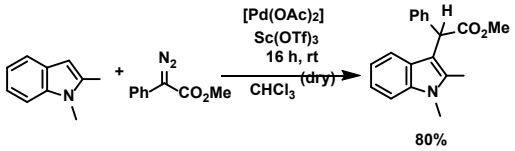


^{1}H NMR (400 MHz, $CDCl_3$):

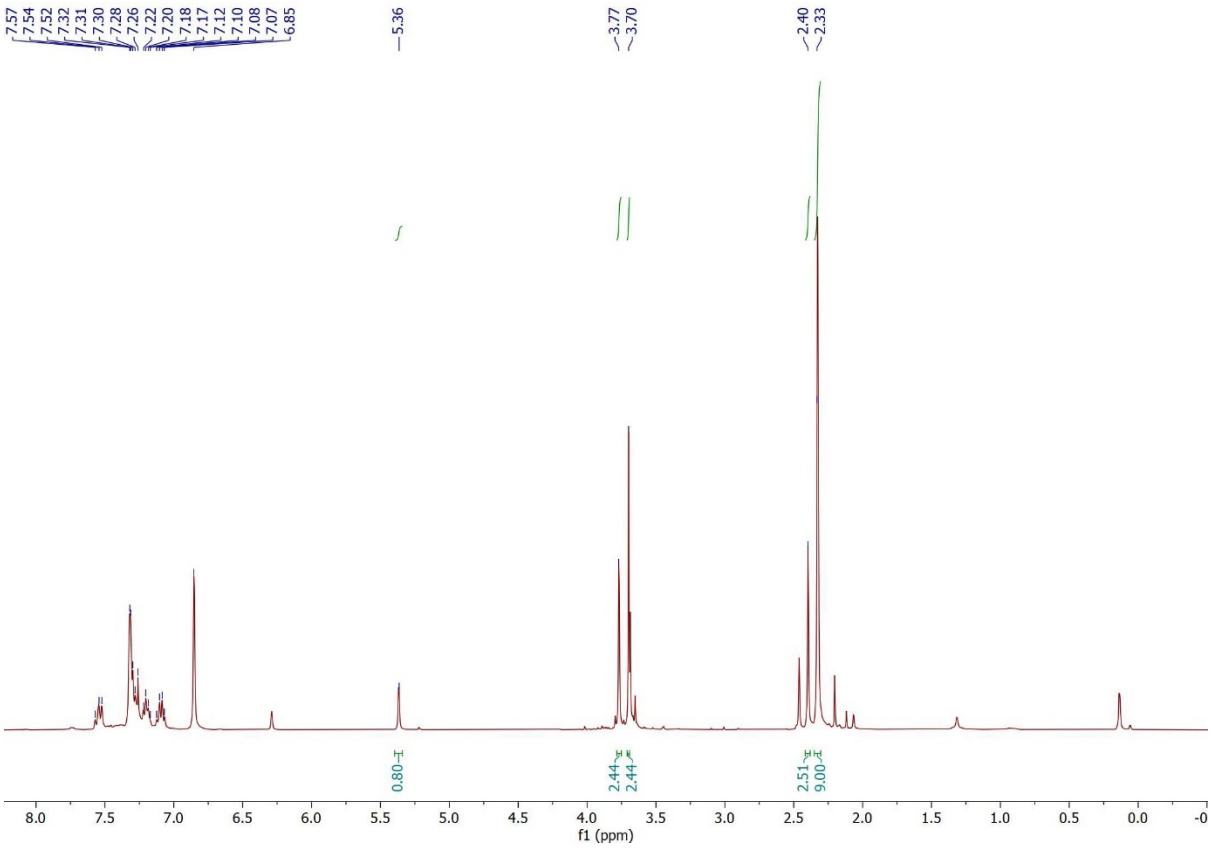


Entry 6

Procedure: Powdered [$Pd(OAc)_2$] (4.5 mg, 0.02 mmol, 10.0 mol%), $Sc(OTf)_3$ (19.7 mg, 0.04 mmol, 20.0 mol%) and 1,2-dimethyl-1*H*-indole (43.6 mg, 0.30 mmol) were introduced into an oven-dried Schlenk tube under argon. After chloroform (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under argon for 1 h. Then methyl-α-diazo-α-phenylacetate (35.4 mg, 0.20 mmol) was introduced, following which the resulting mixture was stirred at 30°C under argon till 16 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. 28 µL mesitylene was added as an internal standard. The crude reaction mixture was subjected to ^{1}H NMR for analysis.

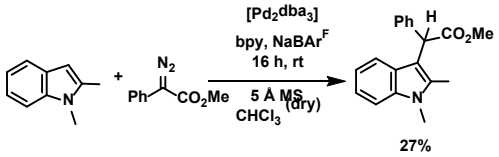


^{1}H NMR (400 MHz, $CDCl_3$):

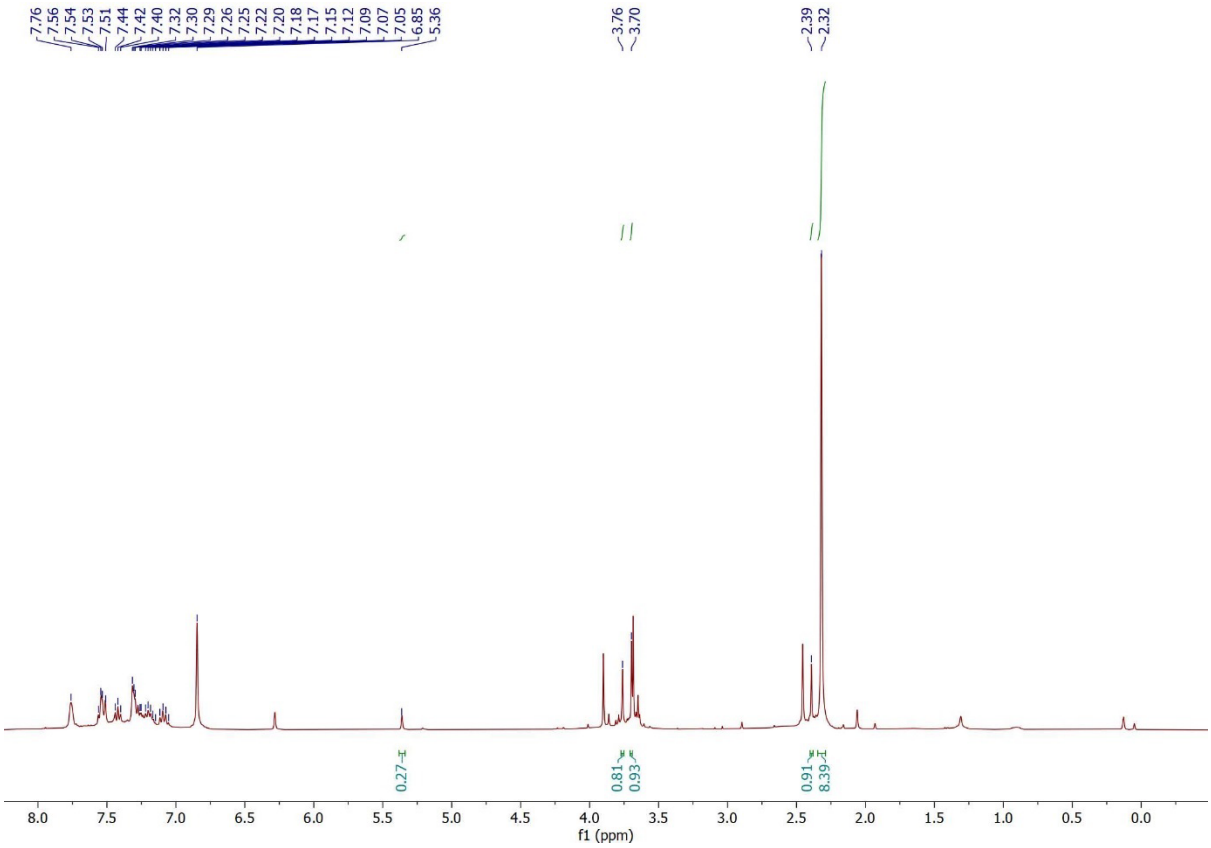


Entry 7

Procedure: Powdered $[Pd_2(dba)_3]$ (4.6 mg, 0.005 mmol, 2.5 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.024 mmol, 12.0 mol%), and 200 mg 5 Å molecular sieves were taken as catalytic mixture and procedure given in entry 1 was followed.

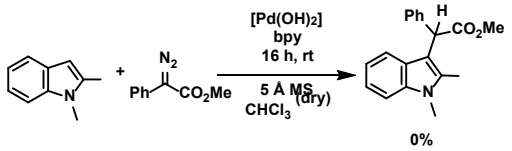


^{1}H NMR (400 MHz, $CDCl_3$):

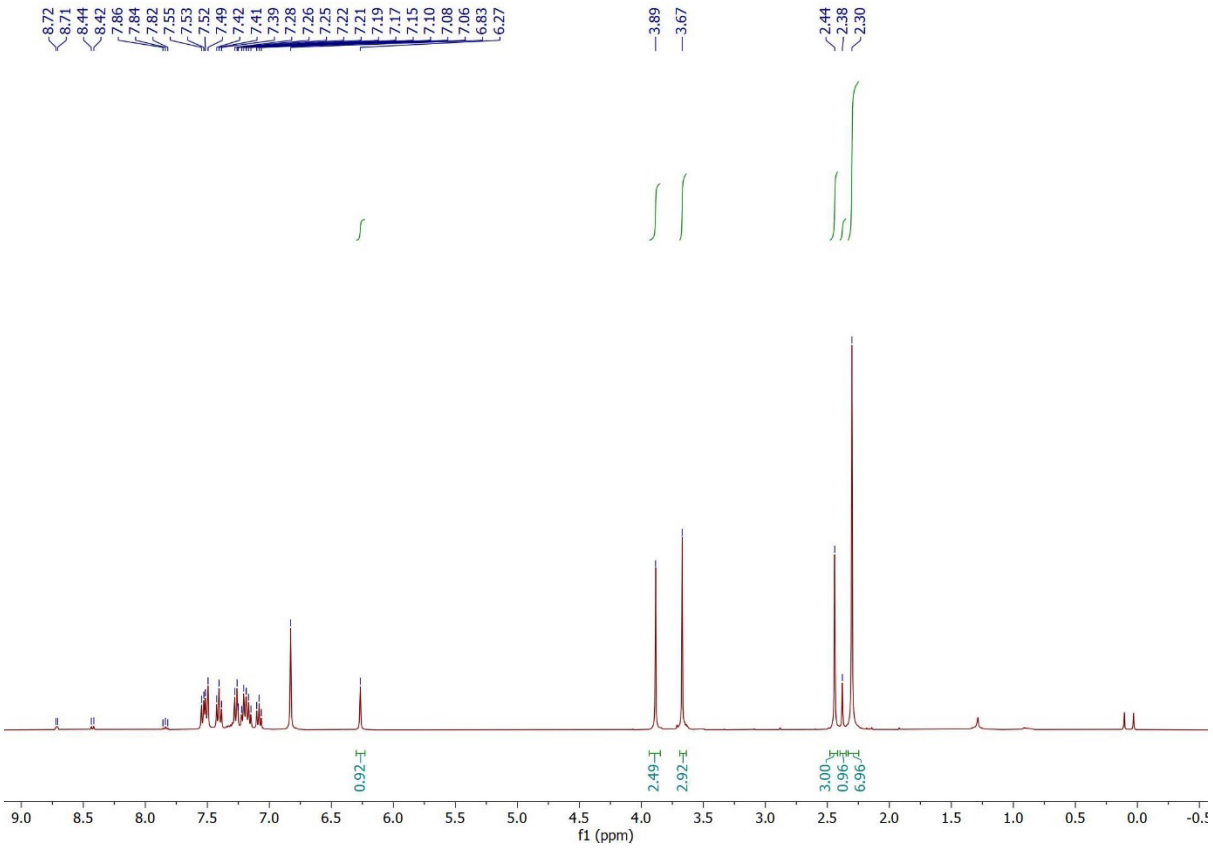


Entry 8

Procedure: Powdered [$Pd(OH)_2$] (20 wt% loading (dry basis), matrix carbon, wet support) (22.4 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), 200 mg 5 Å molecular sieves were taken as catalytic mixture and procedure given in entry 1 was followed.



^{1}H NMR (400 MHz, $CDCl_3$):



3.2. UV-Vis Experiment

Powdered [$Pd(PhCN)_2Cl_2$] (3.9 mg, 0.01 mmol), 2,2'-bipyridine (1.6 mg, 0.01 mmol), $NaBAr^F$ (21.3 mg, 0.024 mmol) was weighted in an oven-dried Schlenk tube under argon atmosphere. Chloroform (1.0 mL) was injected into the Schlenk tube and the solution was stirred at 30°C under argon for 1 h. After 1 h, the solution was diluted with chloroform to make 50 µM of resulting solution and UV-Vis spectra was recorded. Similarly, 50 µM solution of [$Pd(PhCN)_2Cl_2$] as well as [$PdbpyCl_2$] were also prepared and their UV-Vis spectra was also recorded. (**Fig. S1**)

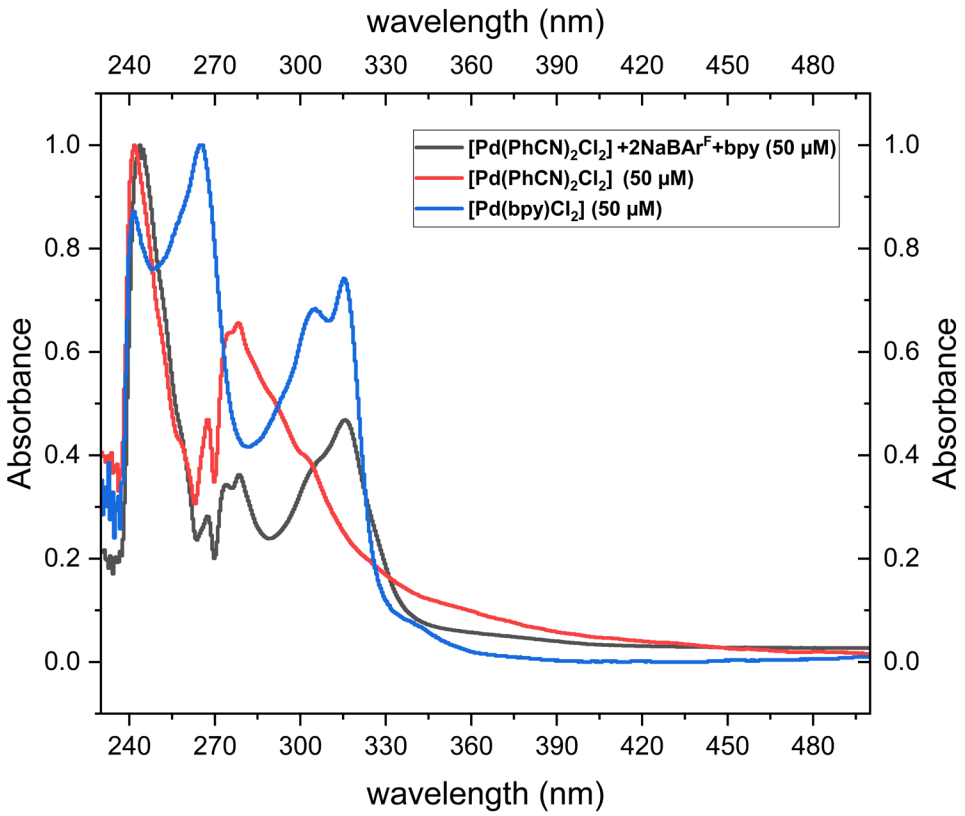


Fig. S1 UV-Vis Spectra for $[Pd(PhCN)_2Cl_2]$ + bpy + $NaBAr^F$ mixture, $[Pd(bpy)Cl_2]$ and $[Pd(PhCN)_2Cl_2]$.

4. Additional Higher Energy Pathways for Active Species A and Stereodetermining TSs

4.1. Oxidative addition pathway

Fig. S2 shows the oxidative addition of Pd(II) into indole C3–H bond with an activation free energy barrier of 52.5 kcal/mol via **TS(X-Y)** and thus was not considered further.

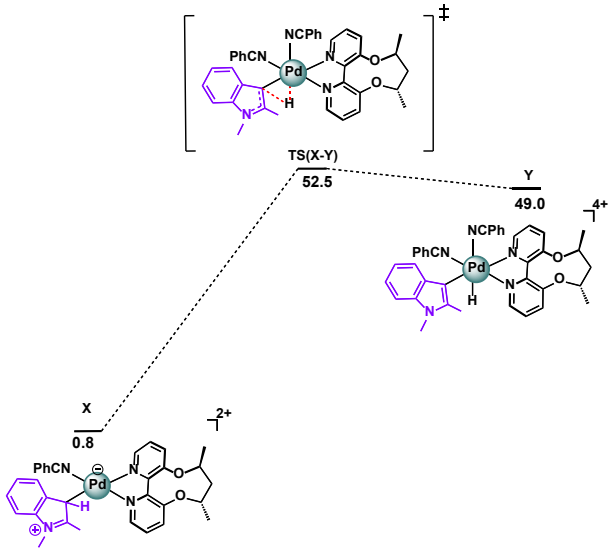


Fig. S2 Free Energy Profile for Oxidative Addition of Indole in Dicationic Pd Pathway showing Formation of Product **P**. Relative Free Energies (kcal/mol) with respect to **A** are at the $SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) Level of Theory.

4.2. 1,2-proton transfer

The 1,2-proton transfer takes place in the zwitterion **D** leading to the formation of product **P**. **TS(D-P)** shows proton transfer from Pd(II) side and **TS(G-P)** shows proton transfer from the face opposite to Pd(II) catalyst. These pathways require an activation free energy barrier of 49.3 kcal/mol, which is not achievable at room-temperature.

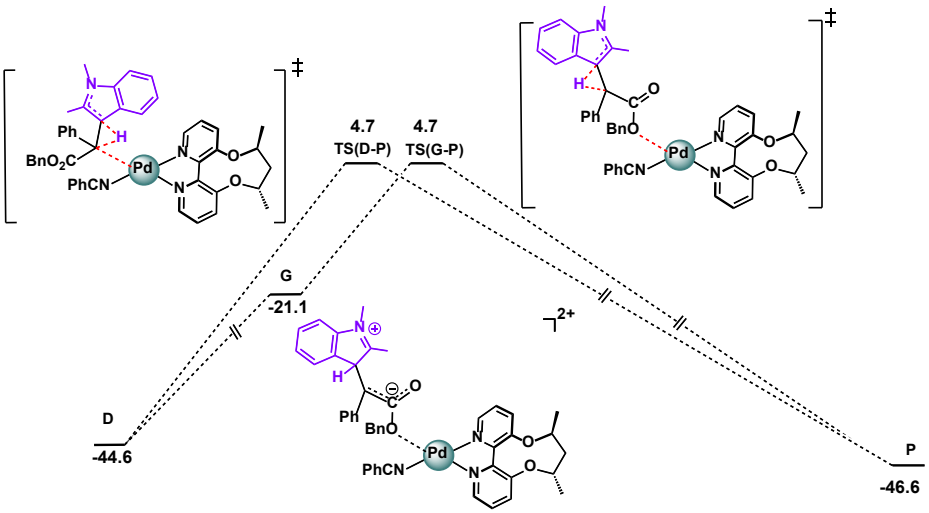


Fig. S3 Free Energy Profile for 1,2-Proton Transfer in Dicationic Pd Pathway showing Formation of Product **P**. Relative Free Energies (kcal/mol) are given at the $SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory.

4.3. 1,2-proton transfer and 1,4-proton transfer in metal enolate species

Fig. S4 shows the formation of the metal-enolate intermediate $\mathbf{D_2}$ from **D**. Once formed, $\mathbf{D_2}$ can undergo a 1,2-proton transfer via $\mathbf{TS(D_2\text{-}P)^b}$ and $\mathbf{TS(D_2\text{-}P)^t}$. $\mathbf{TS(D_2\text{-}P)^b}$ represents proton transfer happening from the same face on which Pd(II) catalyst is present while $\mathbf{TS(D_2\text{-}P)^t}$ represents the one where proton transfer occurs from the face opposite to the Pd(II) catalyst. Both TSs have high activation free energy barriers (41.0 kcal/mol and 47.3 kcal/mol, respectively). $\mathbf{D_2}$ can undergo a 1,4-proton transfer and form the metal associated enol species, $\mathbf{E_b}$. $\mathbf{E_b}$ can be converted to $\mathbf{E_a}$ via dissociation-association of enol from Pd. As discussed in enol pathway in main text already, 1,3-proton transfer from enol species shows preventively high barrier and is not considered further. $\mathbf{D_{free}}$ converges to cyclopropylindoline intermediate.

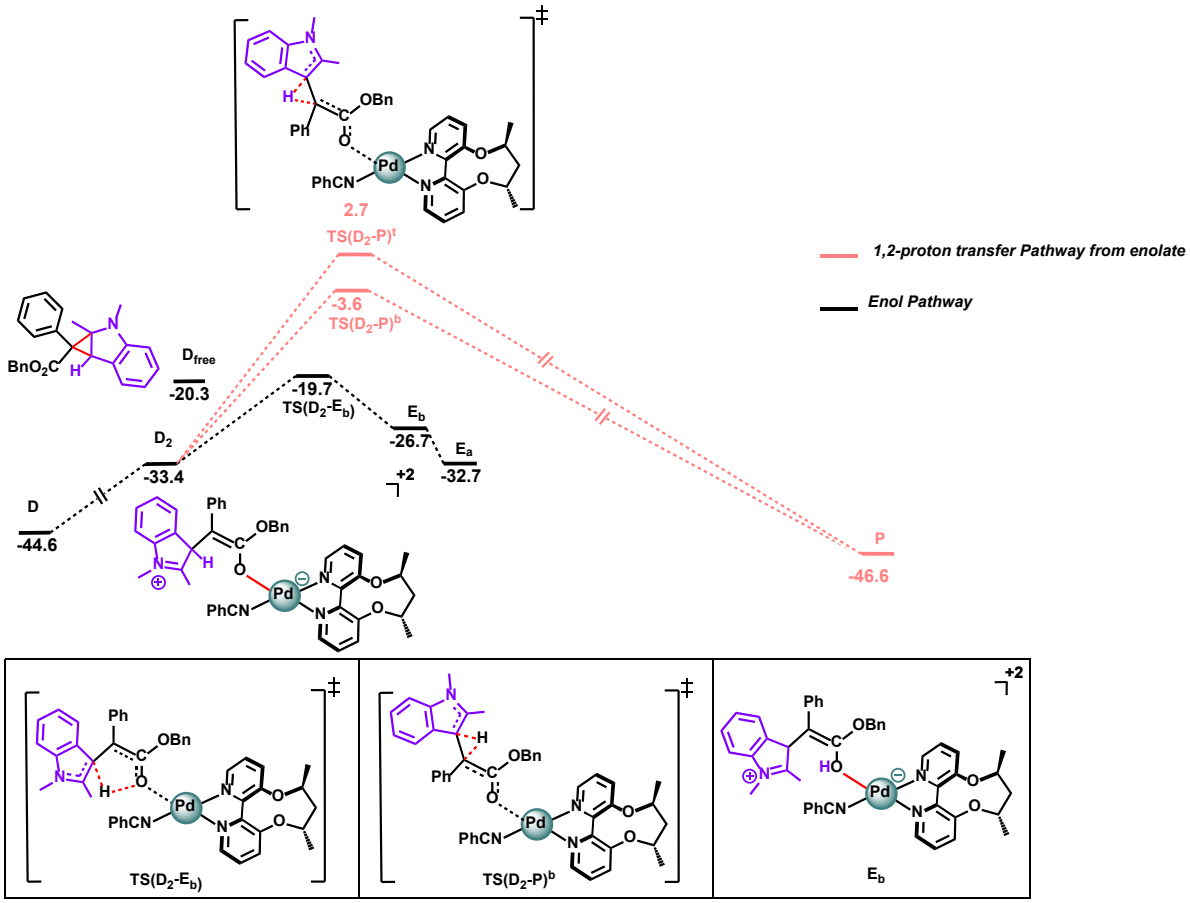


Fig. S4 Free Energy Profile for Metal-enolate Pathway in Dicationic Pd Pathway showing Formation of Product **P**. Relative Free Energies (kcal/mol) are given at the $SMD_{(DCM)}$/B3LYP -D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p), LANL2DZ(Pd) Level of Theory.

4.4. TSs showing unassisted and assisted 1,4-proton transfer from D

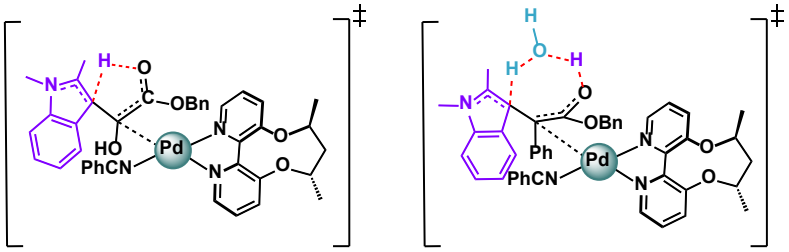


Fig. S5 Relative Free Energies (kcal/mol) (w.r.t. **A**) of TSs leading to 1,4-Proton Transfer under No Assistance and One Water Molecule Assistance in Dicationic Pd Complex at the $SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) Level of Theory.

4.5. Intermediate E in different binding modes

Following the 1,4-proton transfer in **D**, metal free or metal-associated enol species can be formed. Due to the fluxional metal coordination of such an enol species, several binding modes are possible via the different possible ligating sites in the enol. **Fig. S6** shows the enol intermediates in different binding modes with metal. $\mathbf{E_a}$ and $\mathbf{E_c}$ are the most stable intermediates. Following the formation of these enol species, 1,3-proton transfer happens. We only considered final proton transfer from $\mathbf{E_a}$ as it is the most stable species.

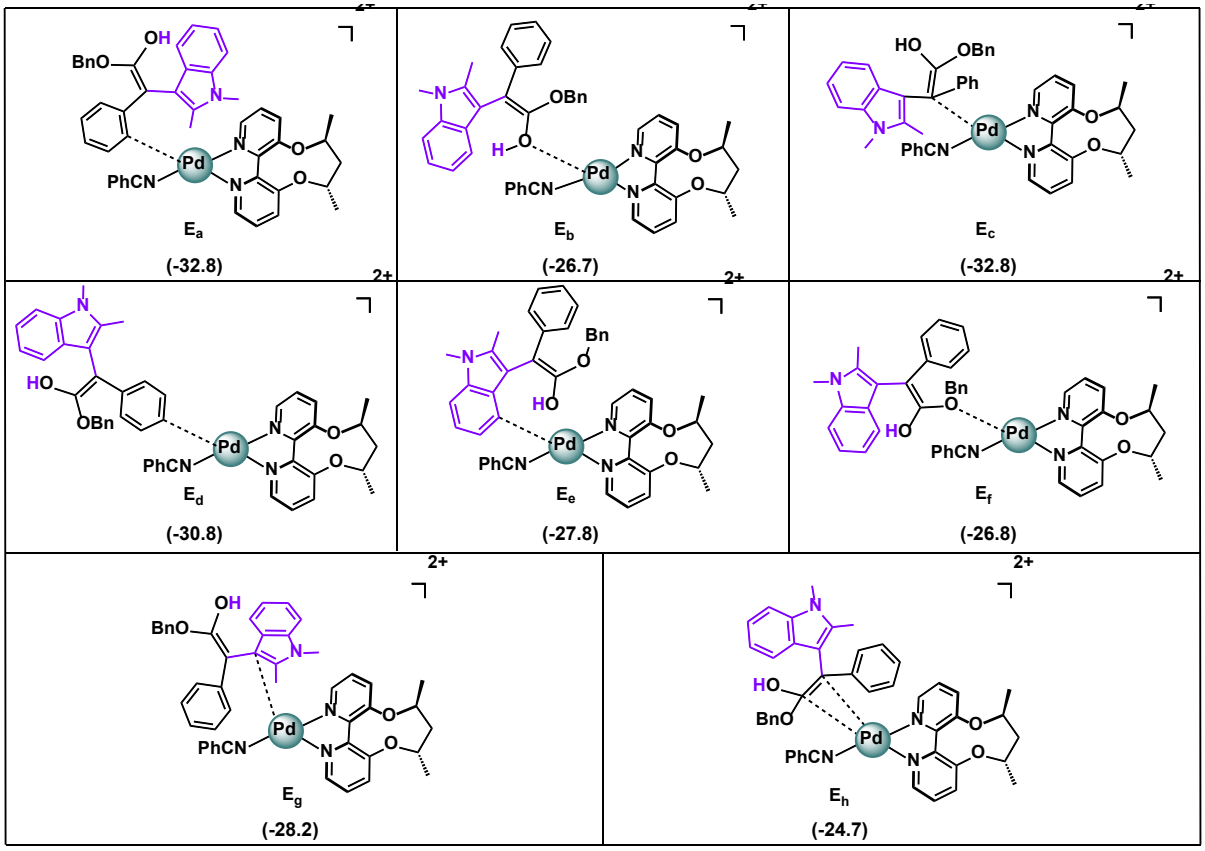


Fig. S6 Relative Free Energies (kcal/mol) (w.r.t. **A**) of Enol Intermediates bound to Dicationic Pd Complex in Different Binding Modes at the $SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) Level of Theory.

4.6. 1,3-proton transfer from $\mathbf{E_a}$

Fig. S7 (a) shows an unassisted and water assisted 1,3-proton transfer from $\mathbf{E_a}$. Two water assisted 1,3-proton transfer is found to be of the lowest energy amongst these. Metal-free unassisted proton transfer and enol assisted proton transfer are also found to be of higher energy. Optimized geometry of $TS(E_a\text{-}P)_{2wat}$ is also given in **Fig. S7(b)**.

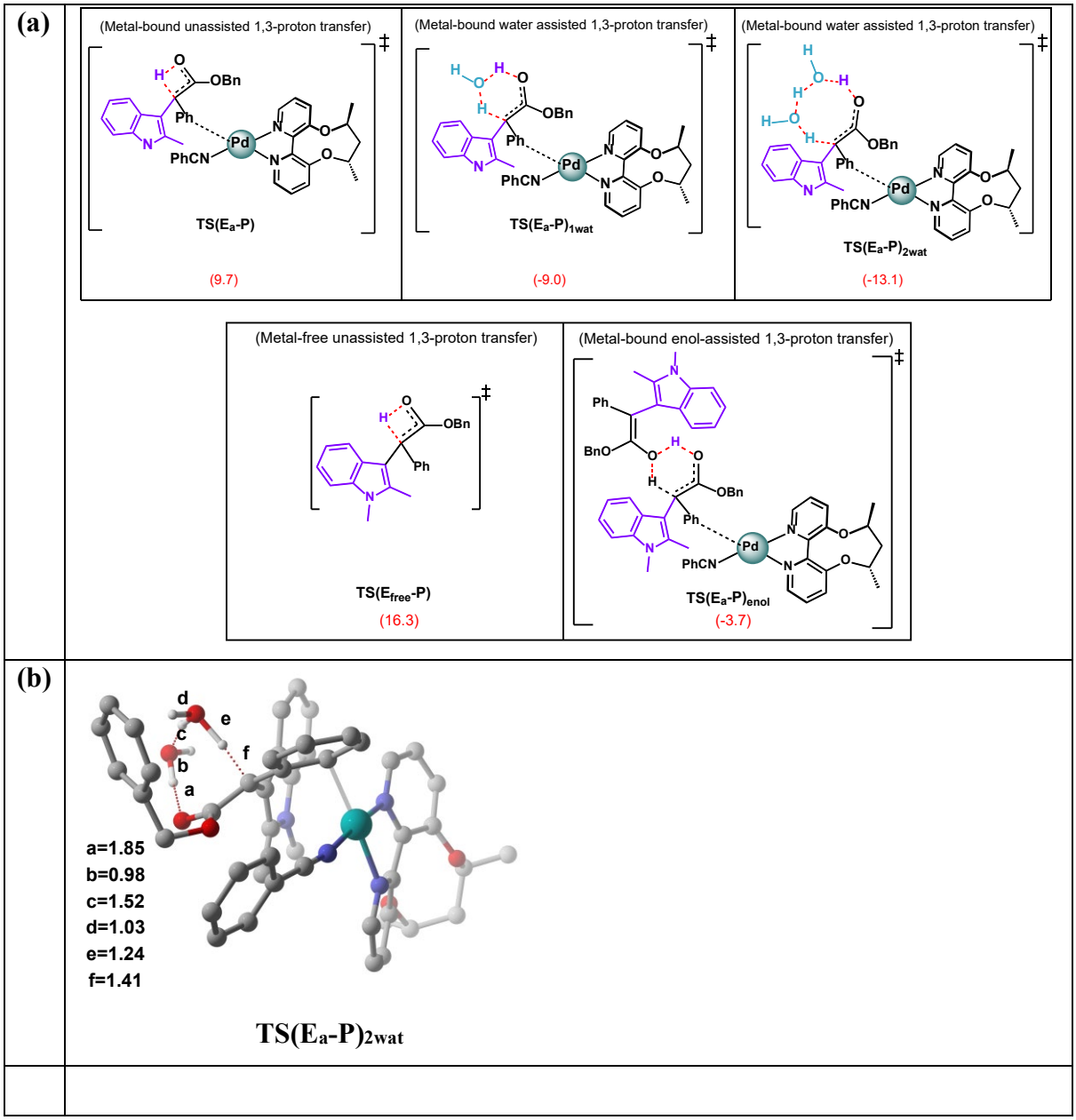


Fig. S7 (a) Relative Free Energies (kcal/mol) (w.r.t. **A**) of 1,3-Proton Transfer TSs with Varying Number of Water molecules at the $SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory. (b) Optimized Geometry of **$TS(E_a\text{-}P)_{2wat}$**. Hydrogens are removed for clarity. Distances are given in Å.

4.7. Optimized geometries corresponding to TS(A-B)$_R$ and TS(A-B)$_S$

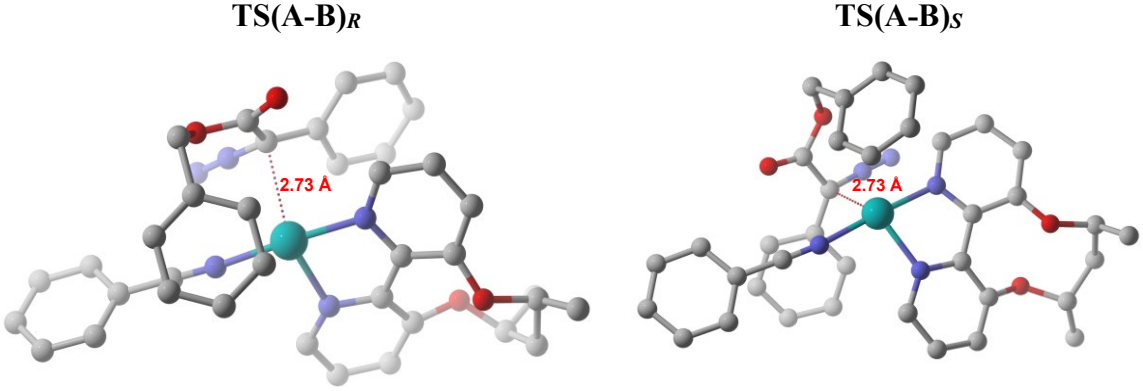
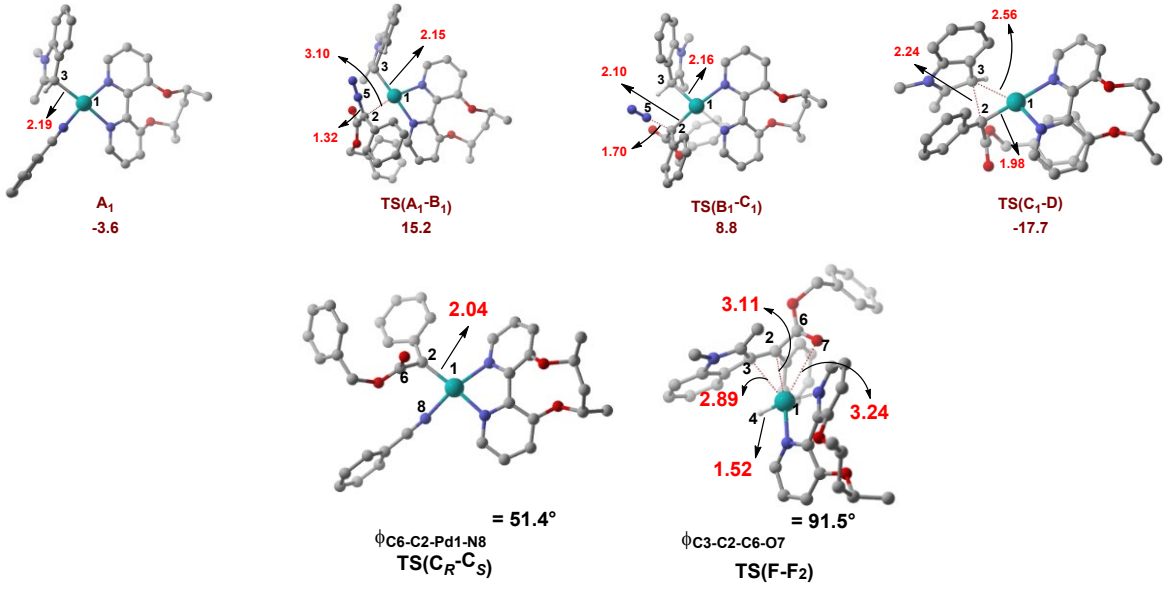


Fig. S8 Optimized Geometries of **TS(A-B)$_R$** and **TS(A-B)$_S$**. Free energies are given at the SMD$_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) Level of Theory. Hydrogens are removed for clarity.

4.8. Optimized Geometries of Additional TSs

(a)



(b) **(c)**

Fig. S9 Optimized Geometries of intermediates and TSs. Hydrogens are removed for clarity and distances are give in Å.

Fig. S9 (a) shows optimized geometries of intermediate **A$_1$** and TSs corresponding to cross-coupling pathway generating zwitterion **D**.

Fig. S9 (b) shows the optimized geometry of **TS(C$_R$-C$_S$)** showing rotation about C=Pd bond. Metallocarbene **C$_R$** can be converted to **C$_S$** (*R* and *S* represents stereochemistry of final product

formed by further reaction on these respective metallocarbenes) via this TS. Dihedral angle about C6-C2-Pd1-N7 is 51.4°. Pd1-C2 bond distance is 2.04 Å.

Fig. S9 (c) shows the optimized geometry of **TS(F-F$_2$)**. This TS involves a conformational change where the indolium species dissociates from the ene and coordinates to the carbonyl oxygen. This in turn allows for a free rotation along the dihedral, C3-C2-C6-O7 so that the indolium species can coordinate from the other prochiral face. In such a scenario, Curtin-Hammett principle will apply, and the final proton transfer will be stereoselective. Bond distance between Pd1-C7, Pd1-C2, Pd1-C3 is 3.24 Å, 3.11 Å and 2.89 Å respectively.

5. Relative Free Energies (kcal/mol) and Total Electronic Energies (kcal/mol) for A active species

Table S2 Relative Free Energies (ΔG) in kcal/mol of all the Stationary Points for Dicationic Pd Species at Different Functionals.[a,b,c,d] Functionals ωB97X-D and DLPNO-CCSD(T) were used only for the Lowest Energy pathway and some Key Intermediates and TSs. Stationary Points involved in the Lowest Energy Pathway are highlighted

	B3LYP-D3[a]	M06-D3[b]	ωB97X-D[c]	DLPNO-CCSD(T)[d]
A	0.0	0.0	0.0	0.0
TS(A-B)$_R$	13.6	11.2	15.1	20.1
TS(A-B)$_S$	14.0	11.6	15.6	21.7
B	3.9	-0.3	2.4	1.5
TS(B-C)	6.8	3.4	5.1	1.9
C	-27.1	-27.3	-27.1	-31.2
TS(C-D)[e]	-23.8	-24.3	-20.6	-23.5
D	-44.6	-49.1	-51.7	-54.0
TS(D-F)	-23.2	-29.1	-31.1	-35.7
F	-24.7	-29.6	-29.8	-32.1
TS(F-F$_1$)	-23.2	-25.6	-28.4	-32.0
F$_1$	-26.4	-29.5	-29.9	-34.4
TS(F$_1$-P$_1$)	-26.3	-30.3	-31.7	-34.0
P$_1$	-41.5	-45.9	-48.6	-48.6
TS(F-F$_2$)	-15.0	-12.5	-15.6	
F$_2$	-29.9	-27.1	-31.5	

P	-46.6	-50.9	-54.3	-61.1
A_1	-3.6	-5.9	-4.0	0.8
TS(A_1-B_1)	15.2	11.9	15.6	27.2
B_1	6.6	0.3	4.0	7.8
TS(B_1-C_1)	8.8	2.8	6.1	6.7
C_1	-29.7	-30.7	-29.8	-29.4
TS(C_1-D)	-17.7	-19.8	-18.5	-19.8
TS-C_{rot}	3.2	4.9		
TS(D-E_a)	-25.5	-33.2	-31.5	-32.8
TS(D-E_a)$_{1wat}$	-22.1	-28.0		
E_a	-32.8	-40.8	-37.2	-37.6
E_b	-26.7	-27.2		
E_c	-32.8	-40.2		
E_d	-30.8	-36.4		
E_e	-27.8	-33.2		
E_f	-26.8	-27.0		
E_g	-28.2	-33.2		
E_h	-24.7	-32.0		
E_{free}	-28.1	-28.2		
TS(E_{free}-P)	16.3	14.6		
TS(E_a-P)	9.7	-0.4		
TS(E_a-P)$_{1wat}$	-9.0	18.2		
TS(E_a-P)$_{2wat}$	-13.1	-21.6	-17.0	-14.3
TS(E_{free}-P)$_{2wat}$	-4.8	-4.4	-7.5	-11.9
TS(E_a-P)$_{enol}$	-3.7	-16.4		
TS(E_a-P)$_{CPA}$	-18.9	-24.0	-20.6	-16.1
TS(E_{free}-P)$_{CPA}$	-25.0	-25.5	-29.2	-32.7
D_{free}	-20.3	-26.9		
D_2	-33.5	-35.4		
TS(D_2-P)^t	2.7	0.9		
TS(D_2-P)^b	-3.6	-7.8		
TS(D_2-E_a)	-19.7	-20.7		

TS(D-P)	4.7	-3.8		
G	-21.1	-24.9		
TS(G-P)	4.7	-1.9		
X	0.8	-4.2		
TS(X-Y)	52.5	52.0		
Y	49.0	50.2		
TS_{dimer}	-6.6	-11.0	-6.5	-14.5

[a]$SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd).[b]$SMD_{(DCM)}$/M06-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd).[c]$SMD_{(DCM)}$/ωB97X-D/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p), LANL2DZ(Pd). [d]$SMD_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd). [e]Geometry Optimization is done at the B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory and single-points were done at all the functionals and basis-sets as stated for other intermediates and TSs.

Table S3 Total Electronic Energies (ΔE) in (a.u.) of all the Stationary Points for Dicationic Pd Species at Different Functionals.[a,b,c,d] Functionals ωB97X-D and DLPNO-CCSD(T) were used only for the Lowest Energy Pathway and some key Intermediates and TSs

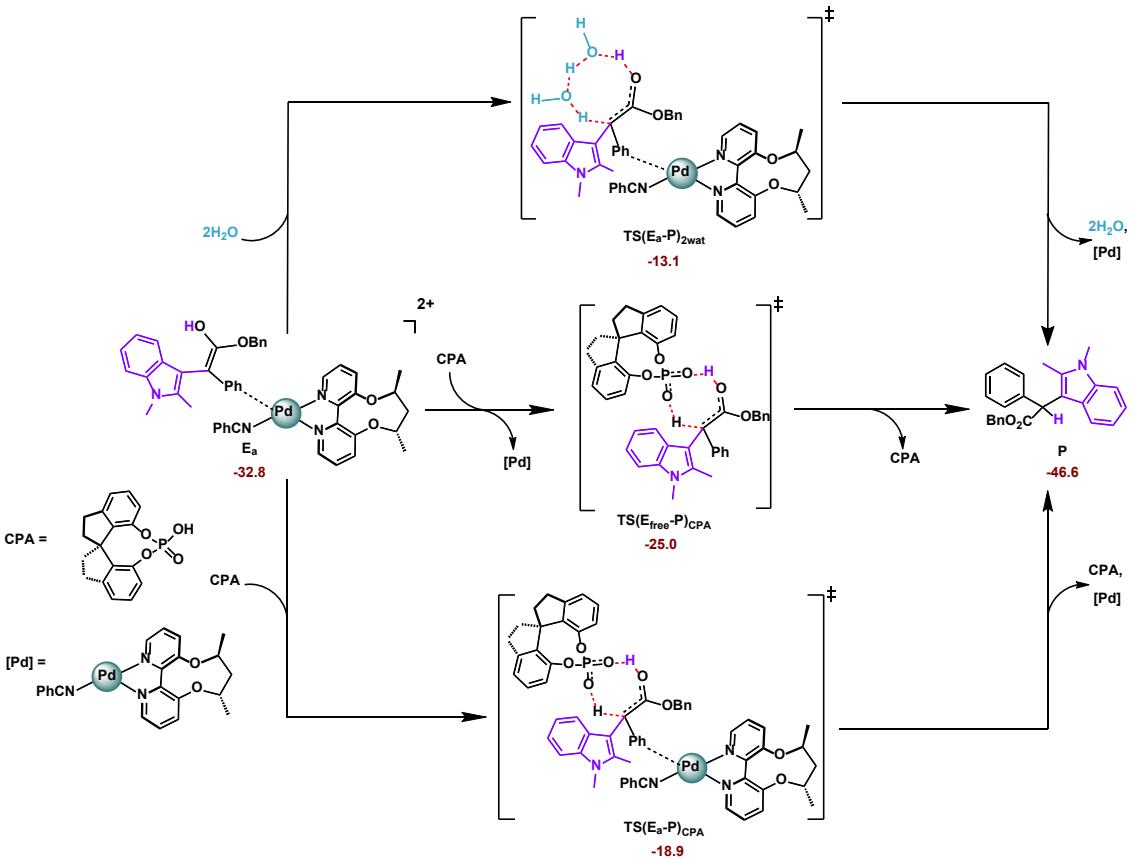
	B3LYP-D3[a]	**M06-D3[b]**	**ωB97X-D[c]**	**DLPNO-CCSD(T)[d]**
A	-1617.135708	-1615.972928	-1616.534283	-1614.7891456
TS(A-B)$_R$	-2131.527804	-2130.01354	-2130.729029	-2128.1411939
TS(A-B)$_S$	-2131.527846	-2130.013501	-2130.728847	-2128.1393519
B	-2131.543455	-2130.031961	-2130.749314	-2128.1708714
TS(B-C)	-2131.537506	-2130.024692	-2130.743707	-2128.1689903
C	-2022.016602	-2020.567802	-2021.261891	-2018.8295641
TS(C-D)[e]	-2464.628329	-2462.814484	-2463.698147	-2460.4597606
D	-2464.669714	-2462.86233	-2463.755993	-2460.5167386
TS(D-F)	-2140.009164	-2138.465984	-2139.230408	-2136.5568718
F	-2140.012457	-2138.467793	-2139.229293	-2136.5520820
TS(F-F_1)	-2140.00789	-2138.459196	-2139.224827	-2136.5497887
F_1	-2140.014242	-2138.466516	-2139.228527	-2136.5546802
TS(F_1-P_1)	-2140.014755	-2138.468539	-2139.23211	-2136.5547834
P_1	-2140.041475	-2138.495913	-2139.261493	-2136.5806356
TS(F-F_2)	-2139.995846	-2138.43932	-2139.20542	

F_2	-2140.01888	-2138.46198	-2139.230117	
P	-1172.128553	-1171.221687	-1171.683454	-1169.6343781
A_1	-1735.141797	-1733.878974	-1734.504005	-1732.50934716
TS(A_1-B_1)	-2249.523735	-2247.907177	-2248.689782	-2245.8494068
B_1	-2249.54043	-2247.928739	-2248.71127	-2245.8832420
TS(B_1-C_1)	-2249.535933	-2247.923702	-2248.706925	-2245.884036
C_1	-2249.582229	-2247.967331	-2248.750434	-2136.543694
TS(C_1-D)	-2140.004965	-2138.455733	-2139.214952	-2136.5361201
TS-C_{rot}	-2021.967579	-2020.515948		
TS(D-E_a)	-2464.633967	-2462.831641	-2463.718486	-2460.4776168
TS(D-E_a)$_{1wat}$	-2541.117452	-2539.271818		
E_a	-2464.649275	-2462.847606	-2463.731356	-2460.4890040
E_b	-2464.639386	-2462.825658		
E_c	-2464.648859	-2462.846172		
E_d	-2464.641591	-2462.836021		
E_e	-2464.64081	-2462.834934		
E_f	-2464.637614	-2462.823441		
E_g	-2464.642857	-2462.836374		
E_h	-2464.636007	-2462.833115		
E_{free}	-1172.095381	-1171.181808		
TS(E_{free}-P)	-1172.01837	-1171.107388		
TS(E_a-P)	-2464.578812	-2462.780395		
TS(E_a-P)$_{1wat}$	-2541.09639	-2539.256015		
TS(E_a-P)$_{2wat}$	-2617.58826	-2615.706178	-2616.617102	-2613.1584697
TS(E_{free}-P)$_{2wat}$	-1325.029279	-1324.033893	-1324.5238756	-1322.259715
TS(E_a-P)$_{enol}$	-3636.723694	-3634.015798		
TS(E_a-P)$_{CPA}$	-3764.17686	-3761.671675	-3762.887358	-3757.6519338

TS(E_{free}-P)$_{CPA}$	-2471.641346	-2470.02938	-2470.823382	-2466.7837011
D_{free}	-1172.085491	-1171.182369		
D_2	-2464.646499	-2462.835065		
TS(D_2-P)^t	-2464.586058	-2462.774502		
TS(D_2-P)^b	-2464.598434	-2462.790627		
TS(D_2-E_a)	-2464.619822	-2462.806994		
TS(D-P)	-2464.584125	-2462.783227		
G	-2464.629789	-2462.821376		
TS(G-P)	-2464.58692	-2462.782813		
X	-2059.753802	-2058.233467		
TS(X-Y)	-2059.666322	-2058.138756		
Y	-2059.673514	-2058.143287		
PhCN	-324.5987776	-324.3367942	-324.4650673	-323.9029635
H_2O	-76.4665348	-76.4260214	-76.44035488	-76.3347120
S_1	-839.0039949	-838.386586	-838.6752025	-837.2784092
S_2	-442.5952318	-442.2296597	-442.424673	-441.6205495
N_2	-109.5543936	-109.4851386	-109.5123517	-109.3713722
TS_{dimer}	-2861.016315	-2858.957036	-2859.93293	-2856.1107269
CPA	-1299.531873	-1298.833071	-1299.164689	-1297.179431

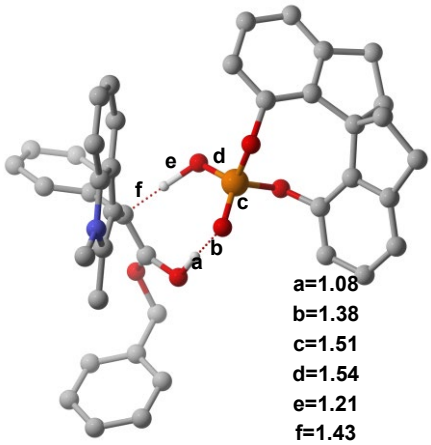
[a]$SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd).[b]$SMD_{(DCM)}$/M06-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd).[c]$SMD_{(DCM)}$/ωB97X-D/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p), LANL2DZ(Pd). [d]$SMD_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd). [e]Geometry Optimization is done at the B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory and single-points were done at all the functionals and basis-sets as stated for other intermediates and TSs.

6. Brønsted Acid Assisted Pathway



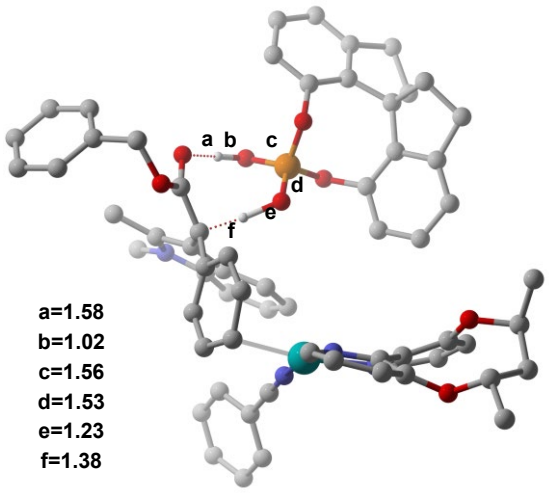
Scheme S1 Formation of Indole Alkylated Product via CPA and Water Assisted Enol Pathway. Free Energies (kcal/mol) are given at the $SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) Level of Theory

$TS(E_{free}\text{-}P)_{CPA}$



-25.0 kcal/mol

$TS(E_a\text{-}P)_{CPA}$

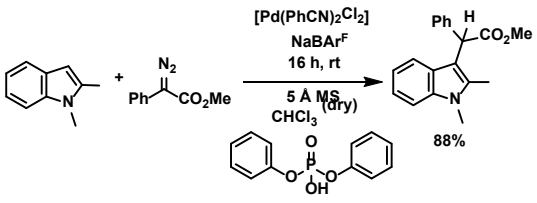


-18.9 kcal/mol

Fig. S10 Optimized Geometries of **TS(E_{free}-P)$_{CPA}$** & **TS(E_a-P)$_{CPA}$**. Free energies (kcal/mol) are given at the SMD$_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) Level of Theory. Hydrogens are removed for clarity. Distances are given in Å.

It is well-reported in literature that enol-keto tautomerization takes place in presence of a co-catalyst, usually a Brønsted acid, also responsible for enantioinduction in these cases.[20] Inspired by this, we considered a TS where a spiro phosphoric acid assists the proton-transfer in the enol to keto transformation, and we found that the activation free energy barrier reduces to 19.6 kcal/mol (w.r.t. **D**). It should be noted that the Pd associated enol had a higher activation free energy barrier. Thus, if the reaction under study is an acid assisted tautomerization, the reaction should have resulted in a racemic mixture. The high *ee* cannot be explained by the free enol model. We also checked the consistency of the calculated barriers at the DLPNO-CCSD(T) functional where we found that the barriers for **TS(F-F$_1$)** and **TS(E_{free}-P)$_{CPA}$** remain unchanged (**Table S2**). This shows that the barrier for 1,3-proton transfer can be significantly reduced in presence of a Brønsted acid. We also confirmed this by carrying out the formation of indole alkylated product in standard reaction conditions (in absence of bpy ligand) with diphenylphosphate (a Brønsted acid), and found high yield *i.e.* 88%, as opposed to without bipy ligand (29% only).

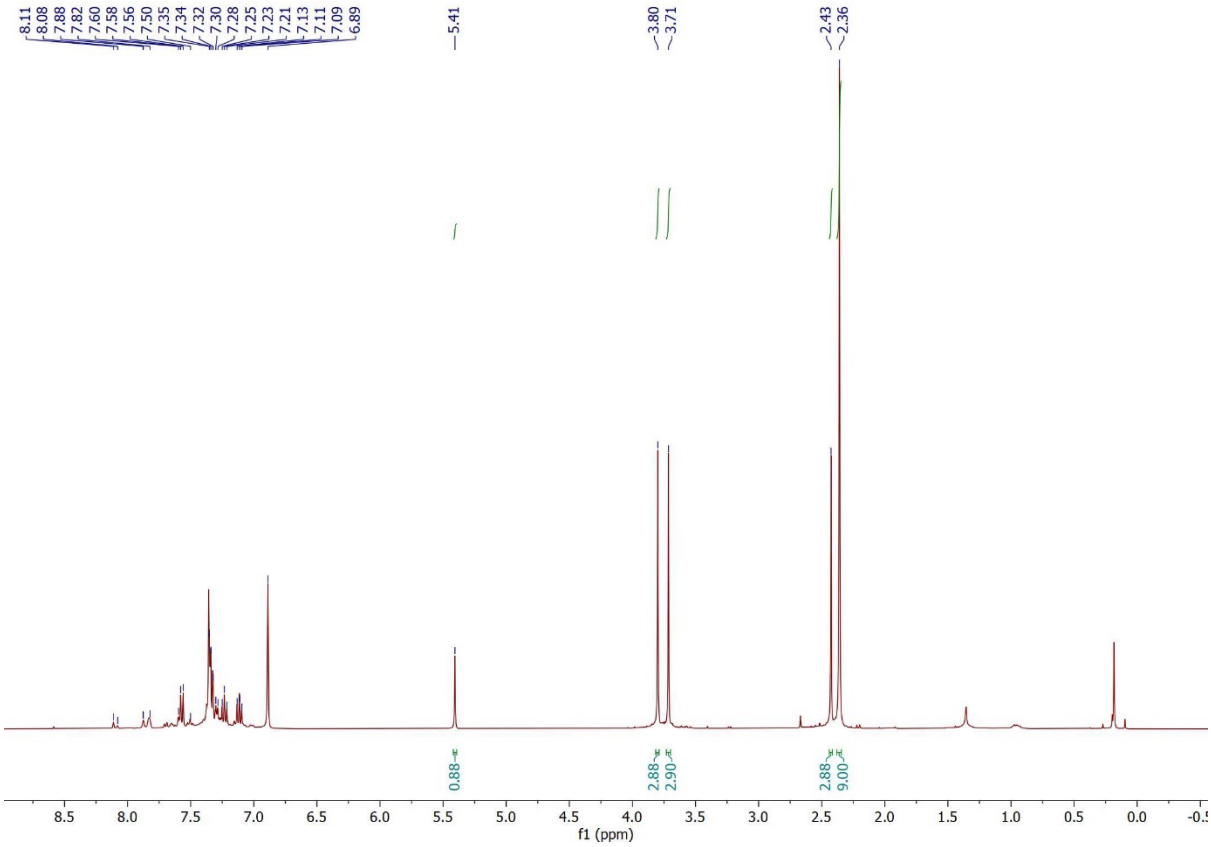
6.1. Formation of Indole Alkylated Product in Presence of Diphenylphosphate and in Absence of bpy Ligand



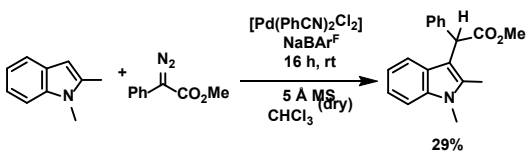
Procedure: Powdered [Pd(PhCN)$_2$Cl$_2$] (3.9 mg, 0.01 mmol, 5.0 mol%), NaBAr^F (21.3 mg, 0.024 mmol, 12.0 mol%), and diphenylphosphate (2.5 mg, 0.01 mmol, 5.0 mol%), and 200 mg

5 Å molecular sieves were introduced into an oven-dried Schlenk tube under argon. After chloroform (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under argon for 1 h. 1,2-dimethyl-1*H*-indole (43.6 mg, 0.30 mmol) and methyl-α-diazo-α-phenylacetate (35.4 mg, 0.20 mmol) was then introduced in one portion. The resulting mixture was stirred at 30°C under argon till 16 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. 28 μL mesitylene was added as an internal standard. The crude reaction mixture was subjected to ^{1}H NMR for analysis.

^{1}H NMR (400 MHz, $CDCl_3$):

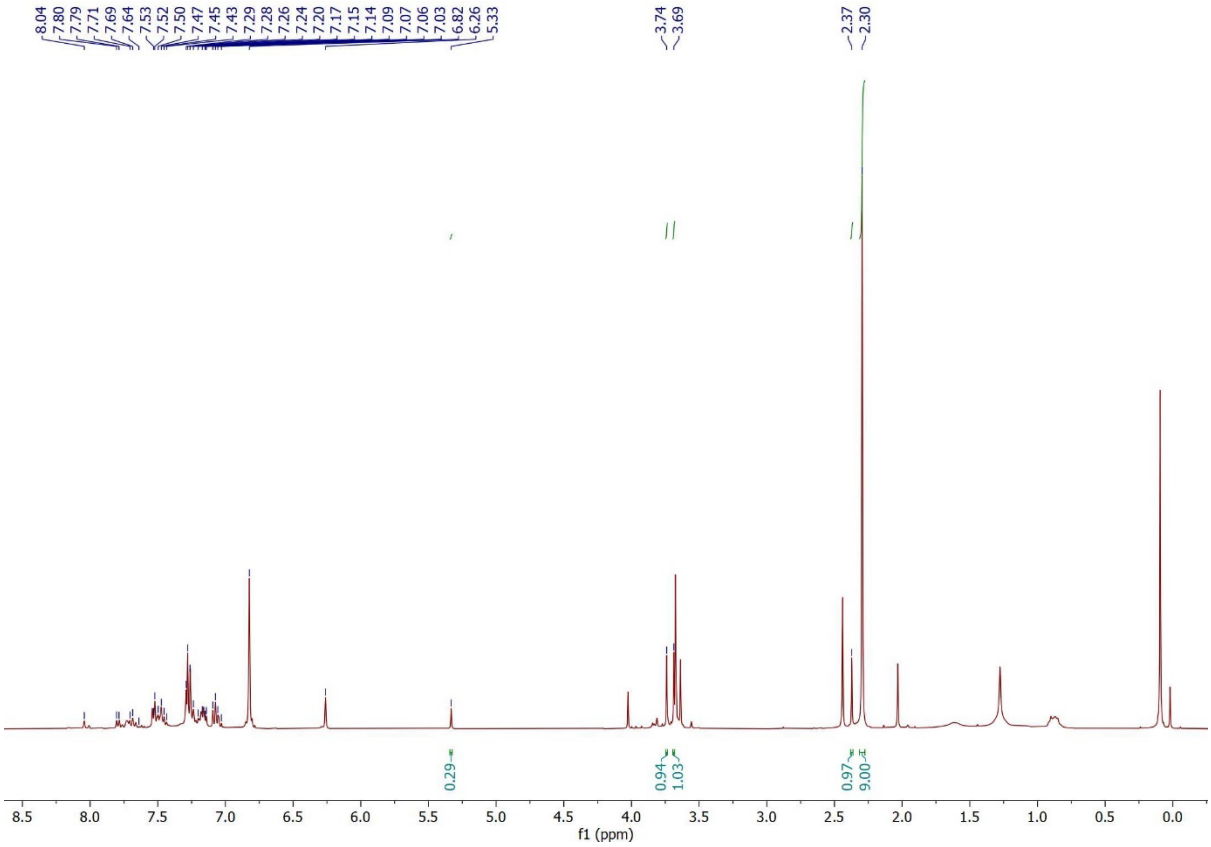


6.2. Formation of Indole Alkylated Product in Absence of Diphenylphosphate and bpy Ligand



Procedure: Powdered [$Pd(PhCN)_2Cl_2$] (3.9 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.024 mmol, 12.0 mol%), and 200 mg 5 Å molecular sieves were introduced into an oven-dried Schlenk tube under argon. After chloroform (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under argon for 1 h. 1,2-dimethyl-1*H*-indole (43.6 mg, 0.30 mmol) and methyl-α-diazo-α-phenylacetate (35.4 mg, 0.20 mmol) was then introduced in one portion. The resulting mixture was stirred at 30°C under argon till 16 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. 28 µL mesitylene was added as an internal standard. The crude reaction mixture was subjected to ^{1}H NMR for analysis.

^{1}H NMR (400 MHz, $CDCl_3$):



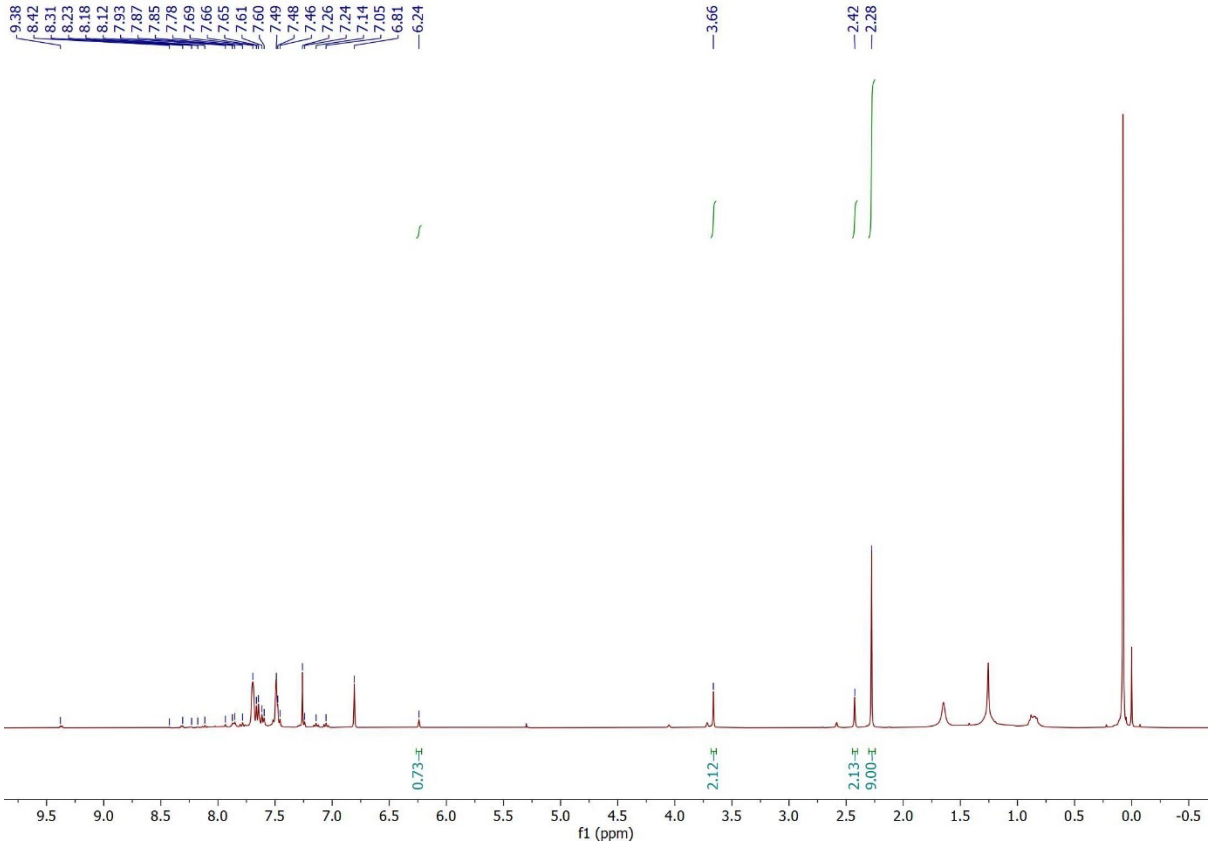
7. Stoichiometric Experiment with 1,2-dimethyl-1*H*-indole

A control experiment was carried out without the diazo substrate in stoichiometric amount for 4 hours to check the formation of any Pd-indole complex employing standard procedure used by Zhou. (citation) Even after 4 hours, 73% indole remains unreacted as seen from ^{1}H NMR.

We were not able to characterize the remaining 27%. It discards the possibility of C–H activation route.

Procedure: Powdered [$Pd(PhCN)_2Cl_2$] (7.7 mg, 0.02 mmol), $NaBAr^F$ (42.5 mg, 0.048 mmol), and 2,2'-bipyridine (3.1 mg, 0.02 mmol) were introduced into an oven-dried Schlenk tube under argon. After chloroform (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under argon for 1 h. Then, 1,2-dimethyl-1*H*-indole (2.9 mg, 0.02 mmol) was introduced, and the resulting mixture was stirred at 30°C under argon for 4 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. 2.8 µL mesitylene was added as an internal standard. The crude reaction mixture was subjected to ^{1}H NMR for analysis.

^{1}H NMR (400 MHz, $CDCl_3$):

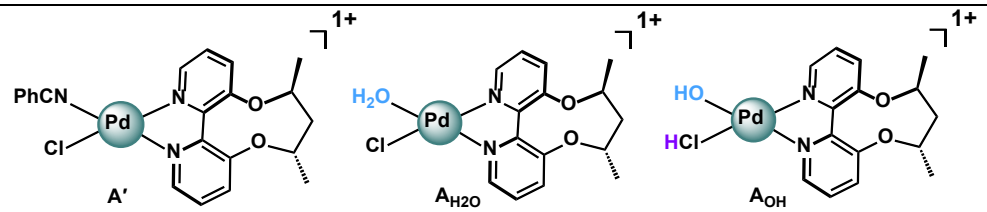


8. Pathways Involving Cationic Pd Catalyst

8.1. Active species

Here, we consider partial abstraction of chloride by $NaBAr^F$ leading to the formation of Pd–Cl species, **A′**. Other complexes that can form due to ligand exchange are $\mathbf{A_{H2O}}$ and $\mathbf{A_{OH}}$. The Pd–Cl complex $\mathbf{A_{H2O}}$ can be hydrolysed by adventitious amount of water present in reaction medium and form Pd–OH complex $\mathbf{A_{OH}}$ that can also act as catalytic species. On comparing their thermodynamic stability, **A′** is found to be more stable than $\mathbf{A_{H2O}}$/$\mathbf{A_{OH}}$ and thus it is considered as active catalytic species. To get a better estimate of energetics, we have done solvent phase optimization of these intermediates and compared their free energy with **A′**. (Table S4)

Table S4 Free Energies (ΔG) in kcal/mol for $\mathbf{A_{H2O}}$ and $\mathbf{A_{OH}}$ relative to **A′** at Different Functionals[a,b]



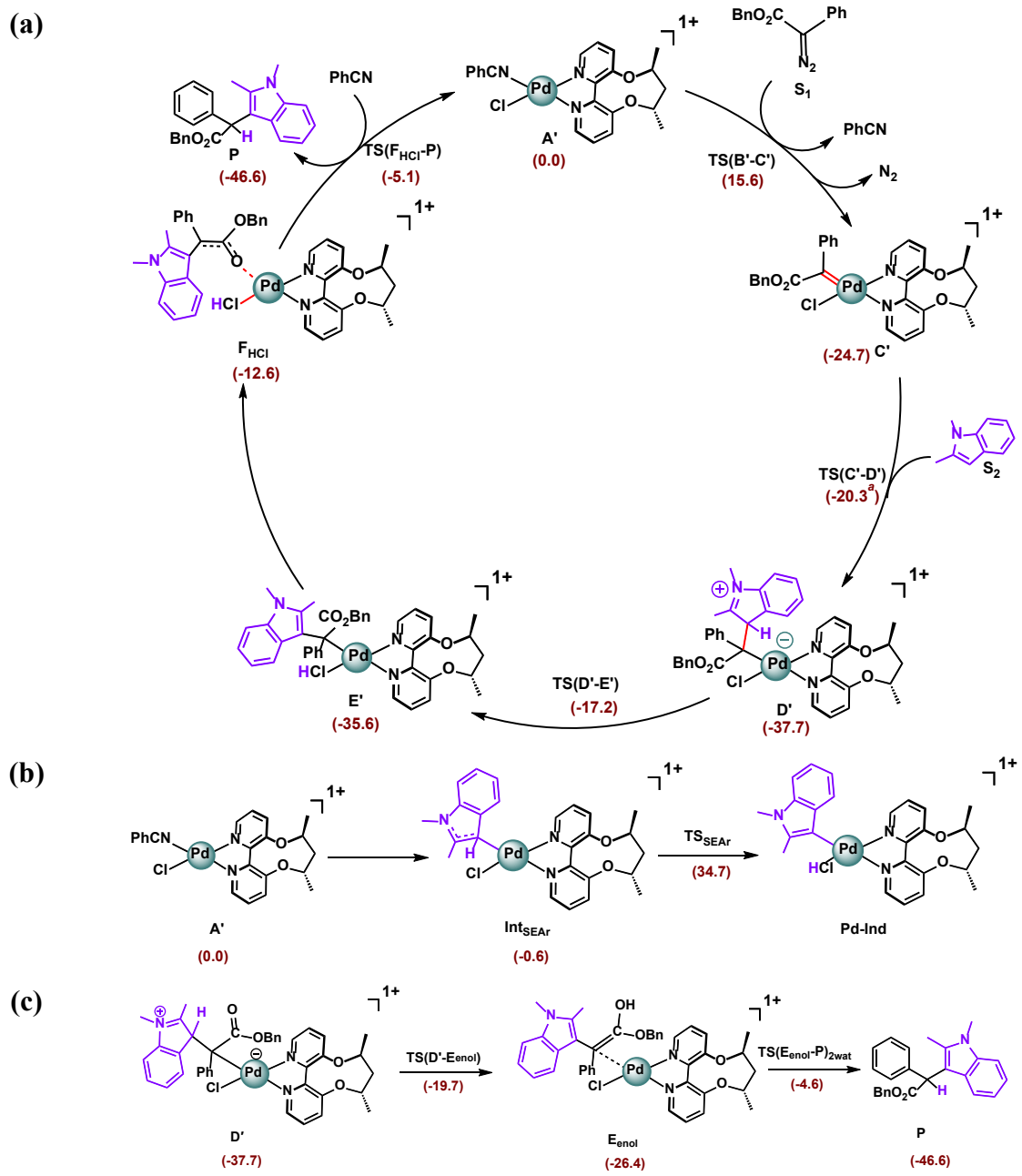
	B3LYP-D3[a]	M06-D3[b]
A′	0.0	0.0
$\mathbf{A_{H2O}}$	6.7	7.4
$\mathbf{A_{OH}}$	44.4	46.3

[a]$SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//$SMD_{(DCM)}$/B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory. [b]$SMD_{(DCM)}$/M06-D3/6-311+G(d,p),LANL2DZ(Pd)//$SMD_{(DCM)}$/B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory.

8.2. Catalytic Cycle with Active species A'

Since, **A'** is the most stable species, we discuss it in the context of the cationic Pd complex. At first N_2 extrusion takes place on complexation of diazoester $\mathbf{S_1}$ with Pd(II) centre via **TS(B′-C′)** followed by nucleophilic attack by indole $\mathbf{S_2}$ via **TS(C'-D')**. Chloride can act as base and abstract proton from indole moiety through 5 member **TS(D'-E')**. Further the proton transfer can happen on carbene carbon by HCl or H_2O via $\mathbf{TS(F_{HCl}\text{-}P)}$ or $\mathbf{TS(F_{H2O}\text{-}P)}$ respectively, releasing the product concomitantly. (Scheme S2(a)) Overall, the free energy barriers of this pathway are high in comparison of Pd(II) pathway and thus this pathway is rejected. (Fig. S11) We failed to get a TS corresponding to CMD. Instead, we found a TS similar to S_EAr (electrophilic aromatic substitution) where a Wheland type intermediate is generated. (Scheme

S2(b)) Subsequently, the C3 proton is abstracted via the Cl^- ligand. However, the activation free energy barrier for this TS was found to be very high (34.7 kcal/mol), also confirmed by DLPNO-CCSD(T) calculations (32.4 kcal/mol). (Fig. S11) (Table S5) Additionally, enol pathway also showed high barrier. (Scheme S2(c))



Scheme S2 (a) Possible Catalytic Cycle for the Formation of Product **P** Starting from Cationic Pd Active Catalytic Species, (b) Possible Pathway via S_EAr, (c) Possible Pathway via Enol Intermediate followed by Tautomerisation. Free Energies (kcal/mol) are given in parenthesis

at the SMD$_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p), LANL2DZ (Pd) level of theory

[a]Free energy is given at the SMD$_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP/6-31G(d,p), LANL2DZ (Pd) Level of Theory

8.3. Free Energy Profile (kcal/mol) for Active Species A'

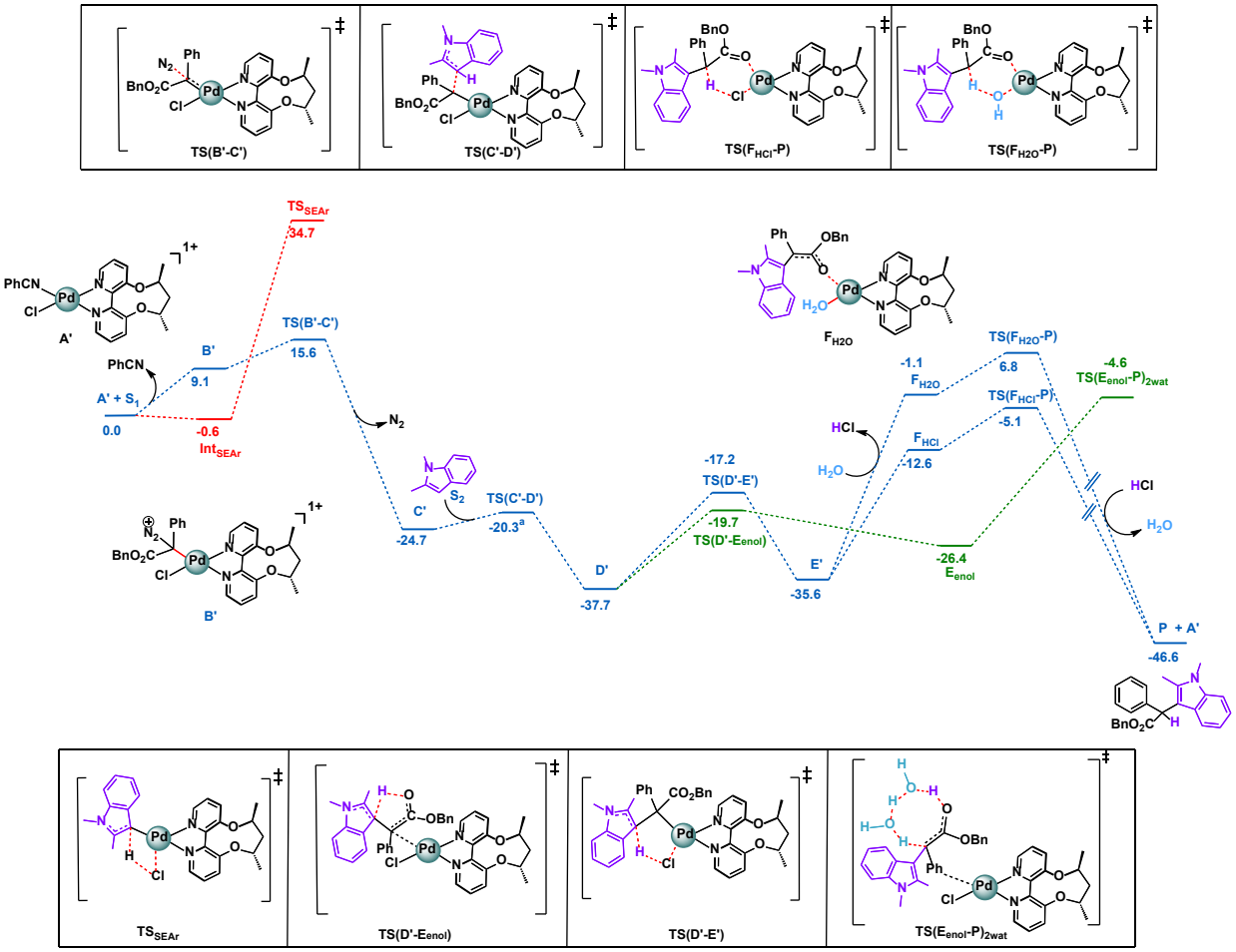


Fig. S11 Free Energy Profile of Cationic Pd Pathway showing Formation of Product **P**. Free Energies (kcal/mol) are given at the SMD$_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) Level of Theory.

[a]Free energy at the SMD$_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP/6-31G(d,p), LANL2DZ (Pd) level of theory.

9. Relative Free Energies (kcal/mol) and Total Electronic Energies (kcal/mol) with Active Species A'

Table S5 Free Energies (ΔG) in kcal/mol of all the Stationary Points for Cationic Pd Species at Different Functionals.[a,b,c] Functional DLPNO-CCSD(T) was used for key TS

	B3LYP-D3[a]	M06-D3[b]	DLPNO-CCSD(T)[c]
A′	0.0	0.0	
B′	9.1	3.8	
TS(B′-C′)	15.6	11.4	
C′	-24.7	-25.0	
TS(C′-D′)[d]	-20.3	-24.2	
D′	-37.7	-44.6	
TS(D′-E′)	-17.2	-23.2	
E′	-35.6	-42.1	
F_{H2O}	-1.1	-2.9	
TS(F_{H2O}-P)	6.8	6.2	
F_{HCl}	-12.1	-20.7	
TS(F_{HCl}-P)	-5.1	-9.0	
Int_{SEAr}	-0.6	-2.9	
TS_{SEAr}	34.7	31.7	32.4
E_{enol}	-26.4	-34.1	
TS(E_{enol}-P)$_{2wat}$	-4.6	-10.5	
TS(D′-E_{enol})	-19.7	-25.4	

[a]$SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd).[b]$SMD_{(DCM)}$/M06-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd). [c]$SMD_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd). [d]Geometry Optimization is done at the B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory and single-points were done at all the functionals and basis-sets as stated for other intermediates and TSs.

Table S6 Total Electronic Energies (ΔE) in (a.u.) of all the Stationary Points for Cationic Pd Species at Different Functionals.[a,b,c] DLPNO-CCSD(T) Functional was used for key TS

	B3LYP-D3[a]	M06-D3[b]	DLPNO-CCSD(T)[c]
A′	-1752.969196	-1752.034342	
B′	-2267.365113	-2266.083392	
TS(B′-C′)	-2267.353443	-2266.069768	
C′	-2157.845085	-2156.624594	

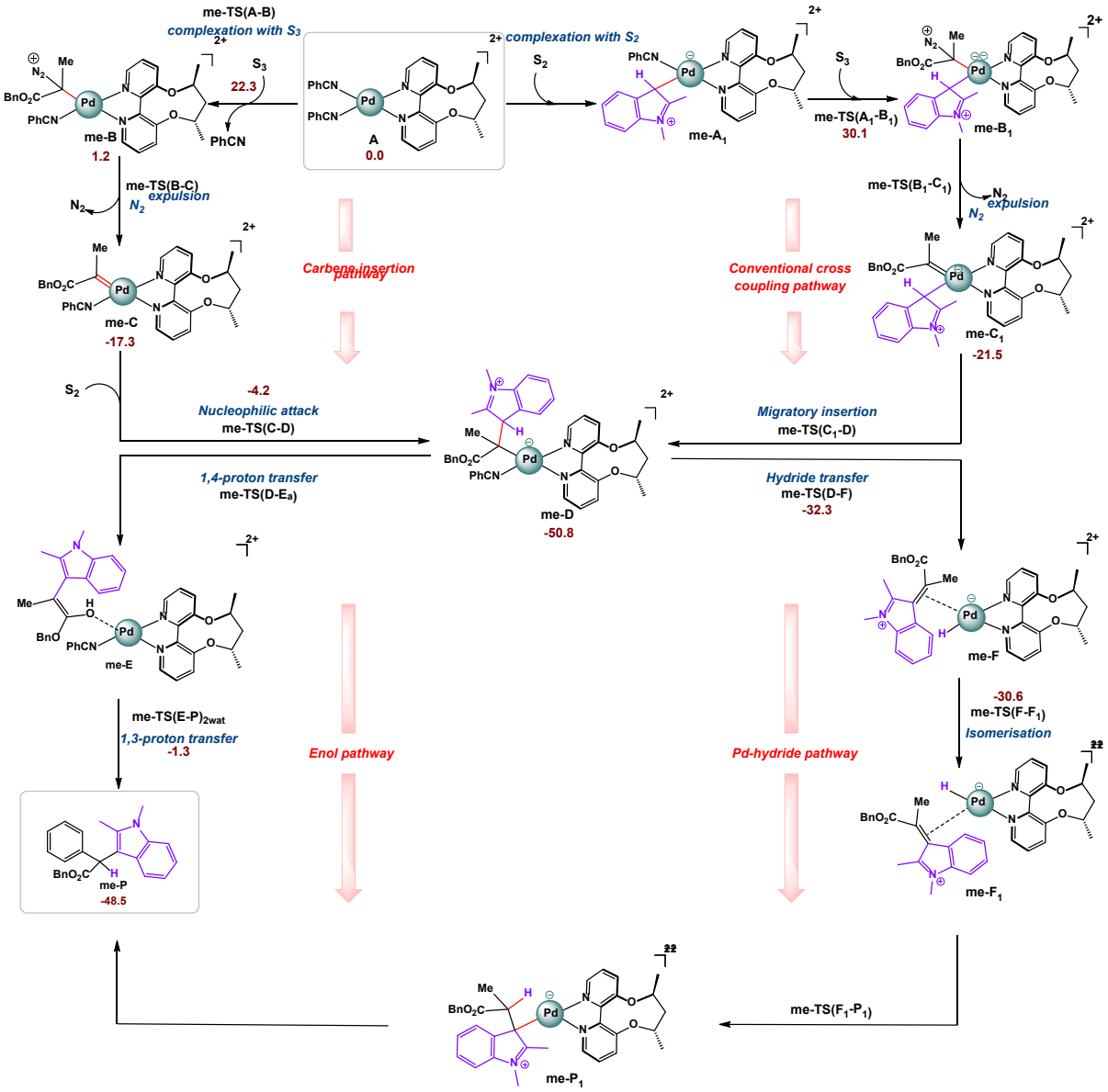
TS(C′-D′)[d]	-2600.455974	-2598.875614	
D′	-2600.492276	-2598.916610	
TS(D′-E′)	-2600.453373	-2598.876436	
E′	-2600.48361	-2598.907332	
F_{H2O}	-2216.079909	-2214.495684	
TS(F_{H2O}-P)	-2216.064361	-2214.478318	
F_{HCl}	-2600.441503	-2598.868618	
TS(F_{HCl}-P)	-2600.433876	-2598.853407	
HCl	-460.8169958	-460.7769238	
Int_{SEAr}	-1870.971032	-1869.936273	
TS_{SEAr}	-1870.907	-1869.873319	-1868.46918
E_{enol}	-2600.472992	-2598.898634	
TS(E_{enol}-P)$_{2wat}$	-2753.408578	-2751.750833	
TS(D′-E_{enol})	-2600.455529	-2598.878023	

[a]$SMD_{(CH2Cl2)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd). [b]$SMD_{(CH2Cl2)}$/M06-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd). [c]$SMD_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd). [d]Geomtery Optimization is done at the B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory and single-points were done at all the functionals and basis-sets as stated for other intermediates and TSs.

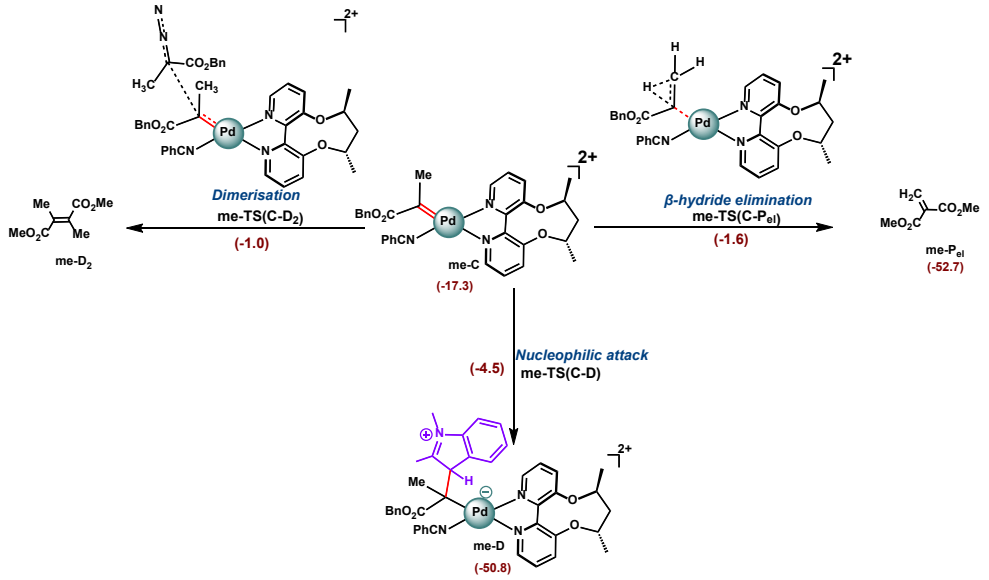
10. Catalytic Cycle with Active species A with benzyl 2-diazopropanoate

To assess the generality of this mechanism, we examined another substrate, α-methyl-α-diazoester (benzyl 2-diazopropanoate), which exhibited a reduced yield and *ee* (34% and 42%, respectively). (citation) Our investigation revealed that the palladium hydride mechanism observed with aryl diazo precursors also applies to alkyl diazo precursors. (Scheme S3) However, side reactions such as dimerization and hydride elimination compete with nucleophilic attack, resulting in a decrease in yield. (Scheme S3) In case of α-phenyl-α-diazoester, the barrier for dimerization is 16.7 kcal/mol w.r.t. **C**, while for α-methyl-α-diazoester, it is 16.3 kcal/mol w.r.t. **me-C**. However, the activation free energy barrier for nucleophilic attack in α-phenyl-α-diazoester is much lower (7.7 kcal/mol w.r.t. **C**) than dimerization at the $SMD_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory, precluding any possibility of dimerization in α-phenyl-α-diazoester.

We have done thorough conformational sampling and the gap between stereodetermining TSs (**me-TS(A-B)**$_R$ and **me-TS(A-B)**$_S$) was found to be 0.4 kcal/mol at the DLPNO-CCSD(T) calculations (corresponding to 40% *ee*) aligns well with experimental results. (Fig. S12)



Scheme S3 Possible Pathways for the formation of Indole Alkylated Product for benzyl 2-diazopropanoate substrate. Free energies (kcal/mol) for respective Intermediates and TSs are given at the SMD$_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) Level of Theory



Scheme S4 Dimerization, Hydride Elimination and Nucleophilic Attack Pathways. Free Energies (kcal/mol) for respective Intermediates and TSs are given in parentheses w.r.t. **A** at the $SMD_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) Level of Theory

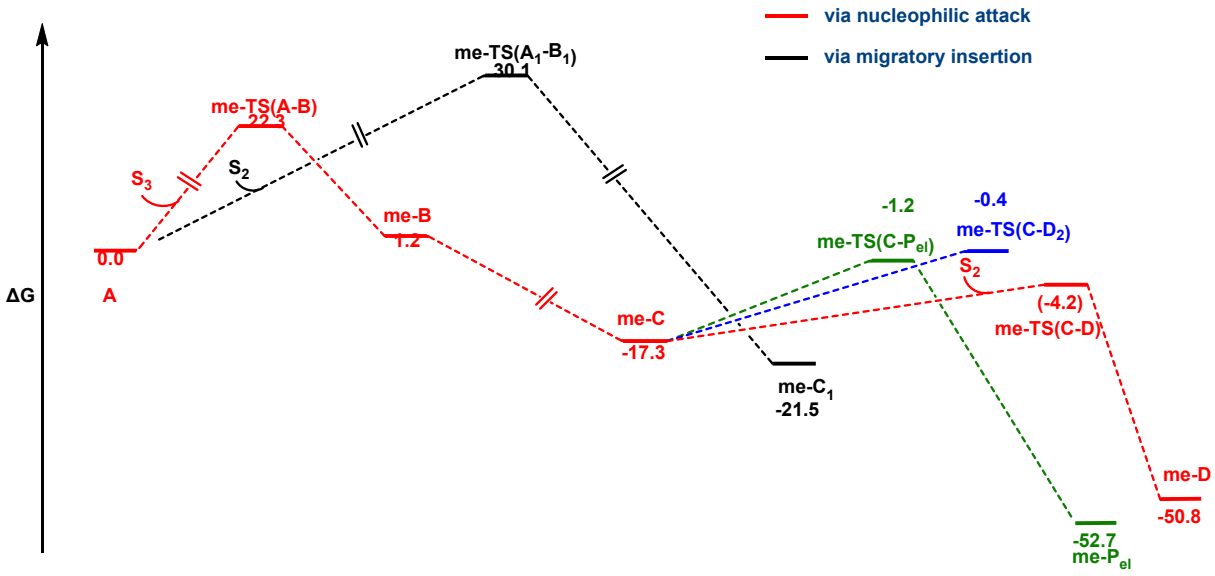


Fig. S12 Free Energy Profile for Active Species **A** with benzyl 2-diazopropanoate. Free energies (kcal/mol) are given at the $SMD_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) Level of Theory.

11. Relative Free Energies (kcal/mol) and Total Electronic Energies (kcal/mol) for Dicationic Pd catalyst for methyl diazoester (benzyl-2-diazopropanoate)

Table S7 Relative Free Energies (ΔG) in kcal/mol of all the Stationary Points for Dicationic Pd for methyl diazoester (benzyl-2-diazopropanoate) at Different Functionals.[a,b,,c,d] Relative Free Energies (ΔG) for all the Stationary Points at the DLPNO-CCSD(T) functional are highlighted

	B3LYP-D3[a]	**M06-D3[b]**	**ωB97X-D[c]**	**DLPNO-CCSD(T)[d]**
A	0.0	0.0	0.0	0.0
me-TS(A-B)$_R$	14.5	13.2	16.9	22.3
me-TS(A-B)$_S$	16.0	14.1	18.7	22.7
me-B	3.5	-0.2	1.8	1.2
me-C	-13.8	-14.9	-14.1	-17.3
me-TS(C-D)[e]	-5.9	-6.3	-3.5	-4.2
me-D	-43.5	-47.7	-49.0	-50.8
me-TS(D-F)	-21.6	-26.8	-28.2	-32.3
me-TS(F-F$_1$)	-24.3	-25.5	-27.8	-30.6
me-C$_1$	-19.6	-24.2	-21.8	-21.5
me-TS(C-P$_{el}$)	5.6	5.0	4.3	-1.2
me-P$_{el}$	-43.4	-38.5	-44.0	-52.7
me-TS(C-D$_2$)	0.5	-3.1	-8.0	-0.4
me-TS(E-P)$_{2wat}$	-6.4	-11.9	-5.5	-1.3
me-TS(A$_1$-B$_1$)	12.8	10.6	14.4	30.1
me-P	-48.5	-52.0	-55.0	-61.9

[a]SMD$_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd).[b]SMD$_{(DCM)}$/M06-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd).[c]SMD$_{(DCM)}$/ωB97X-D/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p), LANL2DZ(Pd). [d]SMD$_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd). [e]Geomtery Optimization is done at the B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory and single-points were done at all the functionals and basis-sets as stated for other intermediates and TSs.

Table S8 Total Electronic Energies (ΔE) in (a.u.) of all the Stationary Points for Dicationic Pd Species at Different Functionals for methyl diazoester (benzyl-2-diazopropanoate)[a,b,c,d,e]

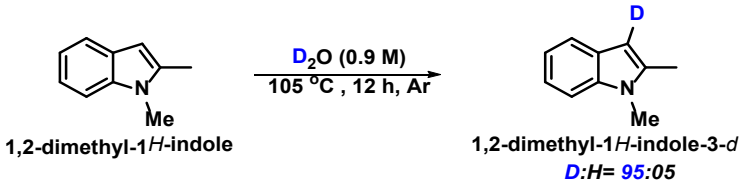
	B3LYP-D3[a]	**M06-D3[b]**	**ωB97X-D[c]**	**DLPNO-CCSD(T)/def2-TZVP[d]**

S_3	-647.207506	-646.747035	-646.9568044	-645.9003914
me-TS(A-B)$_R$	-1939.729083	-1938.369948	-1939.006877	-1936.758866
me-TS(A-B)$_S$	-1939.727036	-1938.368731	-1939.004324	-1936.758371
me-B	-1939.745754	-1938.39033	-1939.030049	-1936.791511
me-C	-1830.194873	-1828.904604	-1829.518987	-1827.425737
me-TS(C-D)[e]	-2272.795531	-2271.138671	-2271.944764	-2269.043305
me-D	-2272.87014	-2271.219365	-2272.032	-2269.132366
me-TS(D-F)	-1948.211591	-1946.82417	-1947.508835	-1945.17483
me-TS(F-F$_1$)	-1948.213643	-1946.819957	-1947.506023	-1945.169928
me-C$_1$	-1948.207826	-1946.819451	-1947.498103	-1945.157125
me-TS(C-P$_{el}$)	-1939.729705	-1938.369494	-1939.013407	-1936.782809
me-P$_{el}$	-537.7027638	-537.3037406	-537.495046	-536.593415
me-TS(C-D$_2$)	-2477.408856	-2475.662106	-2476.480571	-2473.328266
me-TS(E-P)$_{2wat}$	-2425.778824	-2424.049016	-2424.878228	-2421.757605
me-TS(A$_1$-B$_1$)	-2057.730036	-2056.268668	-2056.972298	-2054.46575
me-P	-980.3359064	-979.584795	-979.9671181	-978.2585004

[a]$SMD_{(DCM)}$/B3LYP-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd).[b]$SMD_{(DCM)}$/M06-D3/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd).[c]$SMD_{(DCM)}$/ωB97X-D/6-311+G(d,p),LANL2DZ(Pd)//B3LYP-D3/6-31G(d,p), LANL2DZ(Pd). [d]$SMD_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p),LANL2DZ(Pd). [e]Geomtery Optimization is done at the B3LYP-D3/6-31G(d,p),LANL2DZ(Pd) level of theory and single-points were done at all the functionals and basis-sets as stated for other intermediates and TSs.

12. Isotopic Labeling Experiments

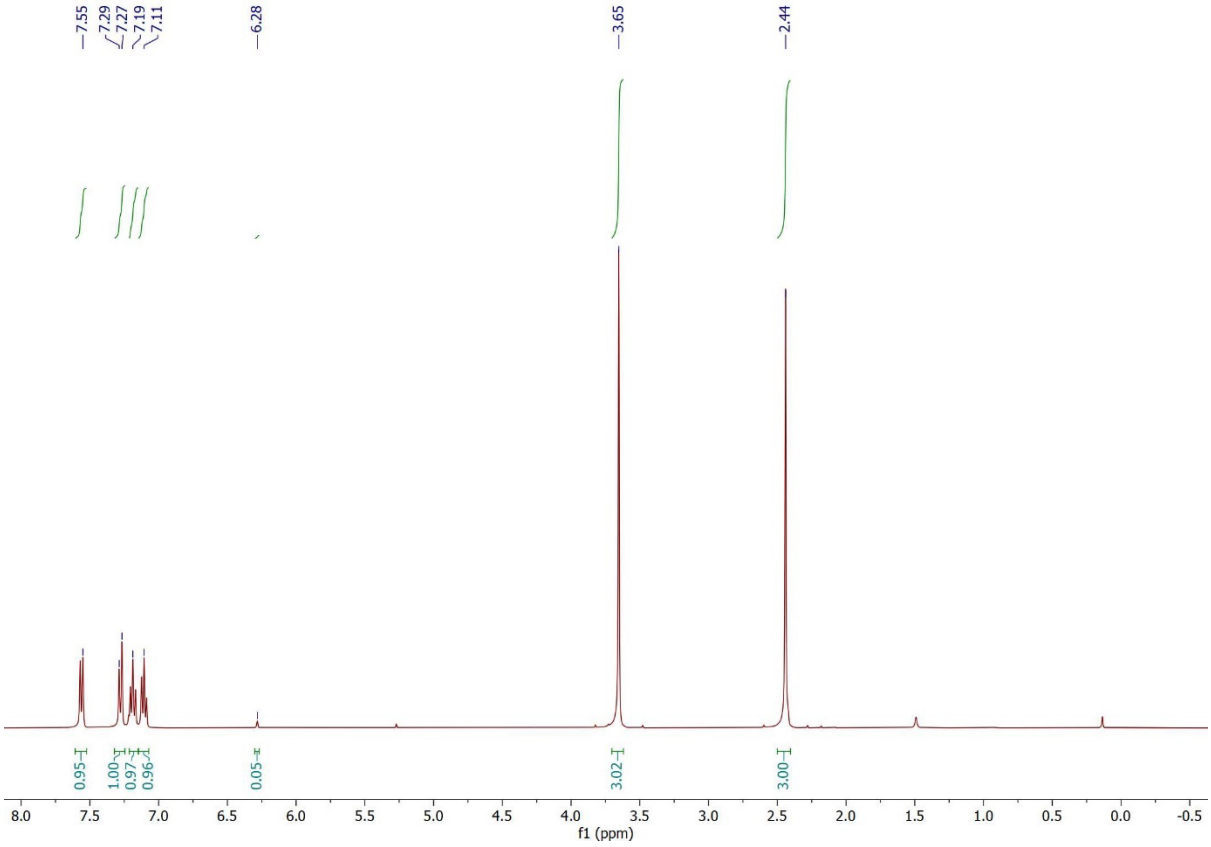
12.1. Synthesis of 1,2-dimethyl-1*H*-indole-3-*d*



Prepared using the following procedure by Lane, B. S. *et al.*[12] A flask is charged with freshly distilled 1,2-dimethyl-1*H*-indole (1 g, 7.6 mmol) and then flushed with argon. To this 2 mL of D_2O is added, and the mixture is heated to 105 °C overnight with very vigorous stirring. After the solution has cooled, it is extracted with hexane (3 times, 5 mL), and dried over Na_2SO_4. The solvent is removed, and the final product was purified by distillation from molecular sieves. The product was completely enriched with deuterium in the 3-position, as determined by ^{1}H NMR.

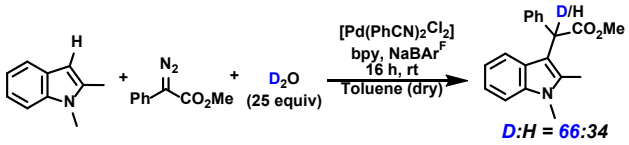
HRMS (ESI+): HRMS (ESI): *m/z* calcd for $C_{10}H_{11}ND$: 146.0970 $[M+H]^+$; found: 146.0967

^{1}H NMR (400 MHz, $CDCl_3$): 7.55 (d, *J* = 7.7 Hz, 1H), 7.27-7.29 (m, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.11 (t, *J* = 7.7 Hz, 1H), 3.65 (s, 3H), 2.44 (s, 3H).



12.2. Deuterium Transfer Experiments

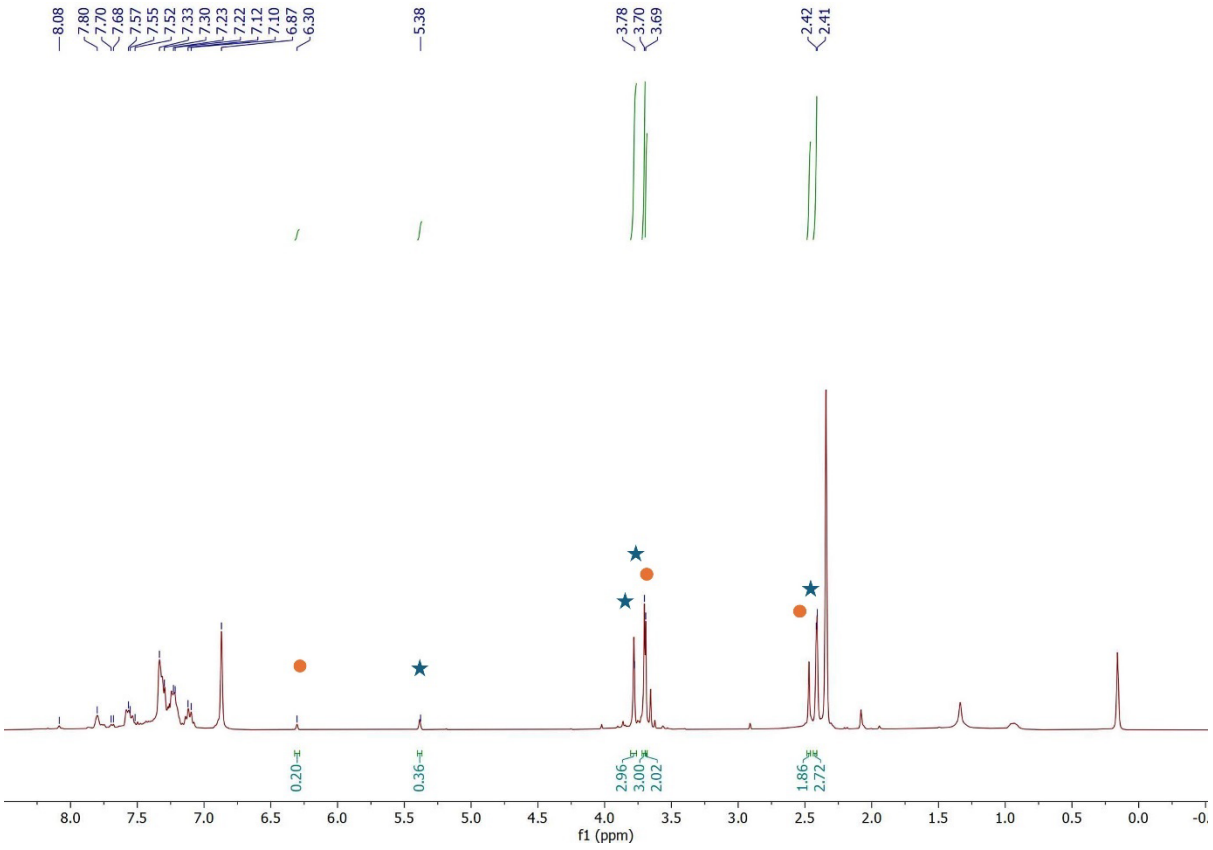
12.2 (a)



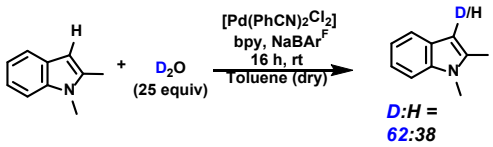
Procedure: Powdered $[Pd(PhCN)_2Cl_2]$ (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%) and $NaBAr^F$ (21.3 mg, 0.024 mmol, 12.0 mol%) were introduced into an oven-dried Schlenk tube under nitrogen. After toluene (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under nitrogen for 1.0 h. 1,2-dimethyl-1*H*-indole (43.6 mg, 0.30 mmol, 1.5 eq), methyl-α-diazo-α-phenylacetate (35.3 mg, 0.20 mmol, 1.0 eq), and D_2O (100 mg, 5.0 mmol , 25 eq) was then introduced in one portion. The resulting mixture was stirred at 30°C under nitrogen till 16 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. 28 μL mesitylene was added as an internal standard. The crude reaction mixture was subjected to ^1H NMR for analysis.

^1H NMR (400 MHz, $CDCl_3$):

● Peaks corresponding to unreacted indole ★ Peaks corresponding to product

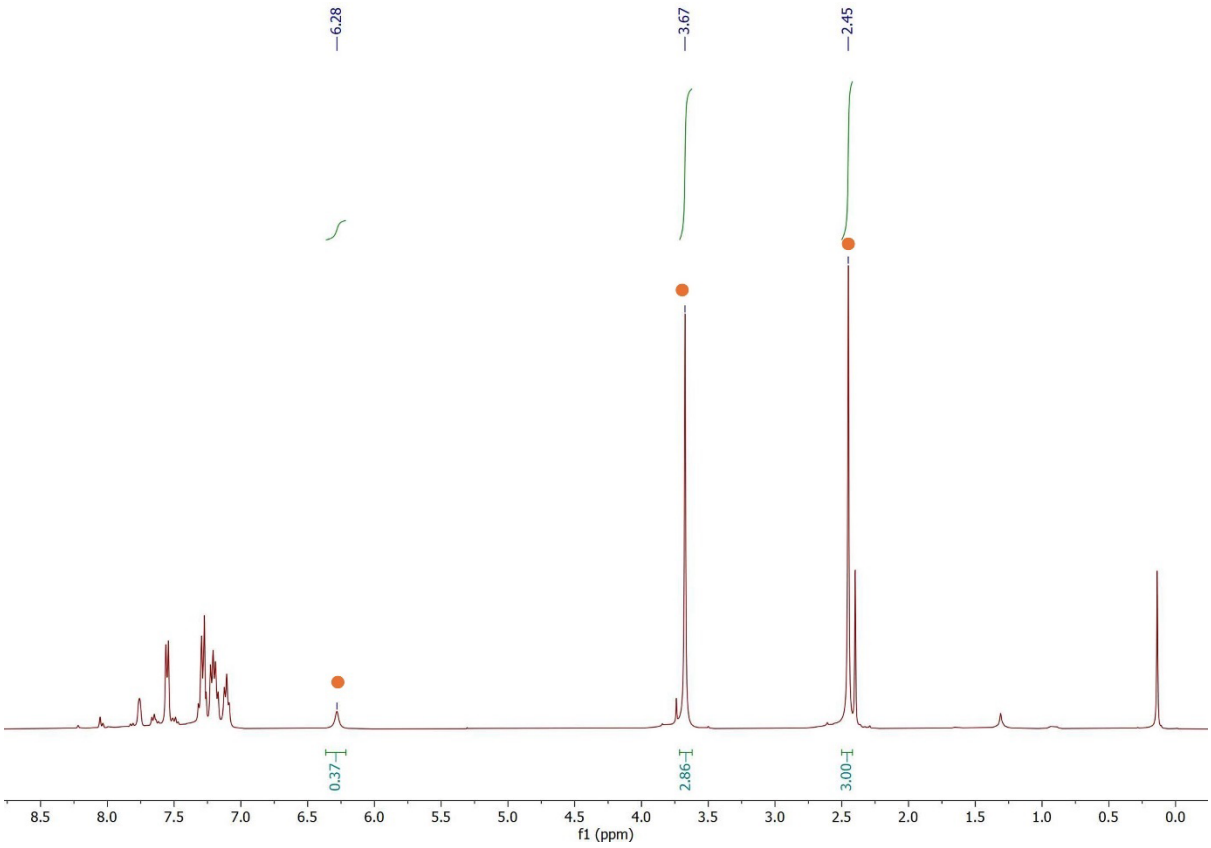


12.2. (b)

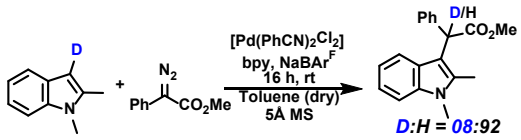


Procedure: Powdered [Pd(PhCN)$_2$Cl$_2$] (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), and NaBAr^F (21.3 mg, 0.02 mmol, 12.0 mol%) were introduced into an oven-dried Schlenk tube under nitrogen. After toluene (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30^{o}C under nitrogen for 1.0 h. 1,2-dimethyl-1*H*-indole (43.6 mg, 0.30 mmol) and D_2O (100 mg, 5.0 mmol , 25 eq) was then introduced. The resulting mixture was stirred at 30^{o}C under nitrogen till 16 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^{1}H NMR for analysis.

^{1}H NMR (400 MHz, CDCl$_3$):

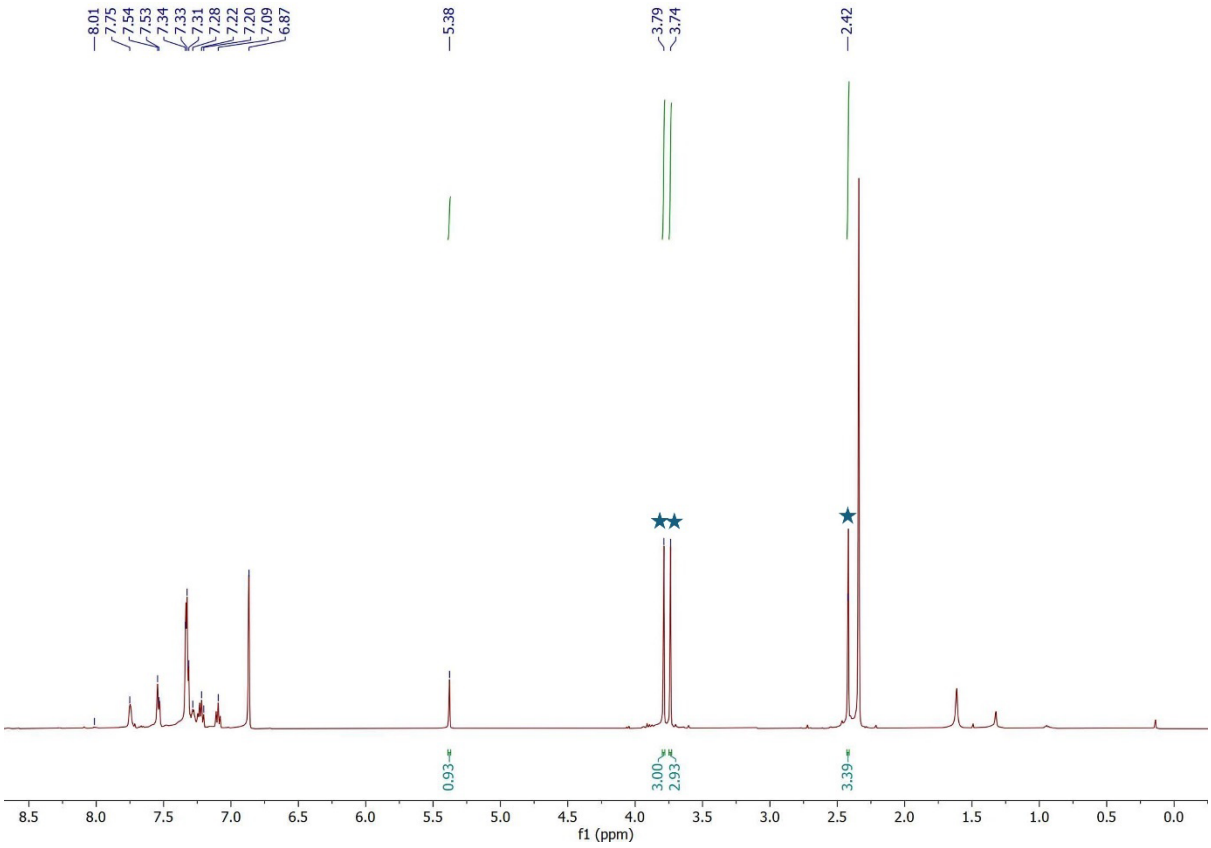


12.2. (c)

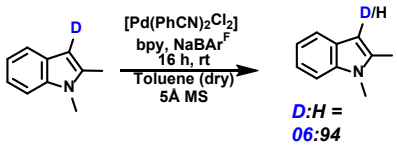


Procedure: Powdered [$Pd(PhCN)_2Cl_2$] (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.02 mmol, 12.0 mol%), and 200 mg 5 Å molecular sieves were introduced into an oven-dried Schlenk tube under nitrogen. After toluene (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under nitrogen for 1.0 h. 1,2-dimethyl-1*H*-indole-3-*d* (43.6 mg, 0.30 mmol) and methyl-α-diazo-α-phenylacetate (35.3 mg, 0.20 mmol) was then introduced in one portion. The resulting mixture was stirred at 30°C under nitrogen till 16 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. 28 µL mesitylene was added as an internal standard. The crude reaction mixture was subjected to ^{1}H NMR for analysis.

^{1}H NMR (400 MHz, $CDCl_3$):

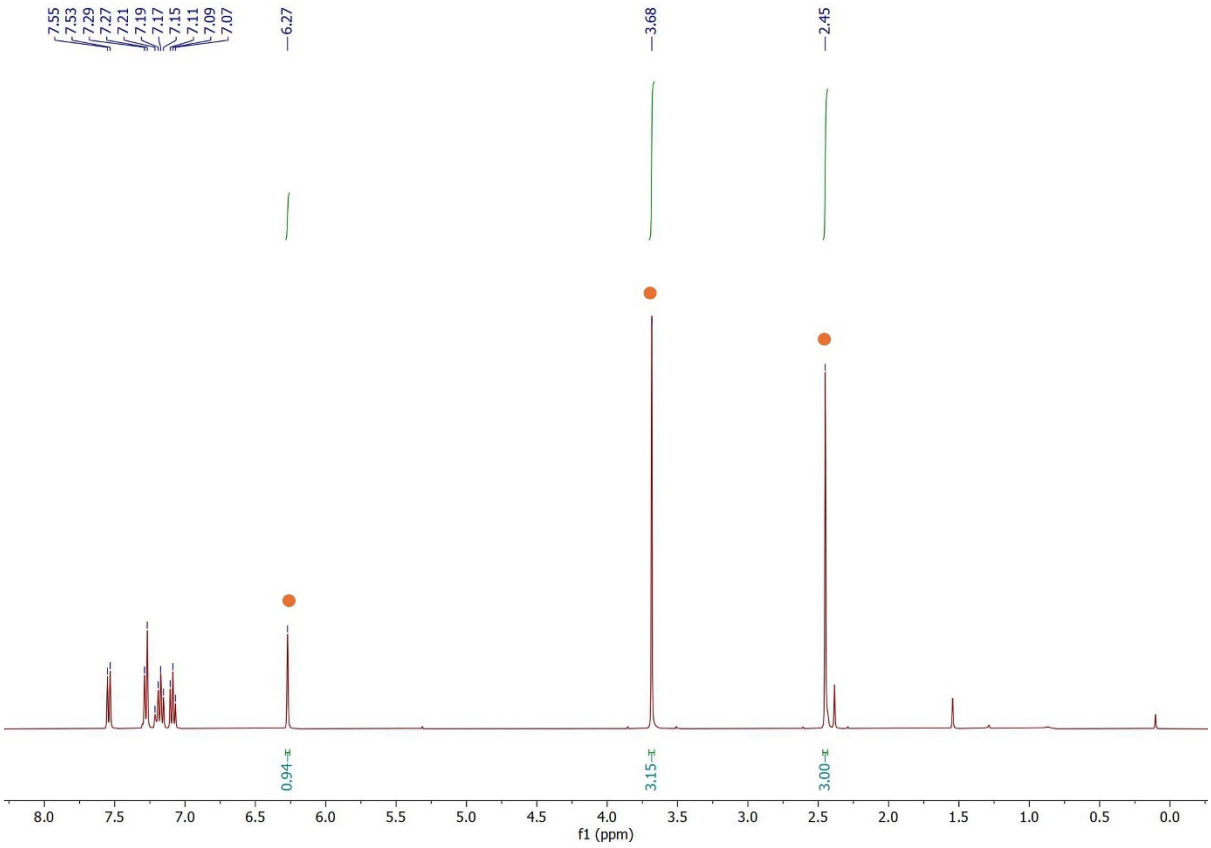


12.2. (d)



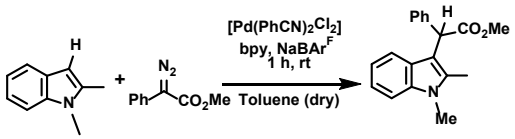
Procedure: Powdered [$Pd(PhCN)_2Cl_2$] (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.02 mmol, 12.0 mol%), and 200 mg 5 Å molecular sieves were introduced into an oven-dried Schlenk tube under nitrogen. After toluene (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under nitrogen for 1.0 h. 1,2-dimethyl-1*H*-indole-3-*d* (43.6 mg, 0.30 mmol) was then introduced. The resulting mixture was stirred at 30°C under nitrogen till 16 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^{1}H NMR for analysis.

^{1}H NMR (400 MHz, $CDCl_3$):



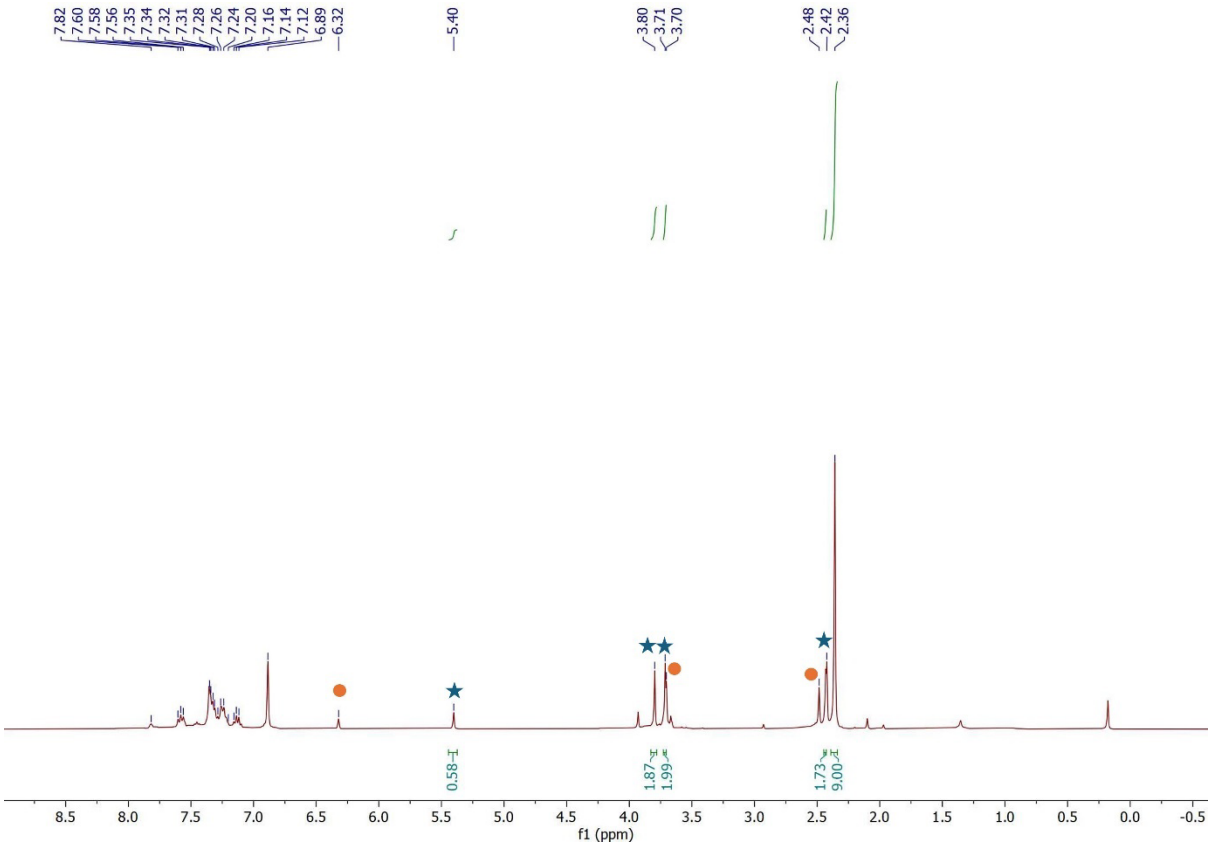
12.3. Control Experiments for Exchange in Indole

12.3 (a) Formation of indole alkylated product in 1h in absence of molecular-sieves (MS)

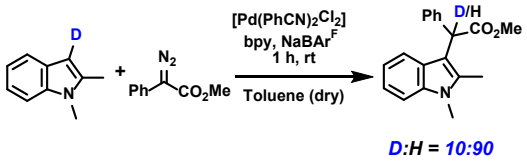


58%

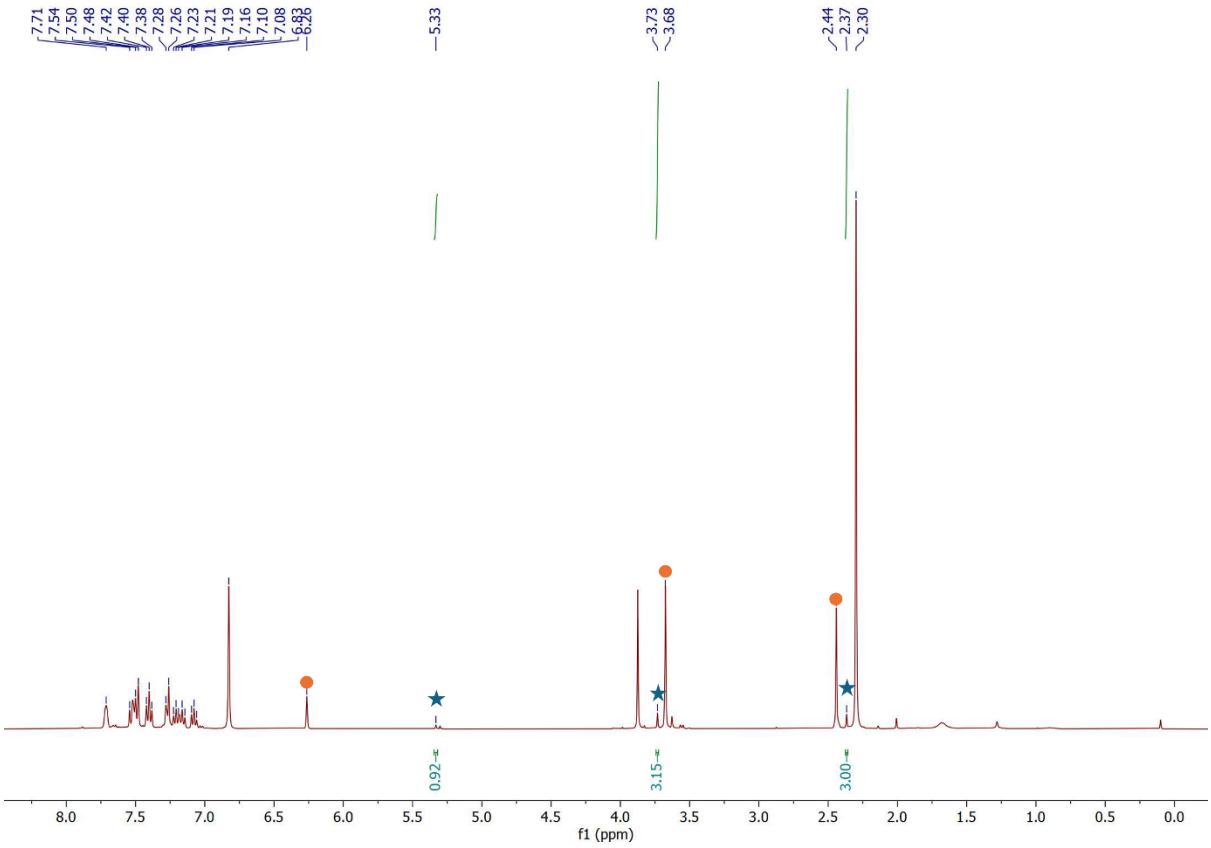
Procedure: Powdered $[Pd(PhCN)_2Cl_2]$ (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), and $NaBAr^F$ (21.3 mg, 0.024 mmol, 12.0 mol%) were introduced into an oven-dried Schlenk tube under argon. After toluene (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under argon for 1 h. 1,2-dimethyl-1*H*-indole (43.6 mg, 0.30 mmol) and methyl-α-diazo-α-phenylacetate (35.4 mg, 0.20 mmol) was then introduced in one portion. The resulting mixture was stirred at 30°C under argon till 1 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. 28 µL mesitylene was added as an internal standard. The crude reaction mixture was subjected to ^1H NMR for analysis.



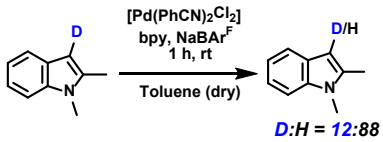
12.3. (b) Exchange in indole alkylated product in 1.0 h in toluene



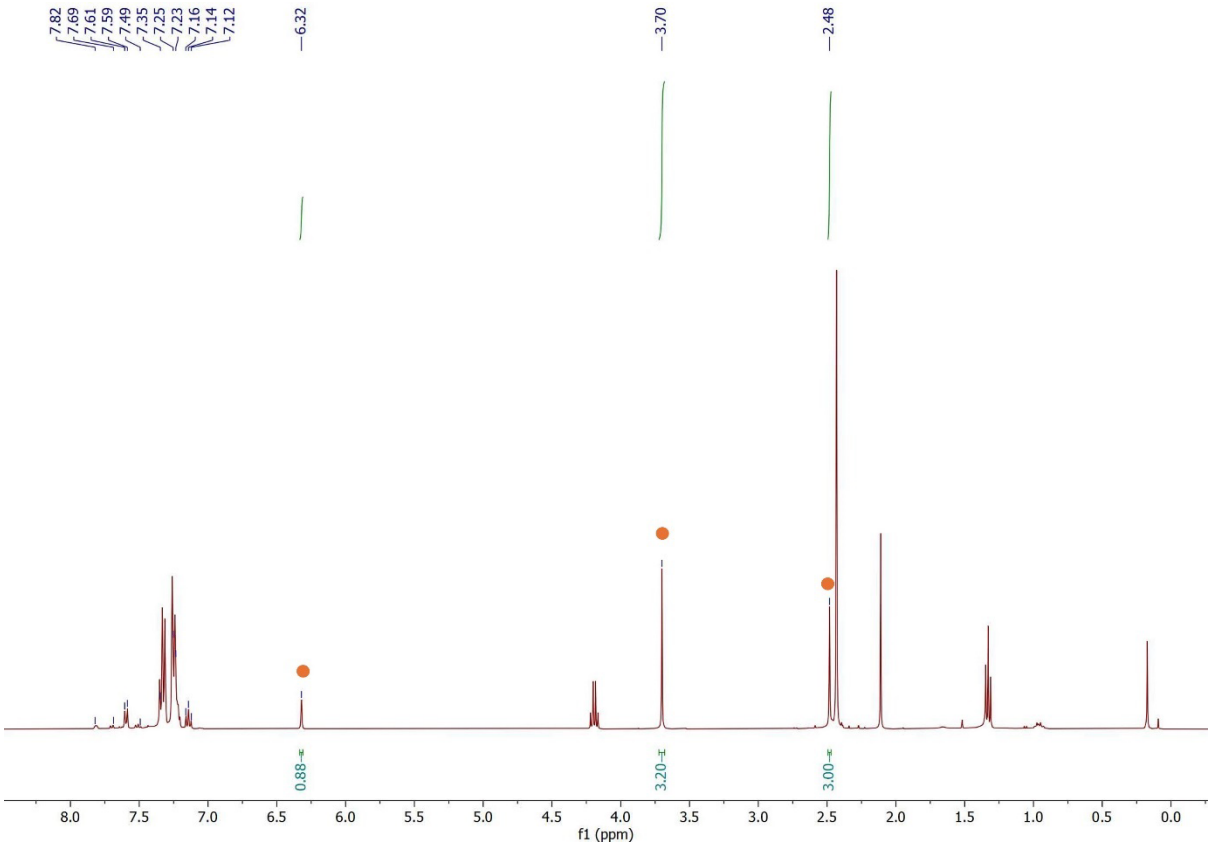
Procedure: Powdered $[Pd(PhCN)_2Cl_2]$ (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.02 mmol, 12.0 mol%) were introduced into an oven-dried Schlenk tube under nitrogen. After toluene (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under nitrogen for 1.0 h. 1,2-dimethyl-1*H*-indole-3-*d* (D:H=95:05)(43.6 mg, 0.30 mmol) and methyl-α-diazo-α-phenylacetate (35.3 mg, 0.20 mmol) was then introduced in one portion. The resulting mixture was stirred at 30°C under nitrogen till 1.0 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. 28 μL mesitylene was added as an internal standard. The crude reaction mixture was subjected to ^1H NMR for analysis.



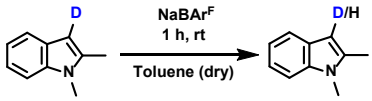
12.3. (c) Exchange in indole in 1.0 h in toluene



Procedure: Powdered [$Pd(PhCN)_2Cl_2$] (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.02 mmol, 12.0 mol%) were introduced into an oven-dried Schlenk tube under nitrogen. After toluene (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under nitrogen for 1.0 h. 1,2-dimethyl-1*H*-indole-3-*d* (D:H=95:05)(43.6 mg, 0.30 mmol) was then introduced. The resulting mixture was stirred at 30°C under nitrogen till 1.0 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^1H NMR for analysis.



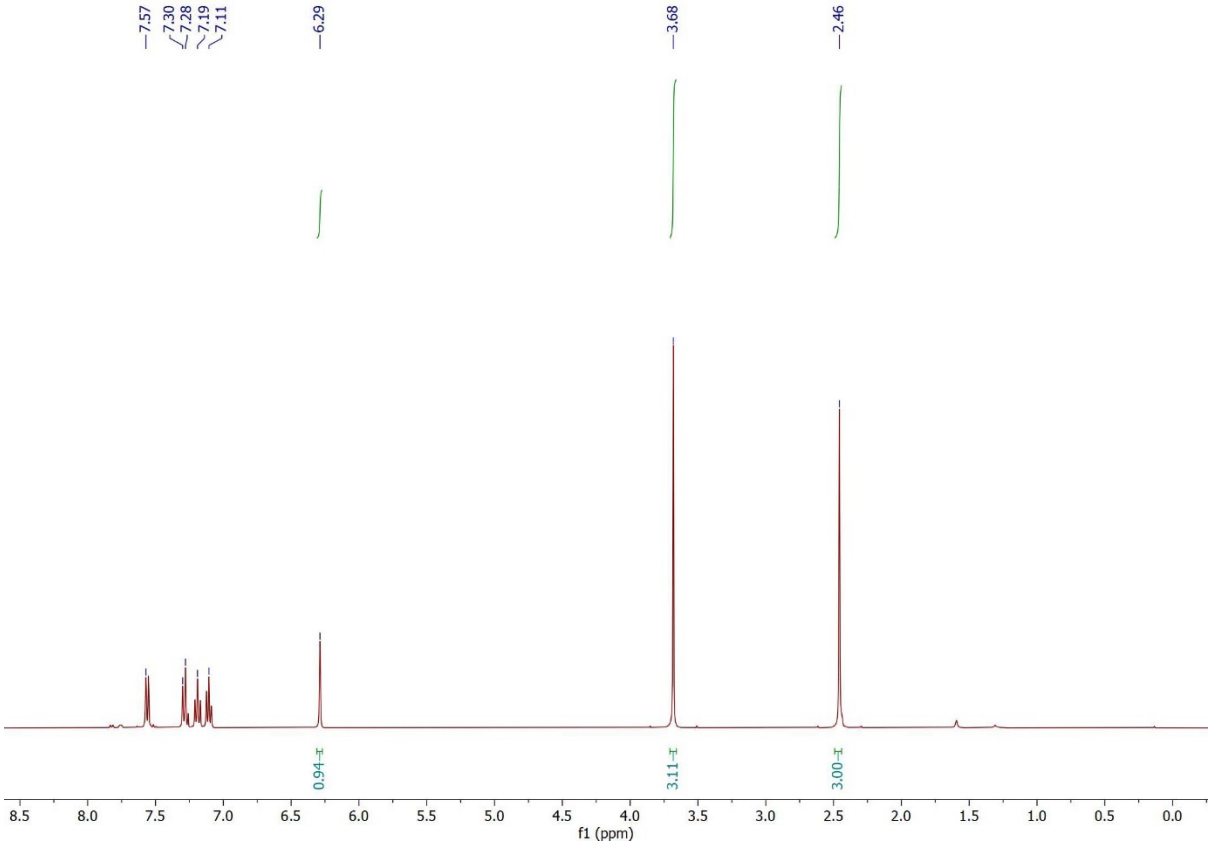
12.3. (d) Effect of $NaBAr^F$ on D:H ratio of indole



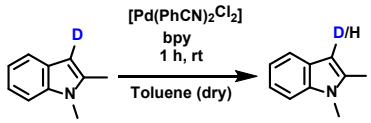
D*:*H* = *07*:*93

Procedure: $NaBAr^F$ (21.3 mg, 0.02 mmol) and 1,2-dimethyl-1*H*-indole-3-*d* (D:H=95:05) (43.6 mg, 0.30 mmol) were introduced into an oven-dried Schlenk tube under nitrogen. Toluene (2.0 mL) was injected into the Schlenk tube and the solution was stirred at 30°C under nitrogen for 1.0 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^{1}H NMR for

analysis.

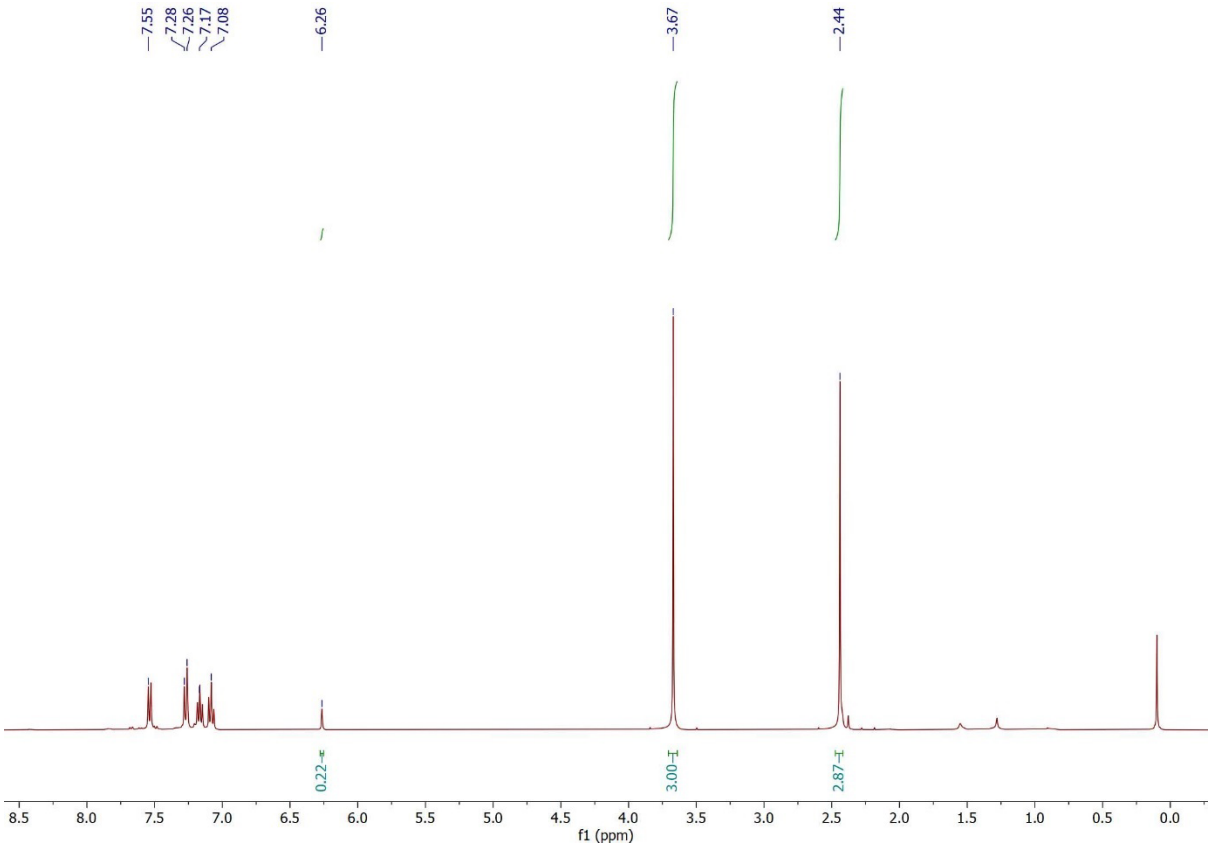


12.3. (e) Effect of $[Pd(PhCN)_2Cl_2]$ and bpy on D:H ratio of indole

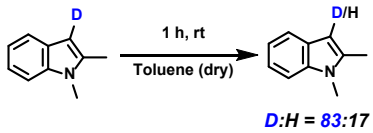


D:H* = *78:22

Procedure: Powdered $[Pd(PhCN)_2Cl_2]$ (3.9 mg, 0.01 mmol), 2,2'-bipyridine (1.6 mg, 0.01 mmol), and 1,2-dimethyl-1*H*-indole-3-*d* (D:H=95:05)(43.6 mg, 0.30 mmol) were introduced into an oven-dried Schlenk tube under nitrogen. Toluene (2.0 mL) was injected into the Schlenk tube and the solution was stirred at 30°C under nitrogen for 1.0 h. T The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^{1}H NMR for analysis.

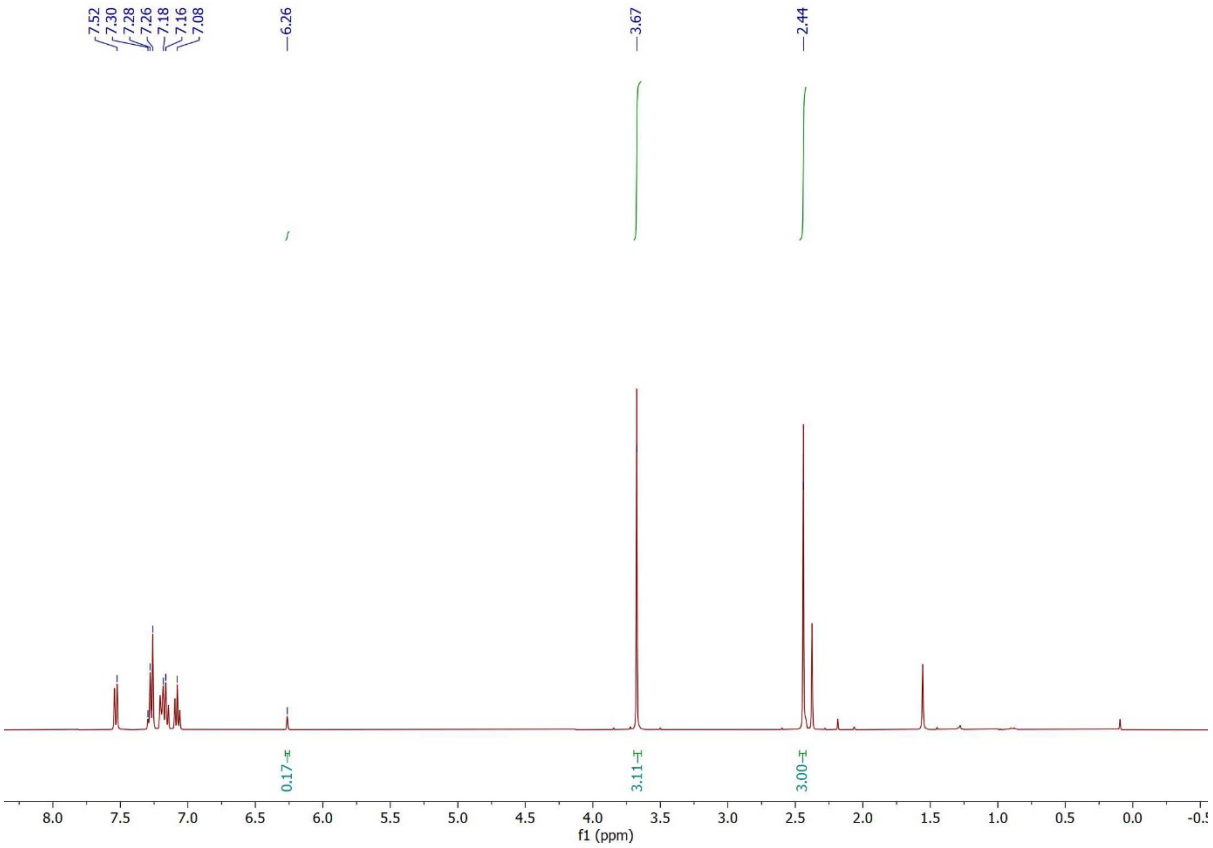


12.3. (f) Exchange in indole due to solvent (toluene)

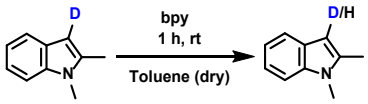


D*:*H* = *83*:*17

Procedure: 1,2-dimethyl-1*H*-indole-3-*d* (D:H=95:05) (43.6 mg, 0.30 mmol) was introduced into an oven-dried Schlenk tube under nitrogen. Toluene (2.0 mL) was injected into the Schlenk tube and the solution was stirred at 30°C under nitrogen for 1.0 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^{1}H NMR for analysis.

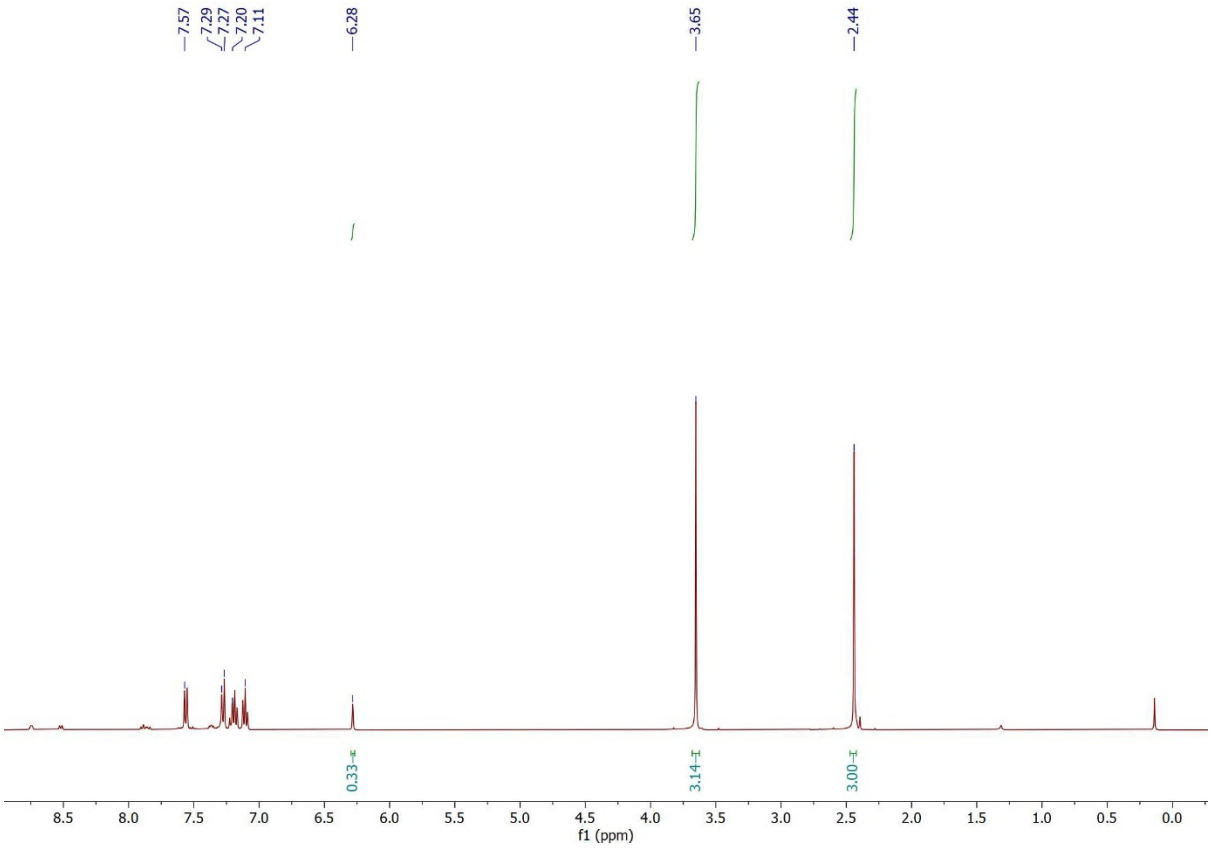


12.3. (g) Exchange in indole due to bpy ligand

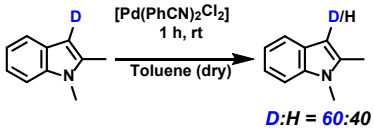


***D*:*H* = 67:33**

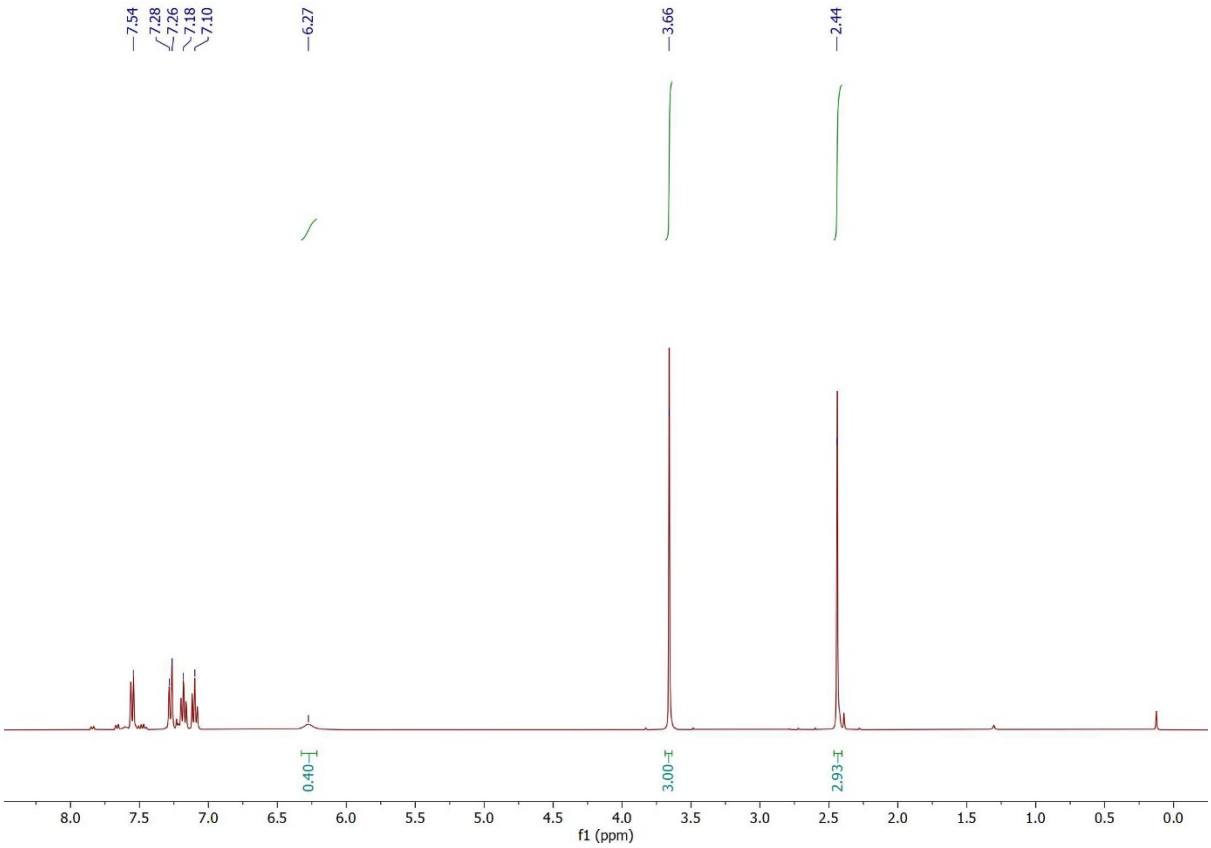
Procedure: 2,2'-bipyridine (1.6 mg, 0.01 mmol), and 1,2-dimethyl-1*H*-indole-3-*d* (D:H=95:05)(43.6 mg, 0.30 mmol) were introduced into an oven-dried Schlenk tube under nitrogen. Toluene (2.0 mL) was injected into the Schlenk tube and the solution was stirred at 30°C under nitrogen for 1.0 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^{1}H NMR for analysis.



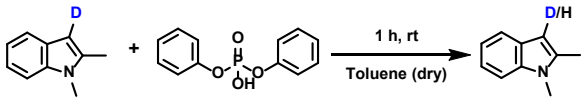
12.3. (h) Exchange in indole due to $[Pd(PhCN)_2Cl_2]$



Procedure: Powdered $[Pd(PhCN)_2Cl_2]$ (3.9 mg, 0.01 mmol) and 1,2-dimethyl-1*H*-indole-3-*d* (D:H=95:05)(43.6 mg, 0.30 mmol) were introduced into an oven-dried Schlenk tube under nitrogen. Toluene (2.0 mL) was injected into the Schlenk tube and the solution was stirred at 30°C under nitrogen for 1.0 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^1H NMR for analysis.

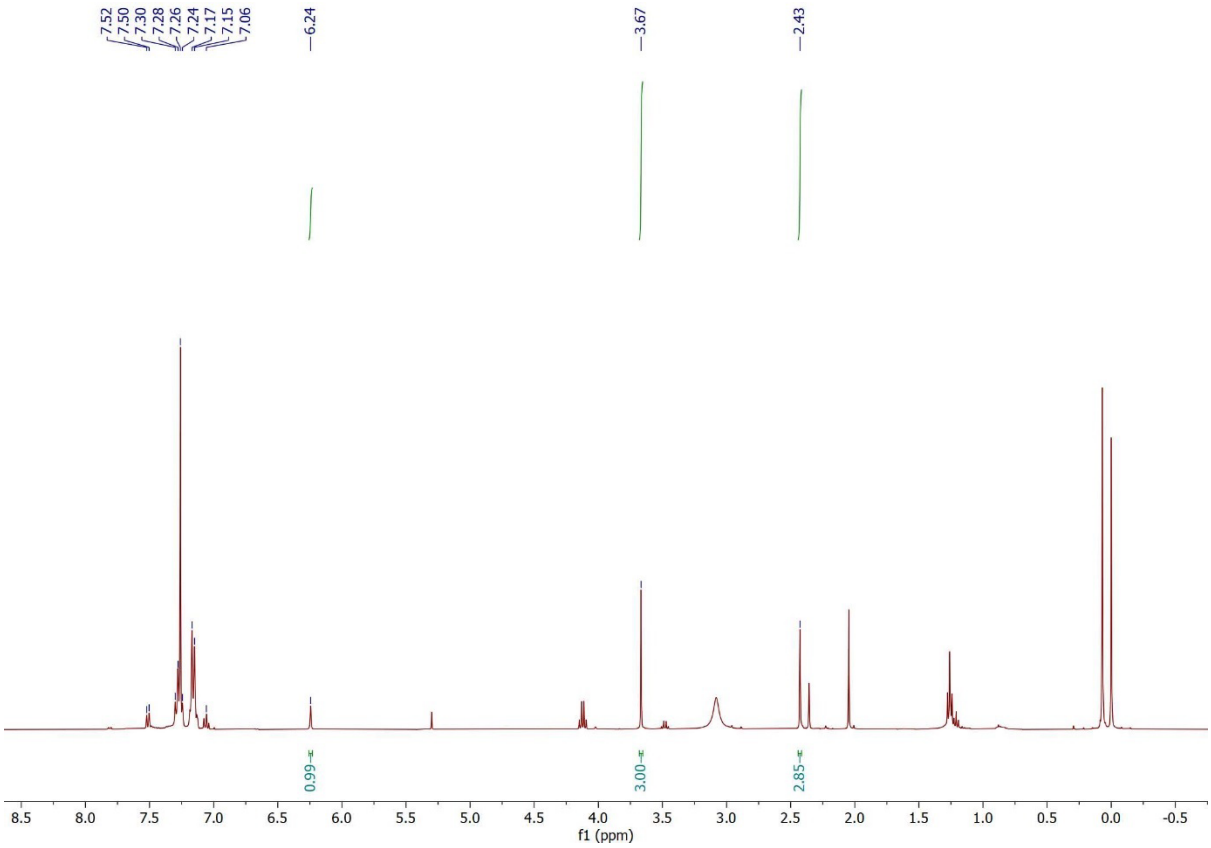


12.3. (i) Exchange in indole due to diphenylphosphate (Brønsted acid)

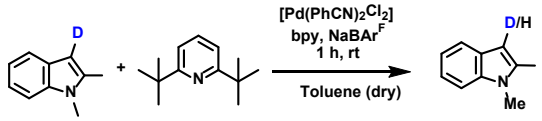


***D*:H = *0*:100**

Procedure: 1,2-dimethyl-1*H*-indole-3-*d* (D:H=95:05) (43.6 mg, 0.30 mmol) and Brønsted acid diphenylphosphate (2.5 mg, 0.01 mmol) were introduced into an oven-dried Schlenk tube under nitrogen. Toluene (2.0 mL) was injected into the Schlenk tube and the solution was stirred at 30°C under nitrogen for 1.0 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^{1}H NMR for analysis.

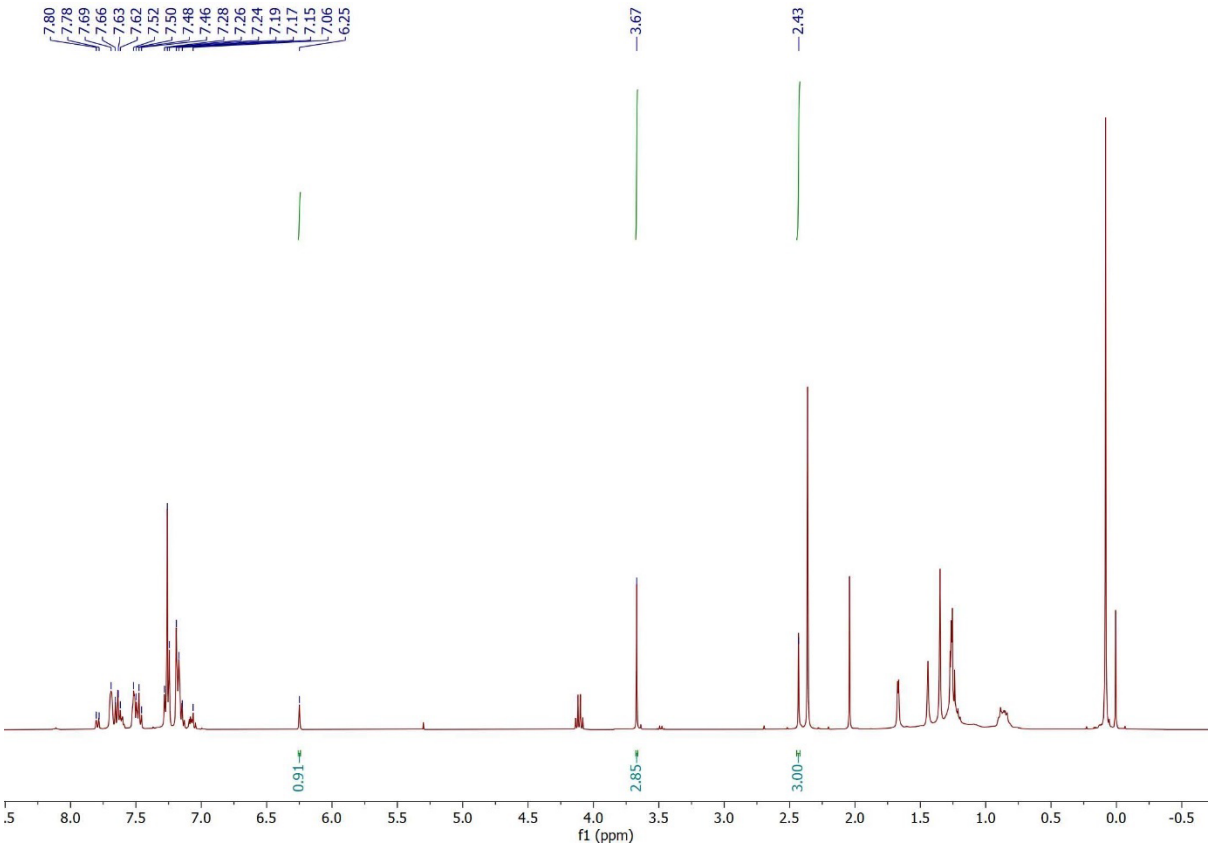


12.3. (j) Exchange in indole in standard reaction conditions in presence of an added base

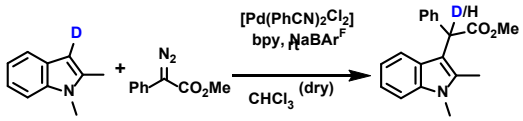


D*:*H* = *10*:*91

Procedure: Powdered $[Pd(PhCN)_2Cl_2]$ (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.02 mmol, 12.0 mol%) were introduced into an oven-dried Schlenk tube under nitrogen. After toluene (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under nitrogen for 1.0 h. 1,2-dimethyl-1*H*-indole-3-*d* (D:H=95:05)(43.6 mg, 0.30 mmol) along with 2,6-Di-*tert*-butylpyridine in stoichiometric amount was then introduced. The resulting mixture was stirred at 30°C under nitrogen till 1.0 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^1H NMR for analysis.



12.4. Monitoring Exchange in Unreacted Indole and Product with Time in Chloroform

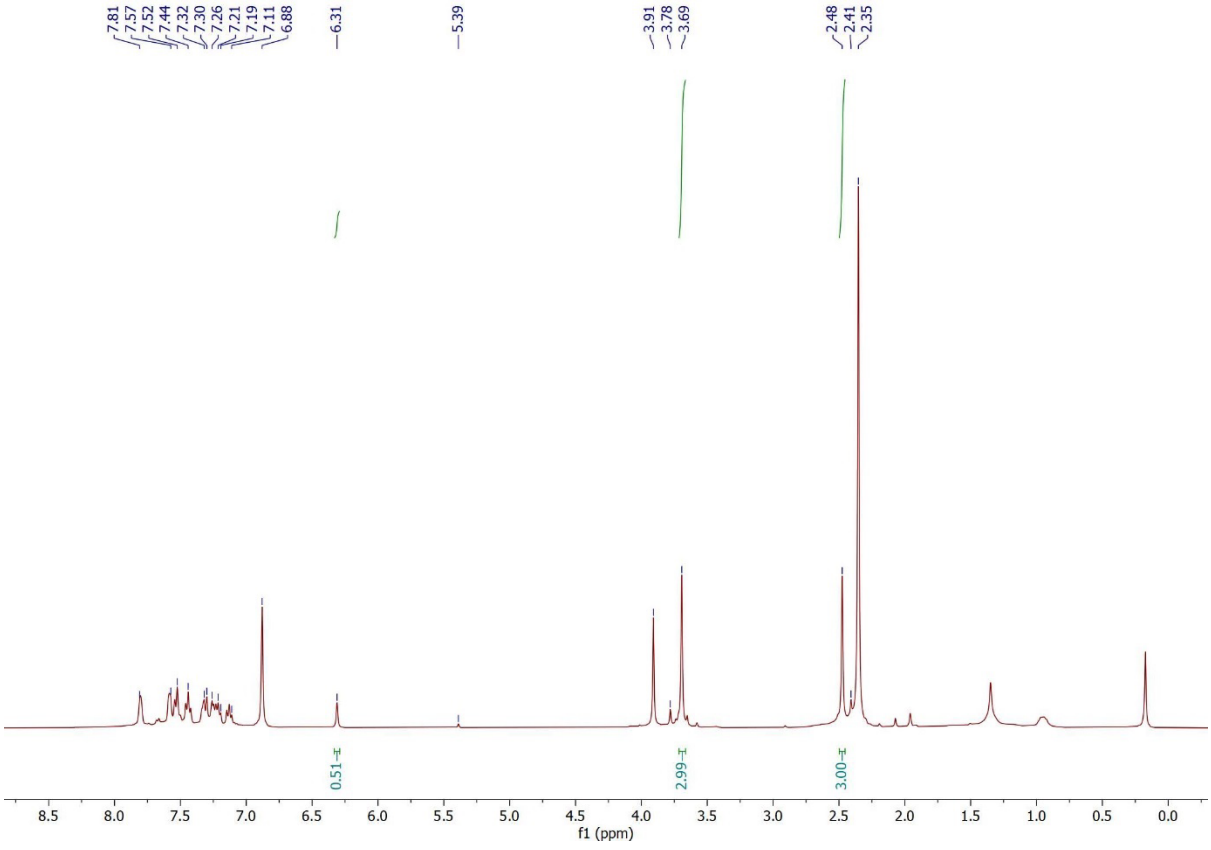


Procedure: Powdered $[Pd(PhCN)_2Cl_2]$ (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.02 mmol, 12.0 mol%) were taken as catalytic mixture and procedure given in section 12.2(c) was followed in chloroform solvent. Four such reactions were set up and were stirred for 10, 20, 30, 60 minutes, respectively. The respective reaction mixtures were then filtered, and the filtrates were concentrated under vacuum. Mesitylene was added in the respective mixtures. The crude reaction mixtures were subjected to ^1H NMR for analysis.

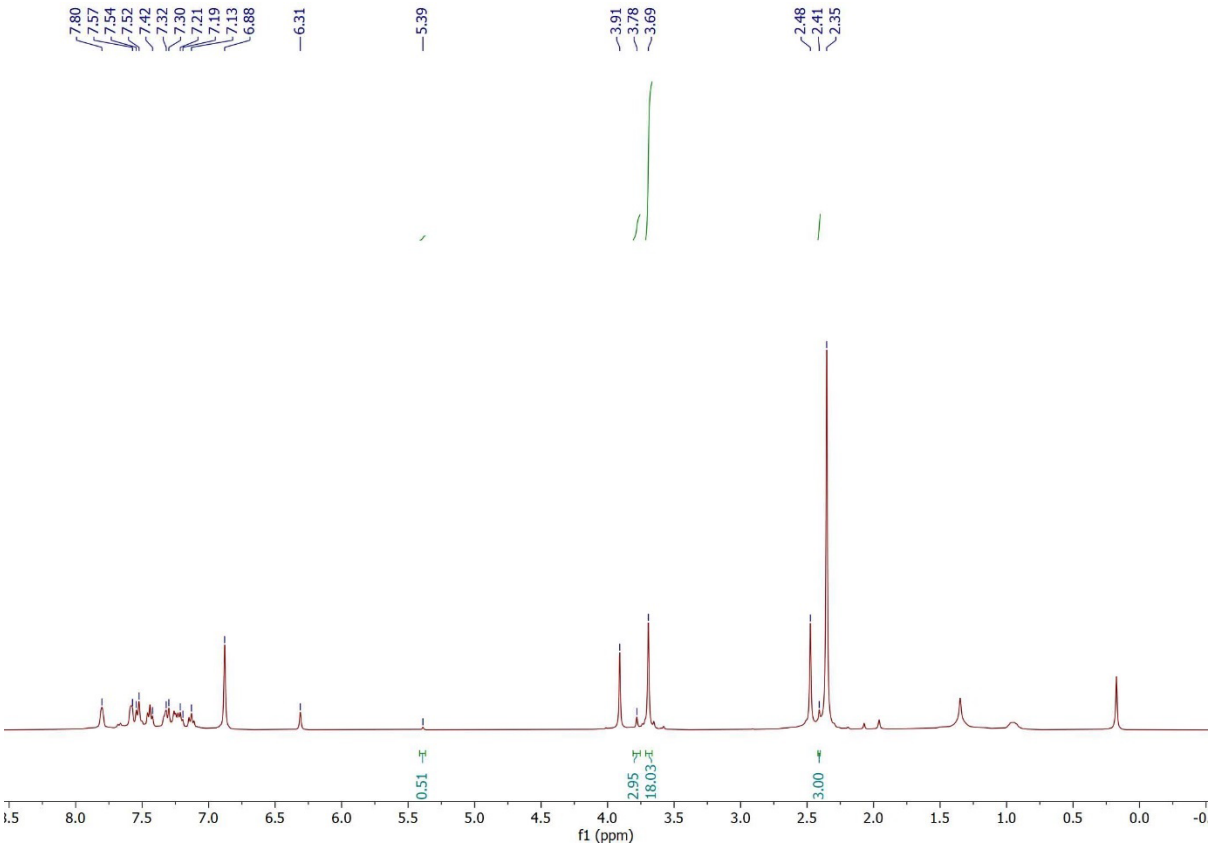
Table S9 D:H Ratio in Unreacted Indole and Product with Time along with respective Yields in Chloroform

t (min)	D:H in unreacted indole	D:H in product	yield
0	75:25	-	-
10	49:51	49:51	14
20	49:51	48:52	24
30	43:57	44:56	34
60	33:67	38:62	40

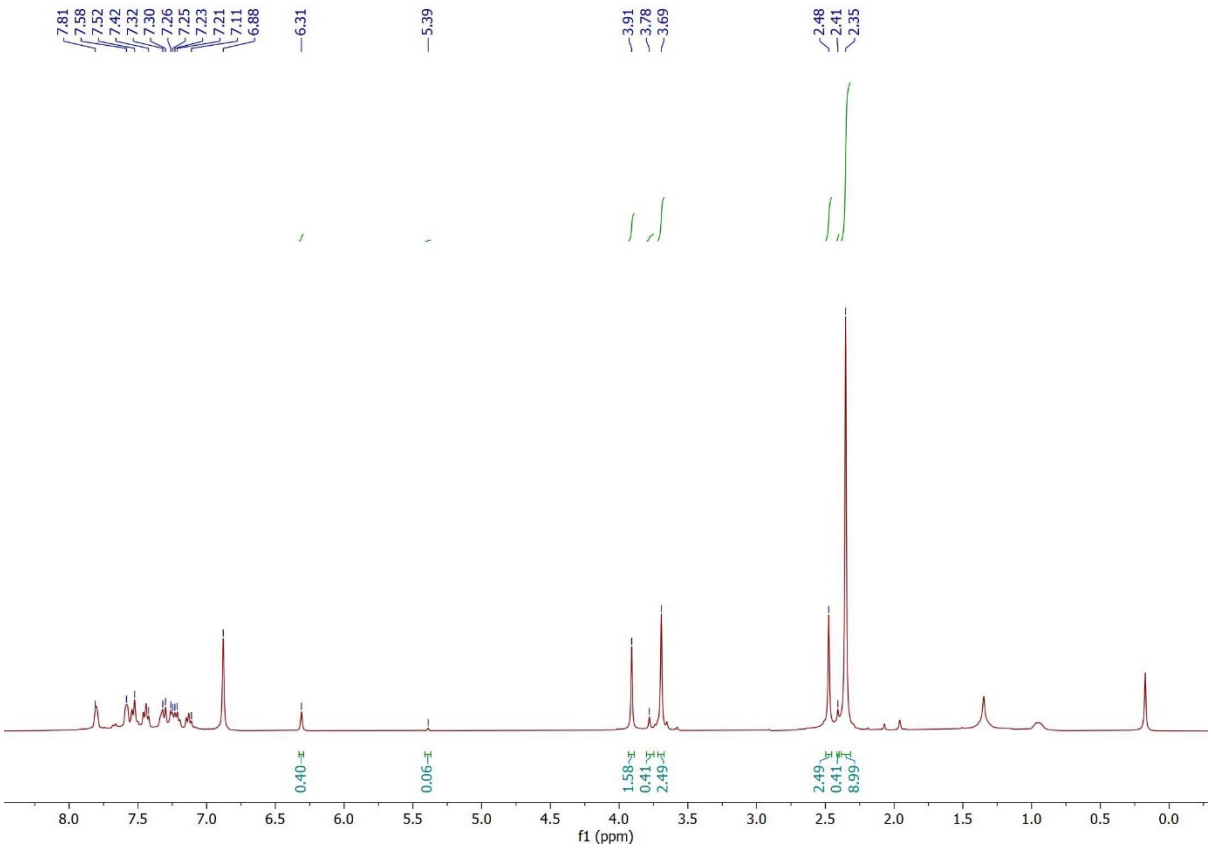
10 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for unreacted indole:



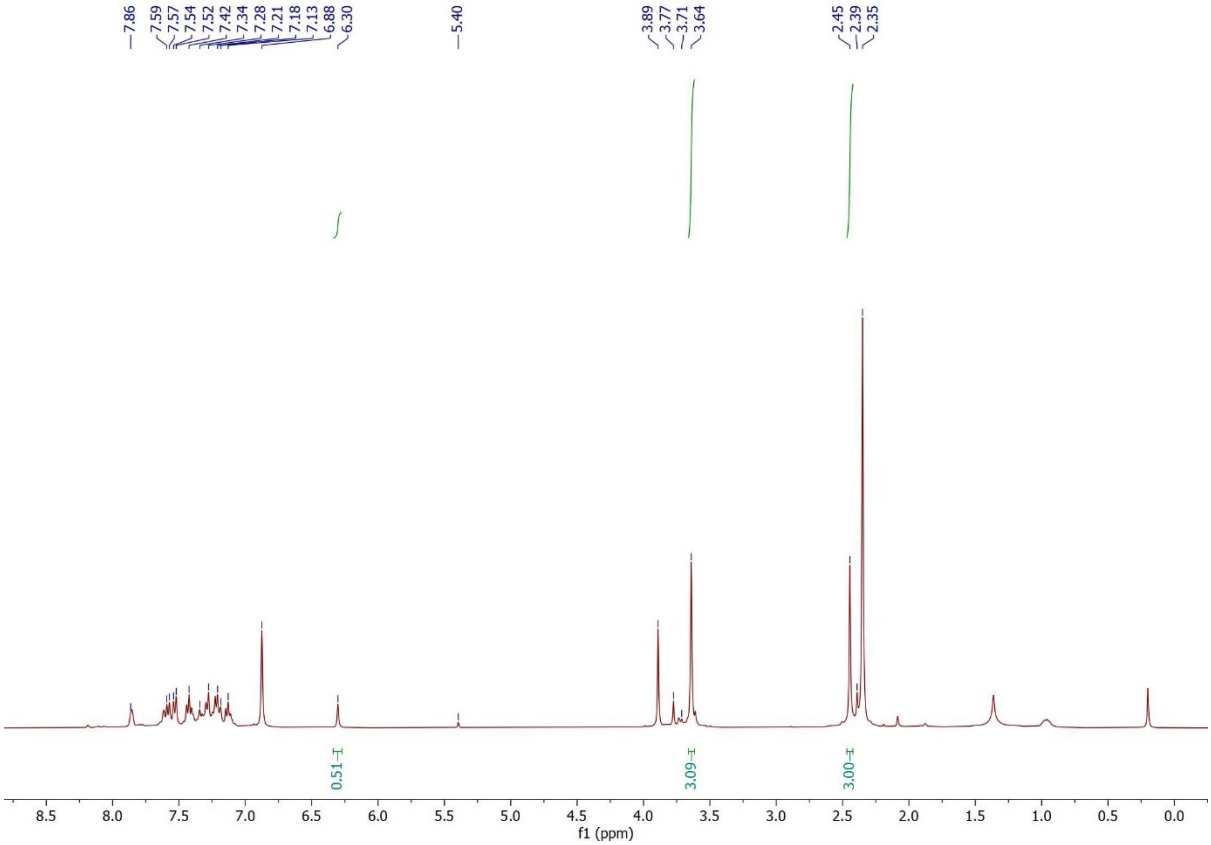
10 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for product:



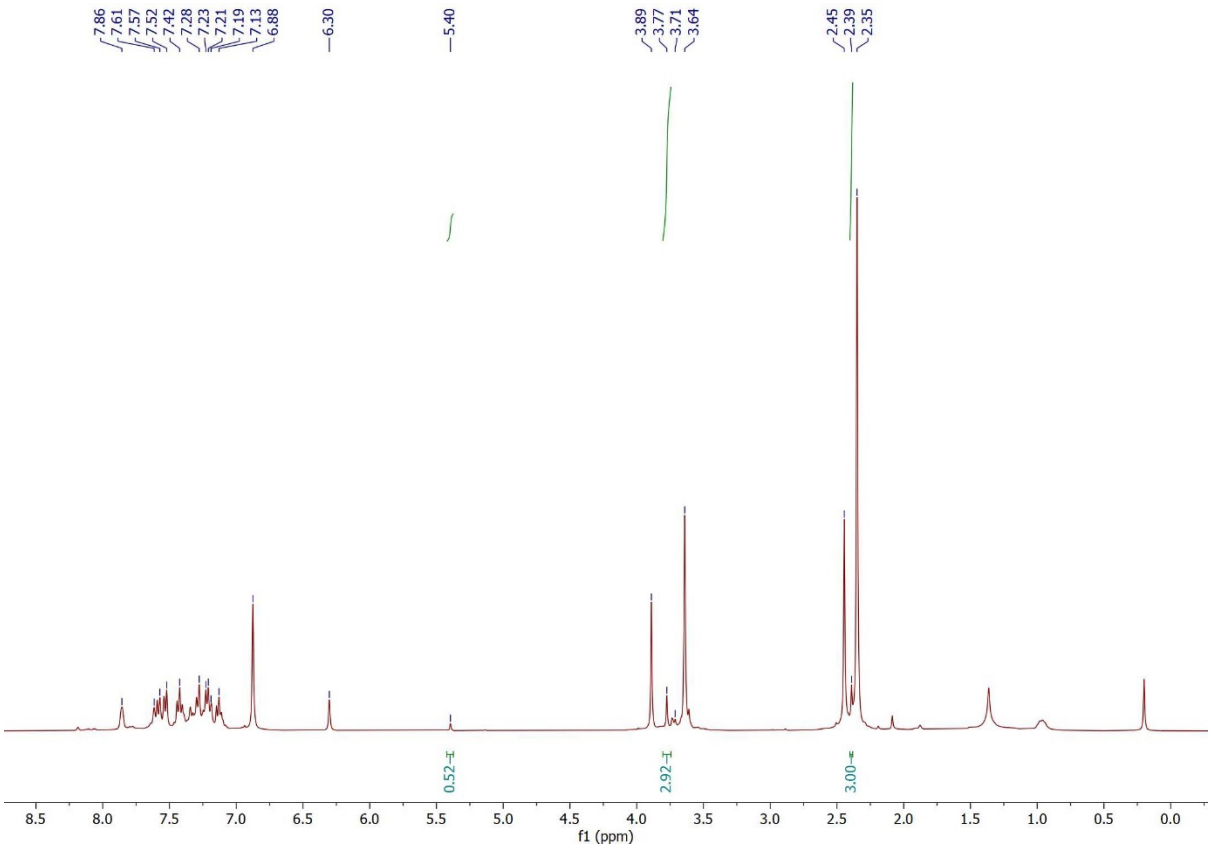
10 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for yield of product:



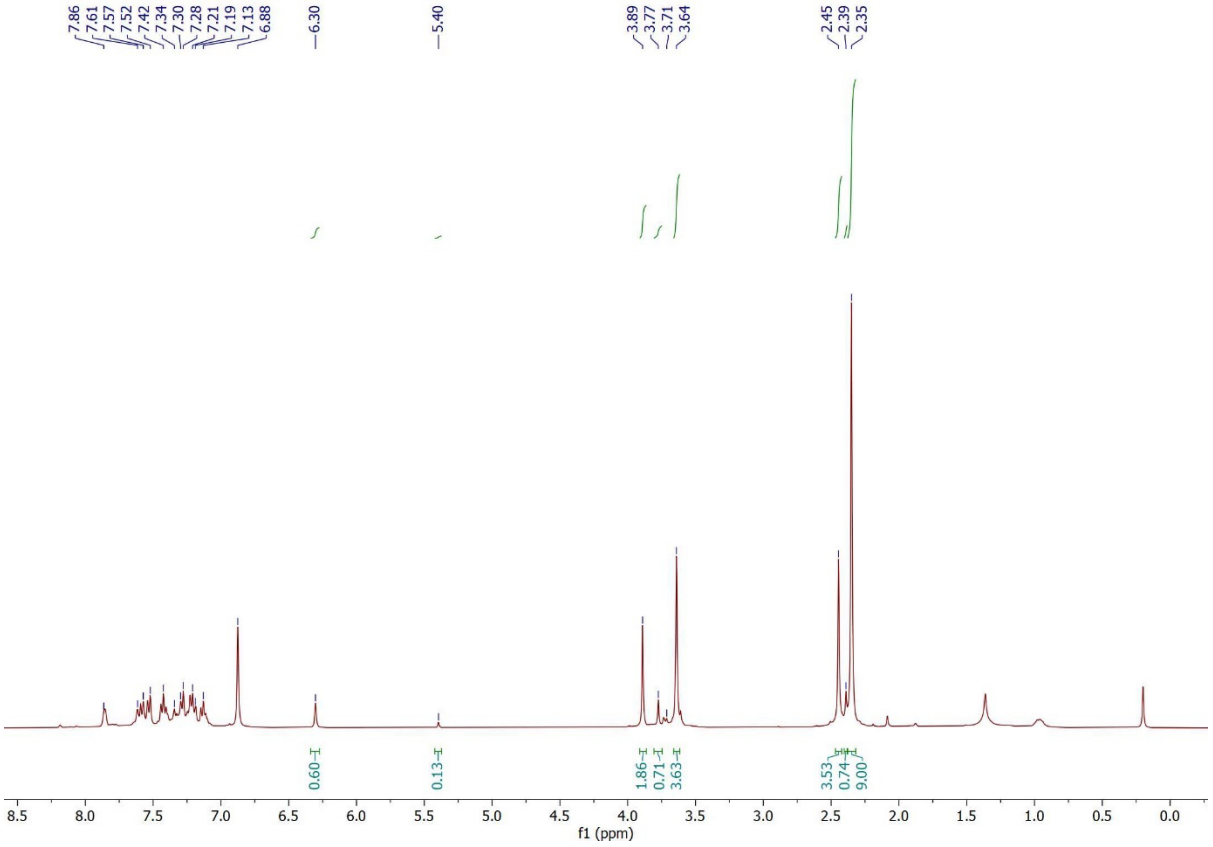
20 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for unreacted indole:



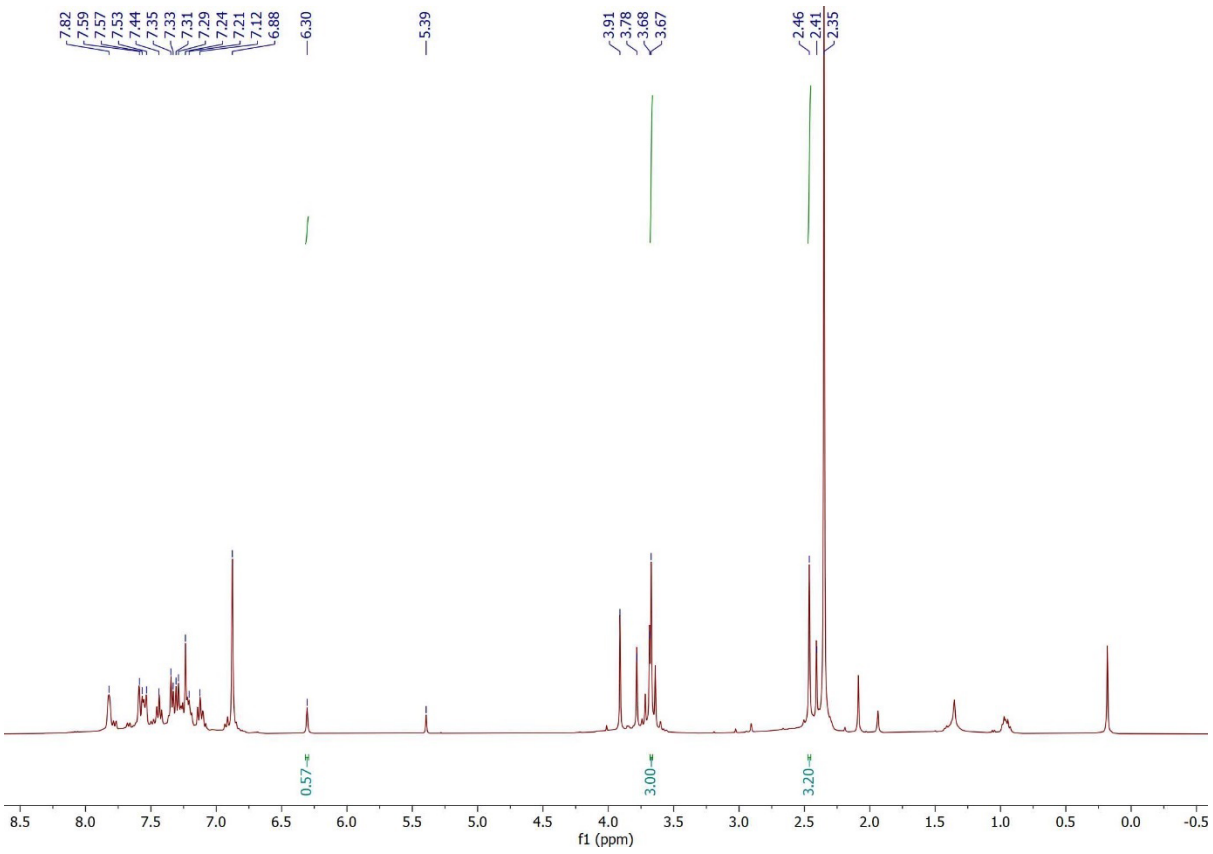
20 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for product:



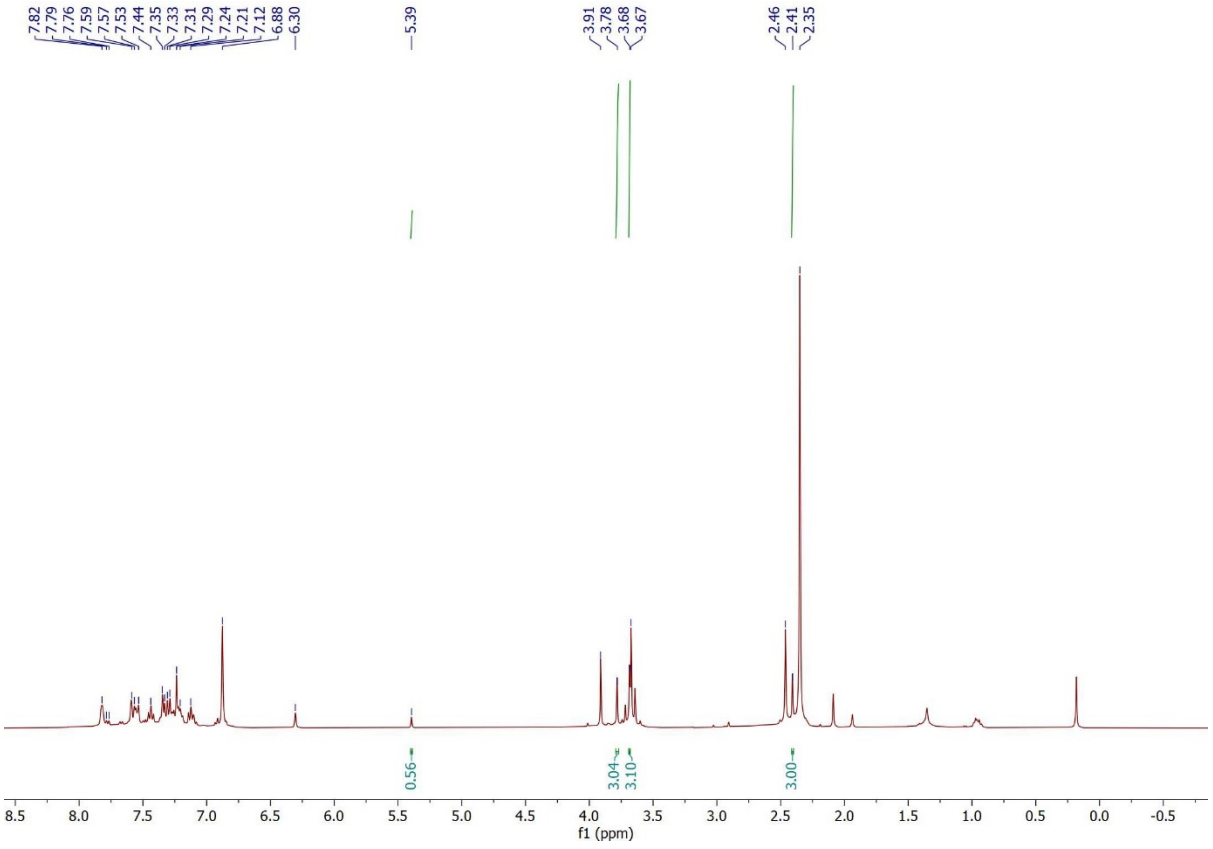
20 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for yield of product:



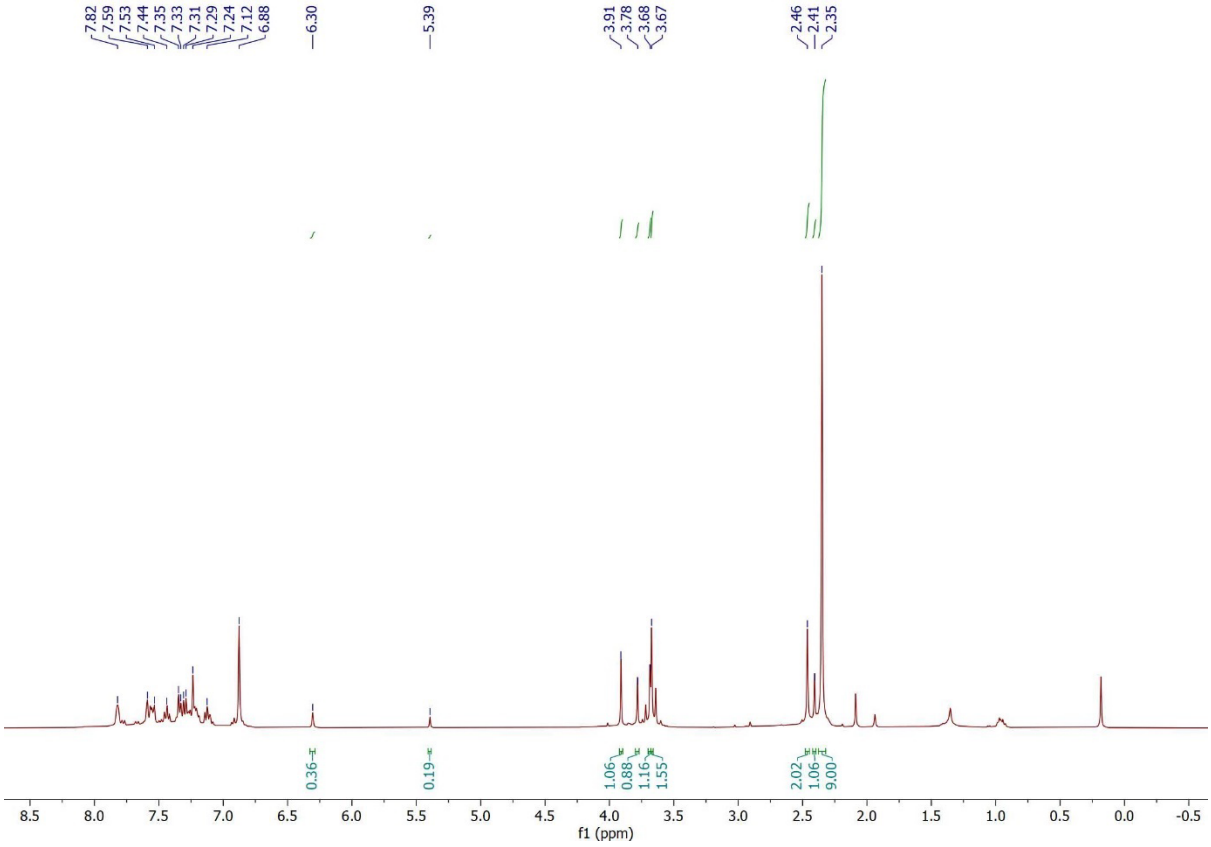
30 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for unreacted indole:



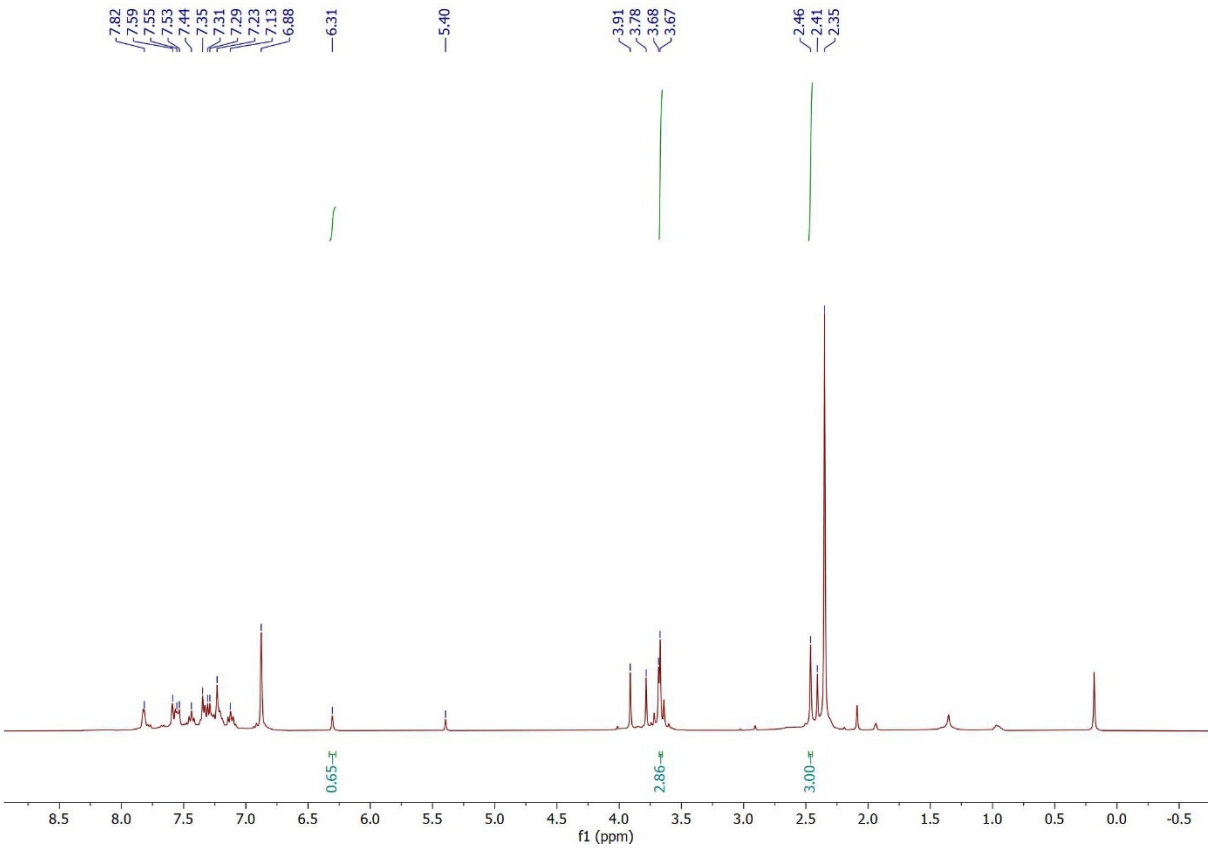
30 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for product:



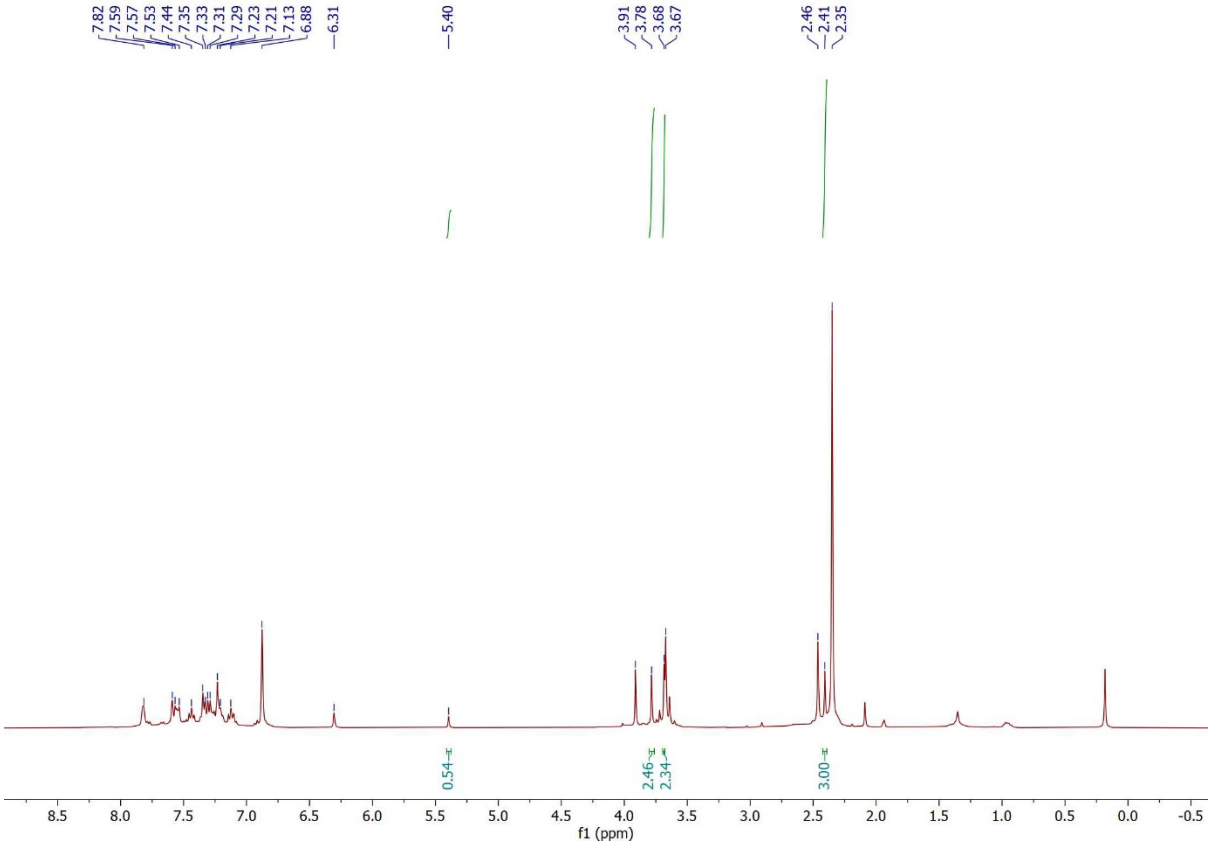
30 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for yield of product:



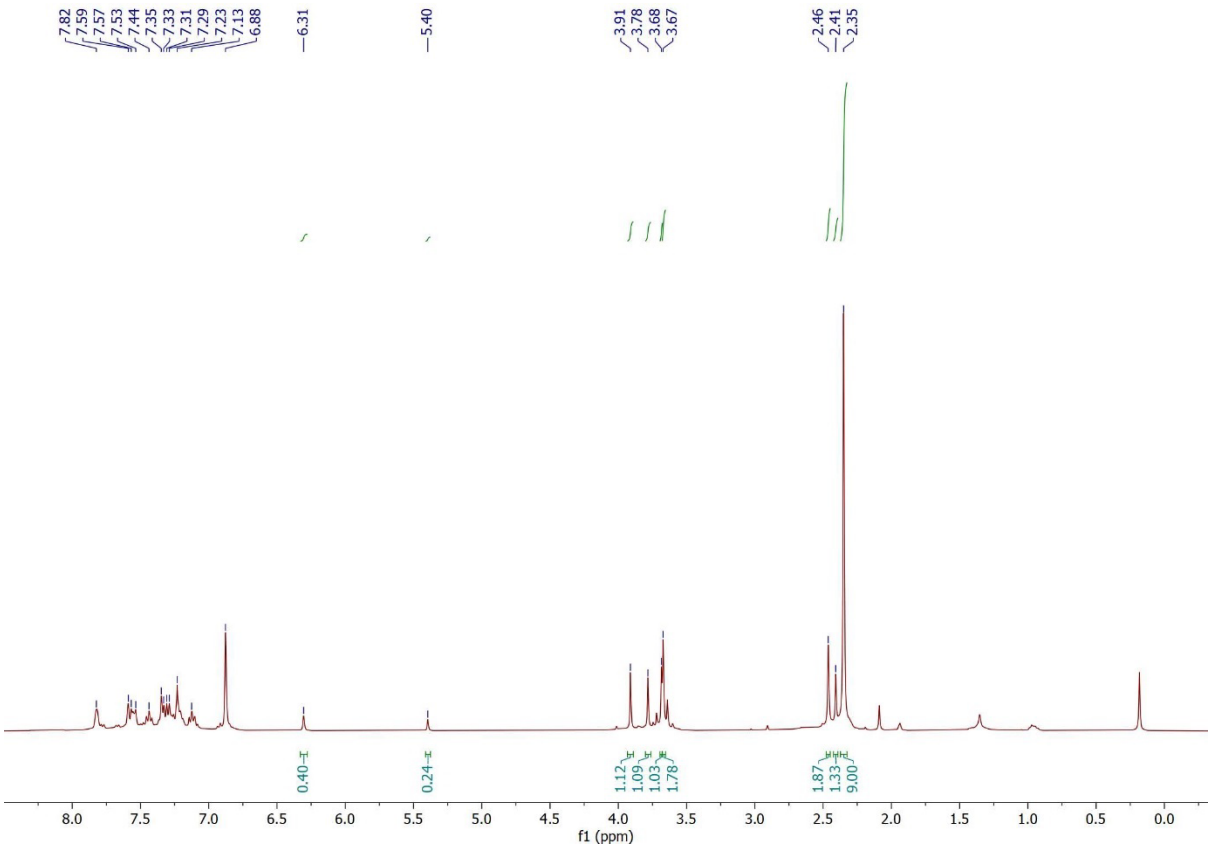
60 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for unreacted indole:



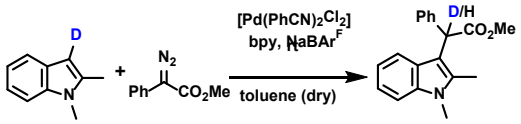
60 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for product:



60 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for yield of product:



12.5. Monitoring Exchange in Unreacted Indole and Product with Time in Toluene



Procedure: Procedure given in section 12.4 was followed in toluene. Five such reactions were set up and were stirred for 10, 20, 40, 50, 60 minutes, respectively. The respective reaction mixtures were then filtered, and the filtrates were concentrated under vacuum. The crude reaction mixtures were subjected to ^{1}H NMR for analysis.

Table S10 D:H ratio in Unreacted Indole and Product with Time in Toluene

t (min)	D:H in unreacted indole	D:H in product
0	61:39	-
10	20:80	30:70
20	20:80	22:78
40	24:76	27:73
50	15:85	25:75
60	14:86	24:76

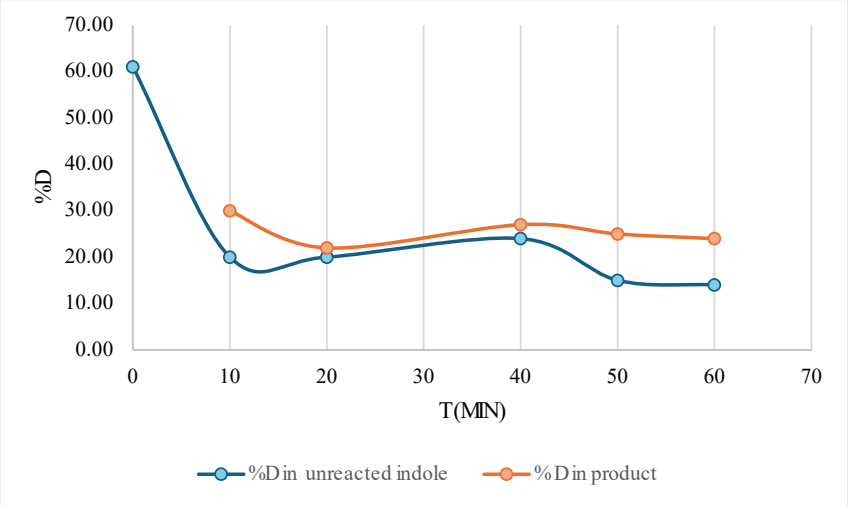
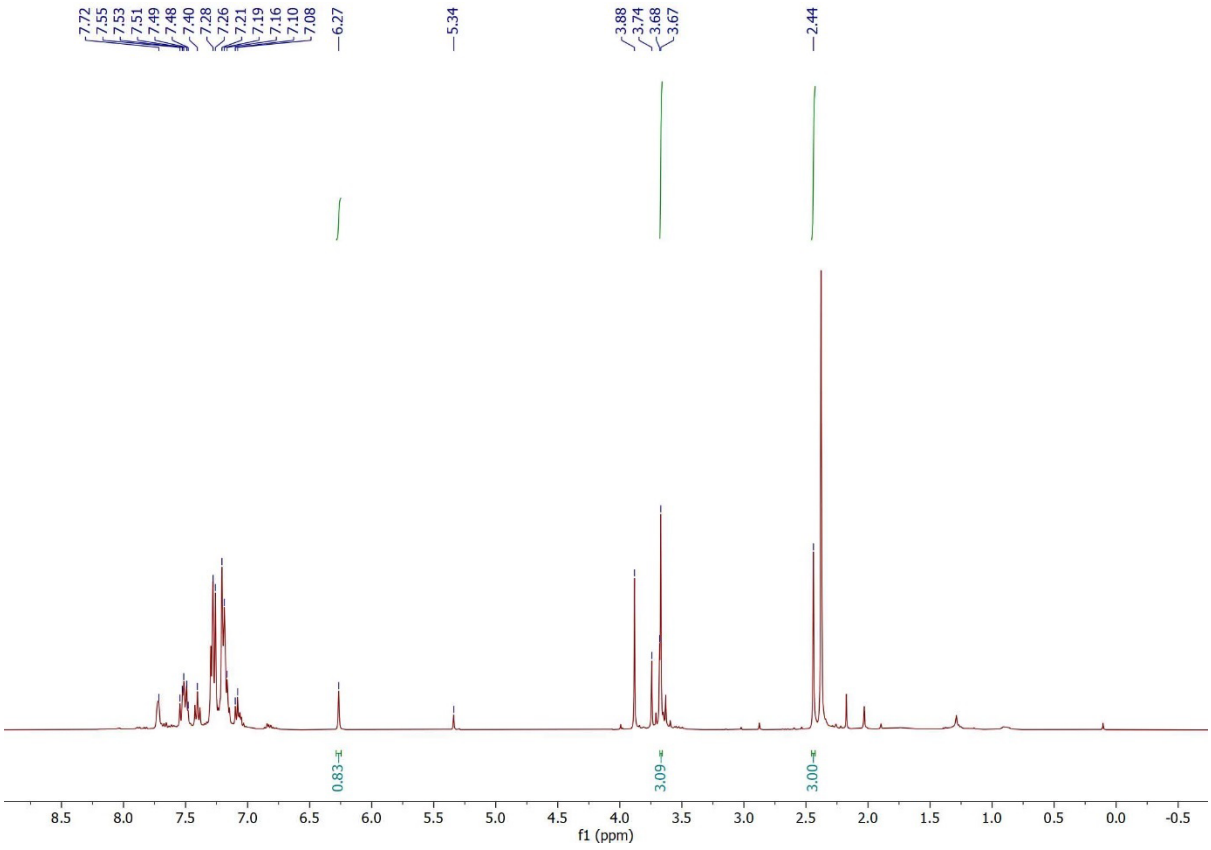
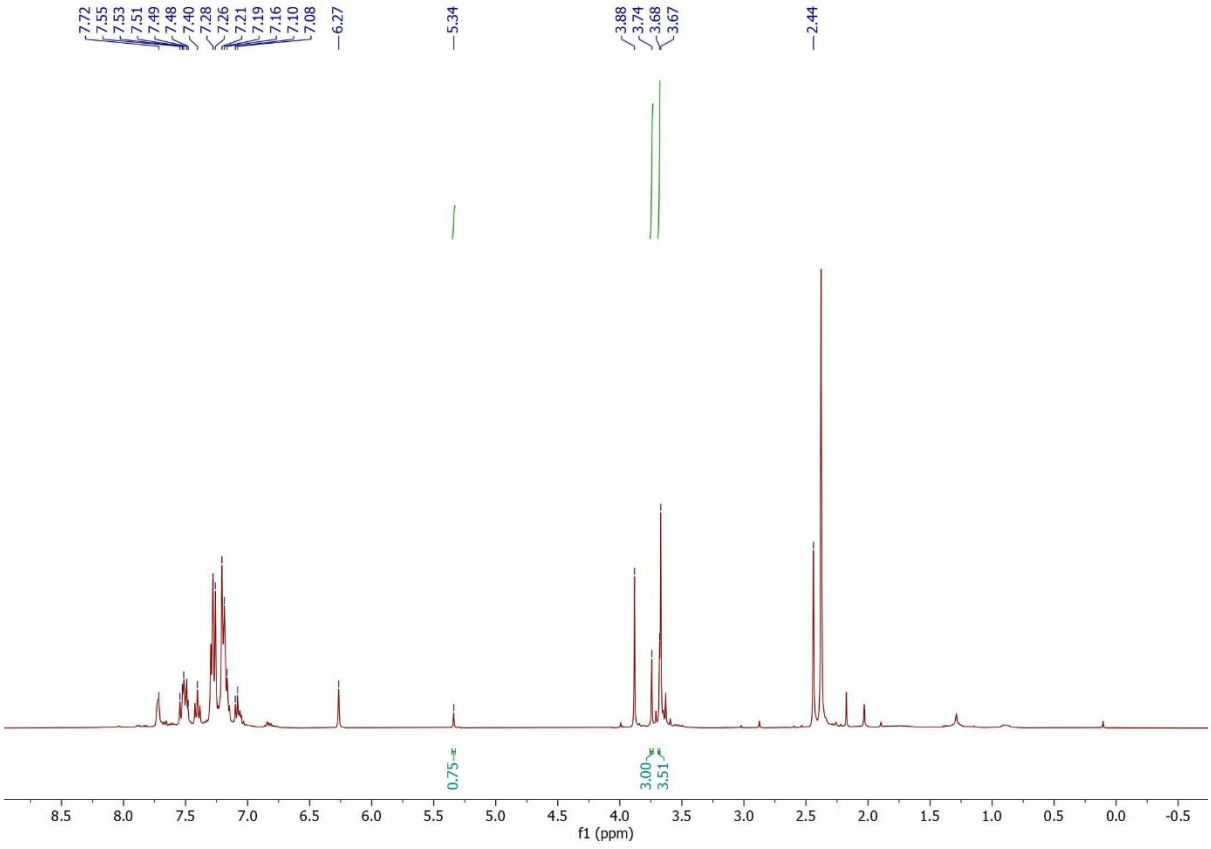


Fig. S13 %D in Unreacted Indole and Alkylated Product with Time.

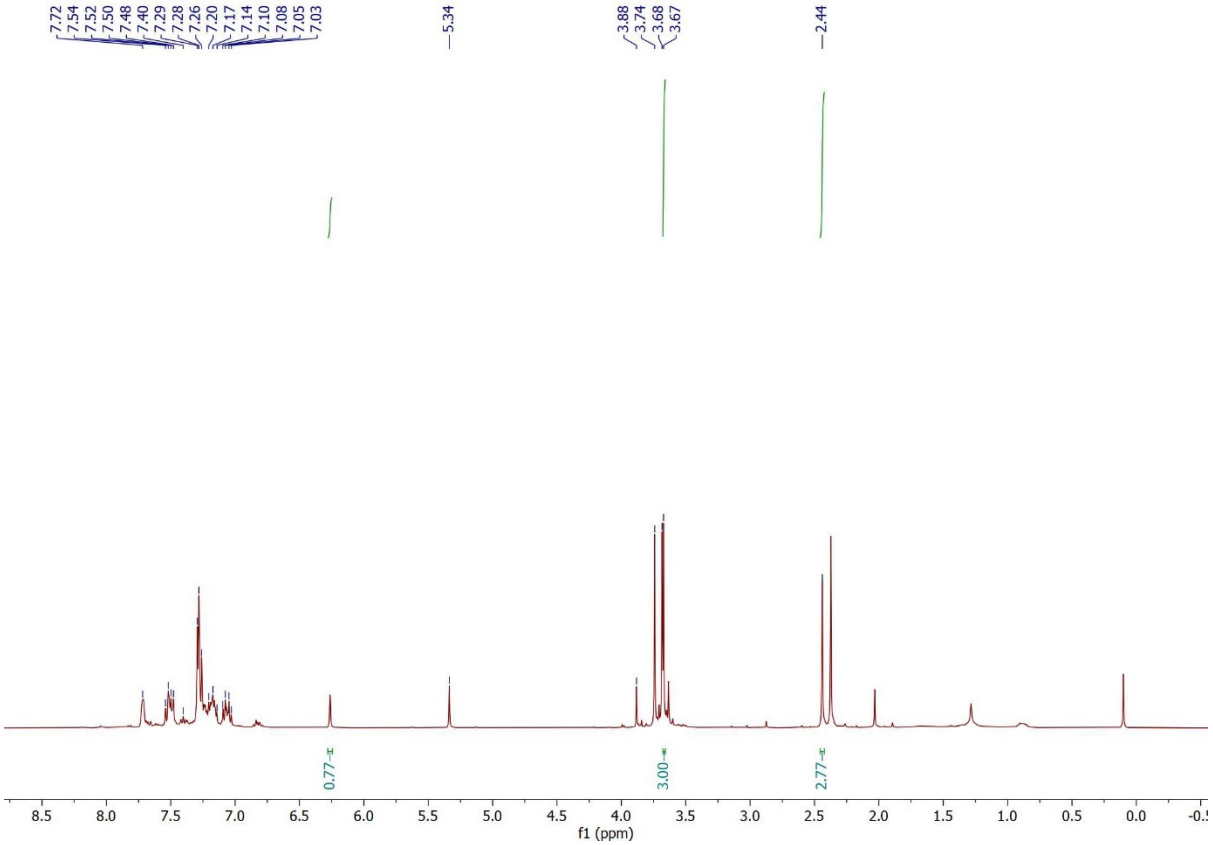
10 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for unreacted indole:



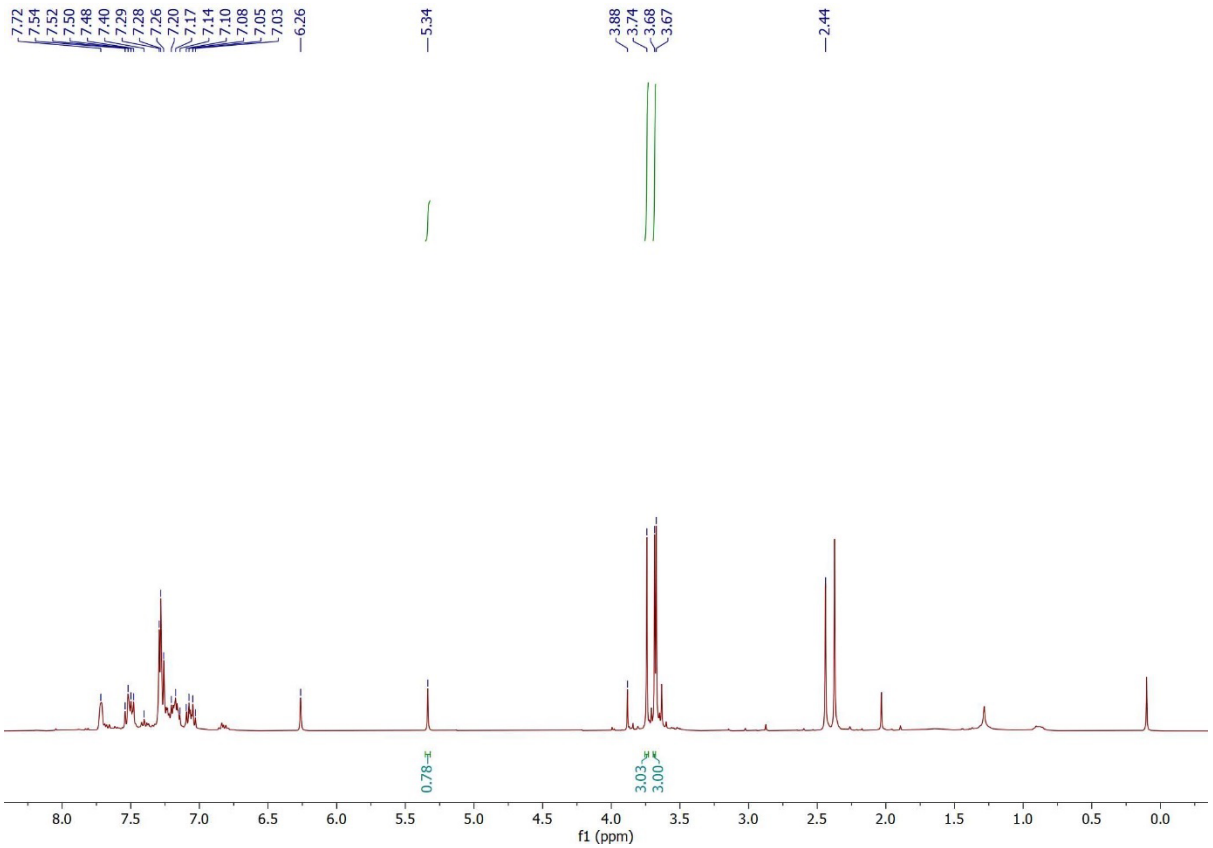
10 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for product:



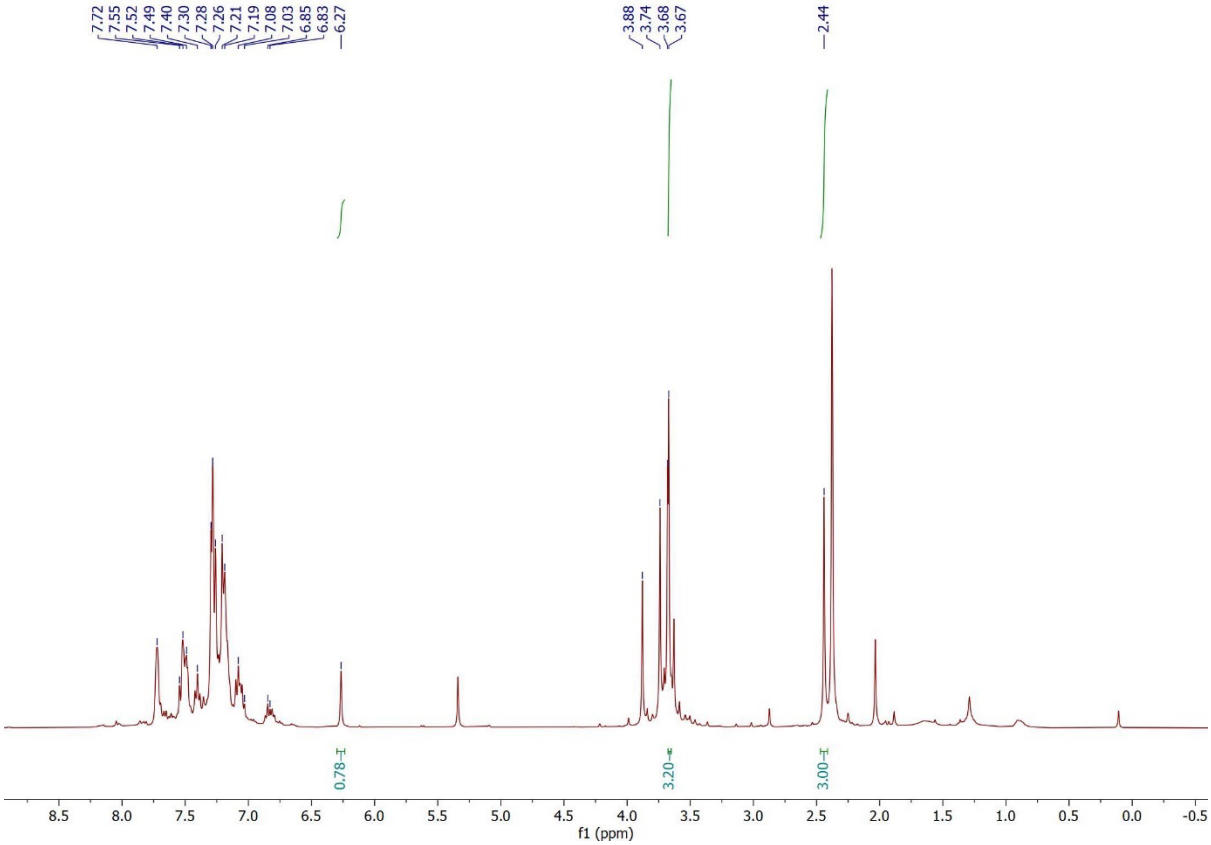
20 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for unreacted indole:



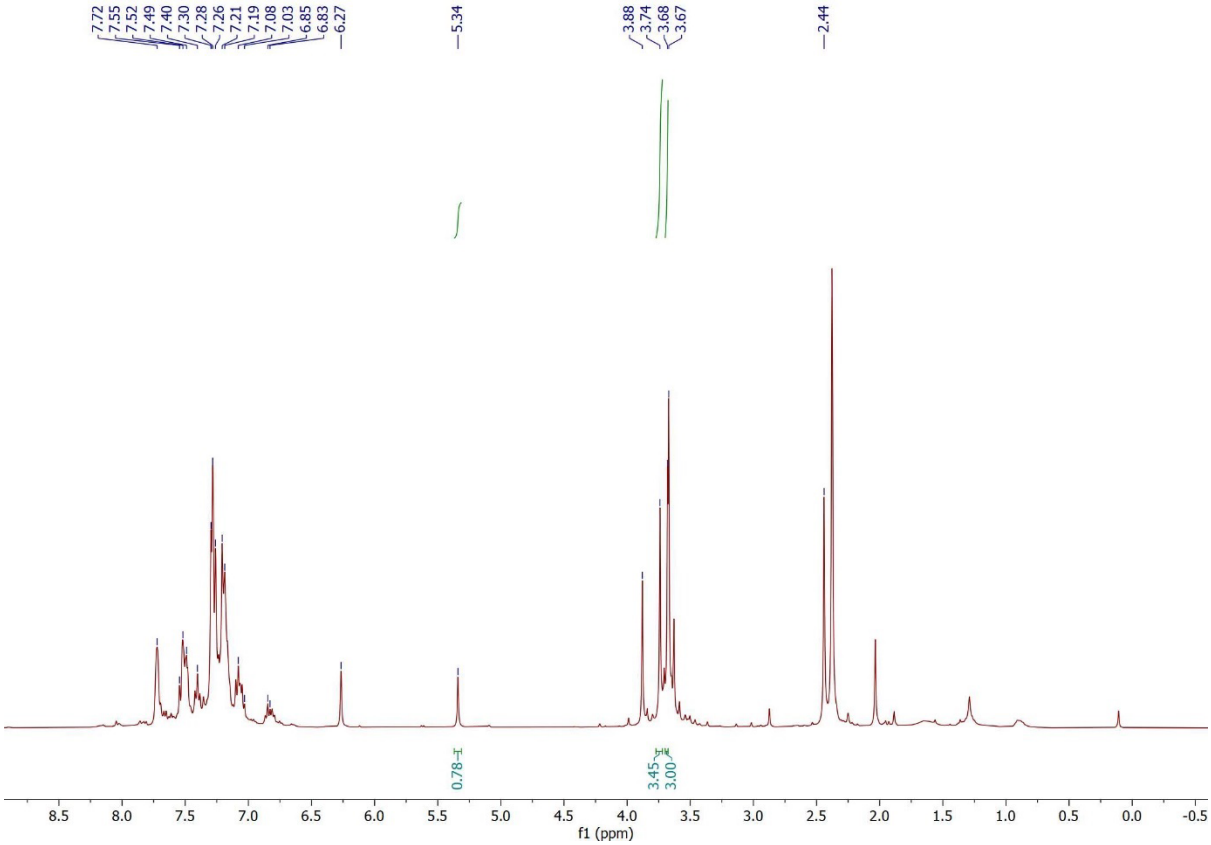
20 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for product:



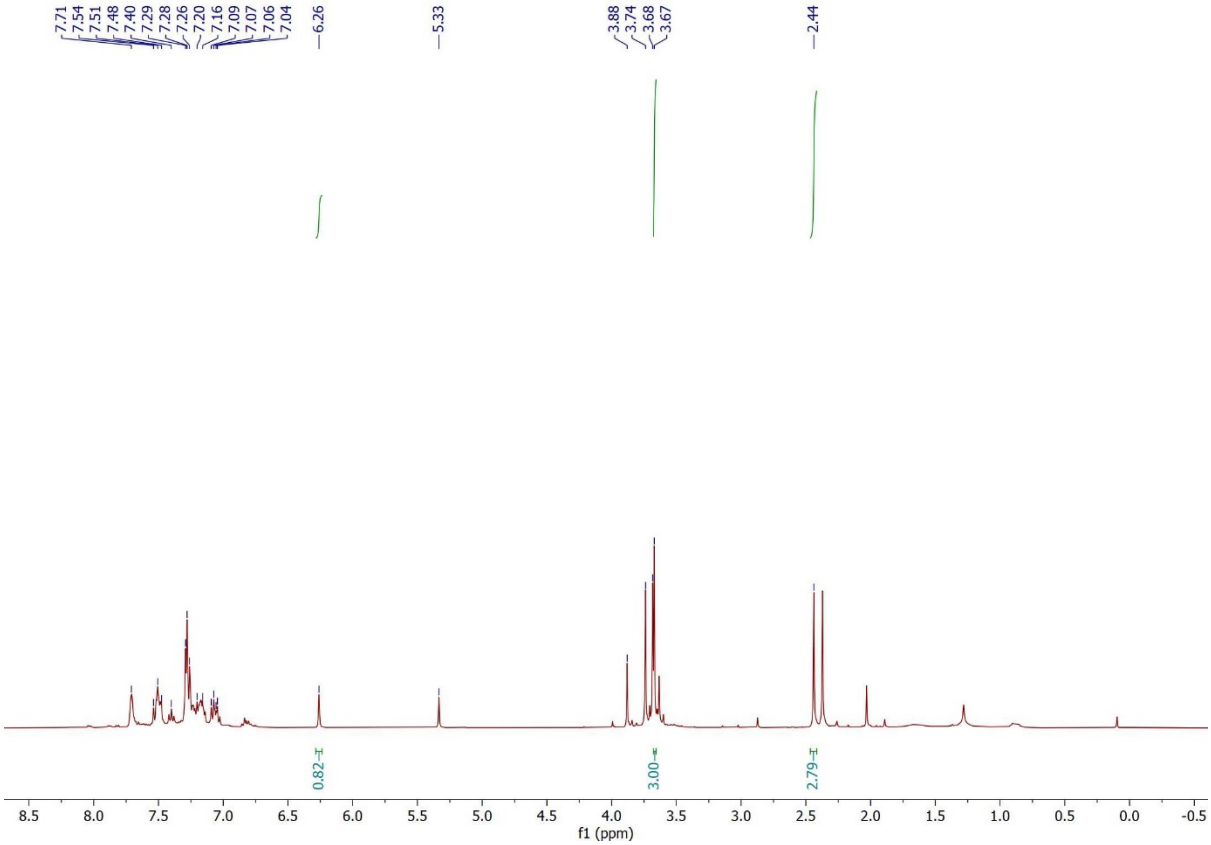
40 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for unreacted indole:



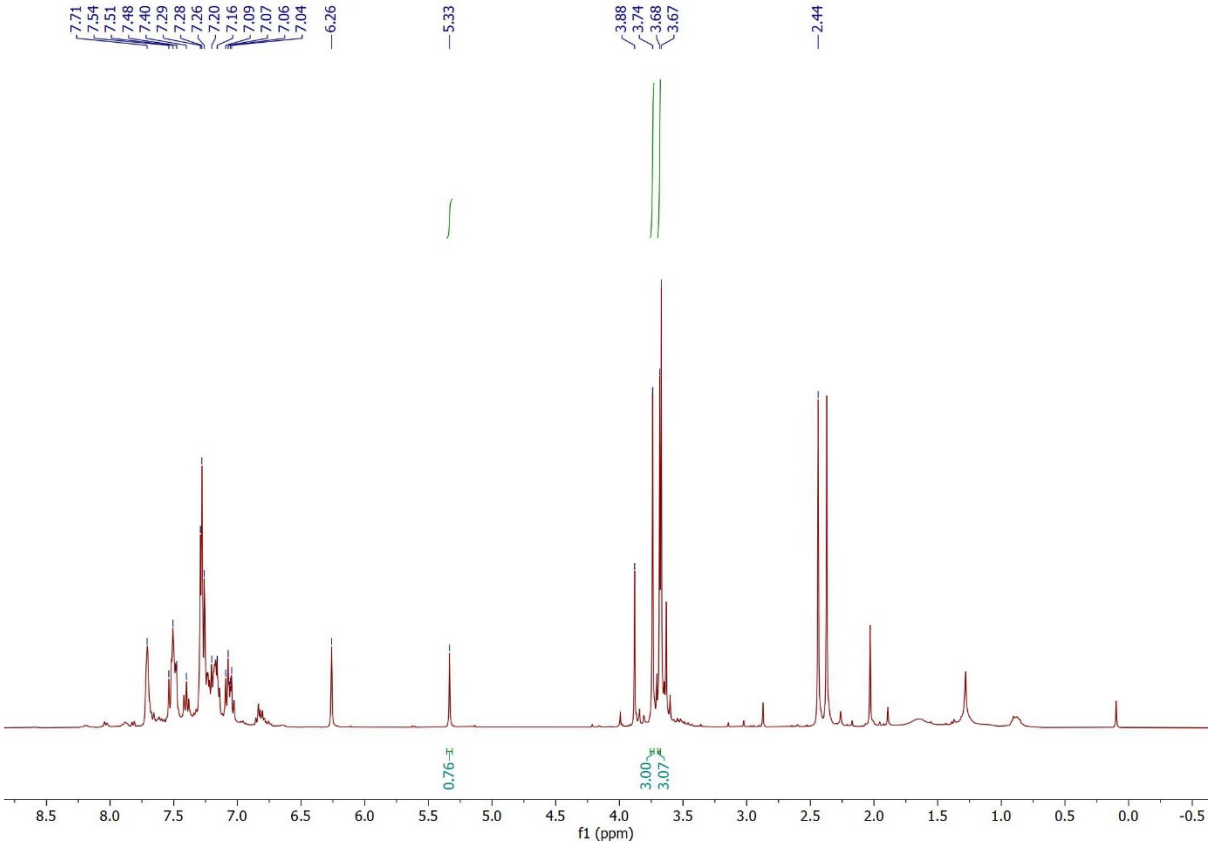
40 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for product:



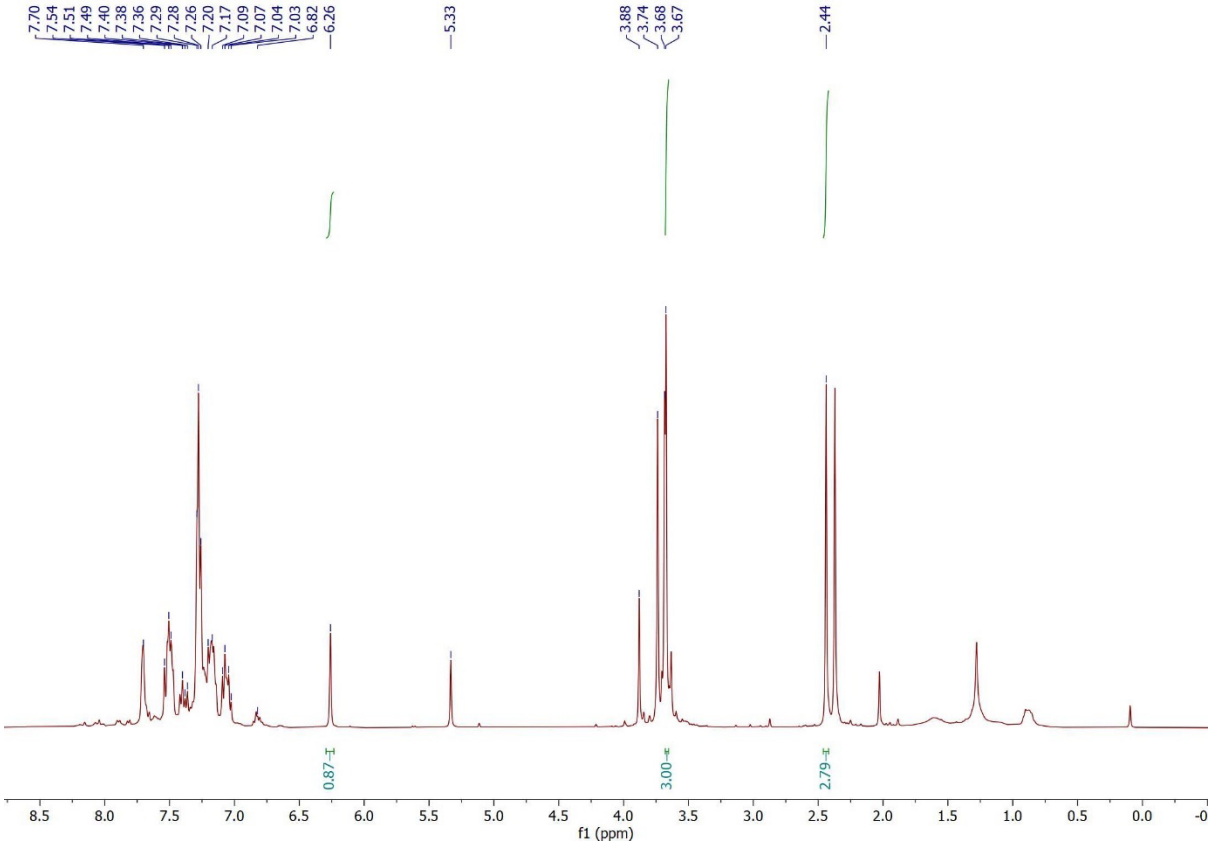
50 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for unreacted indole:



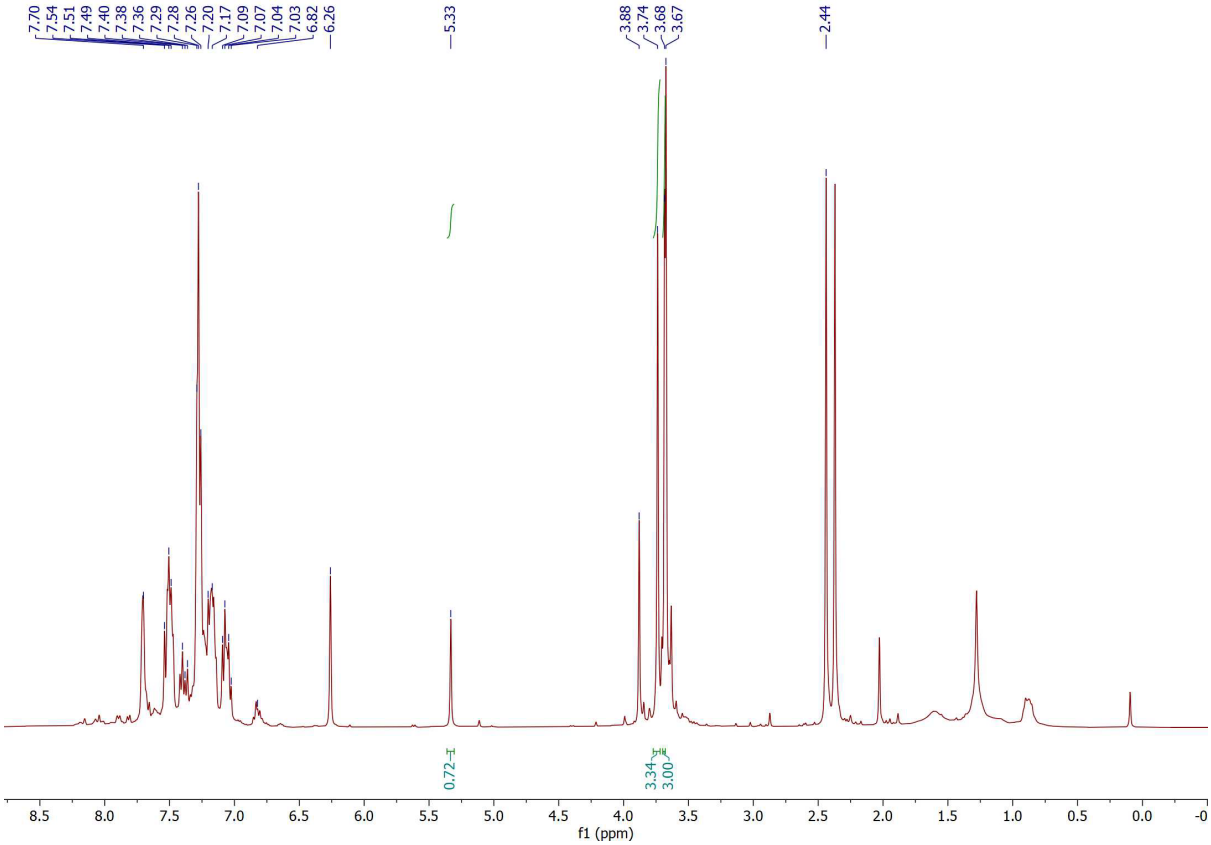
50 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for product:



60 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for unreacted indole:



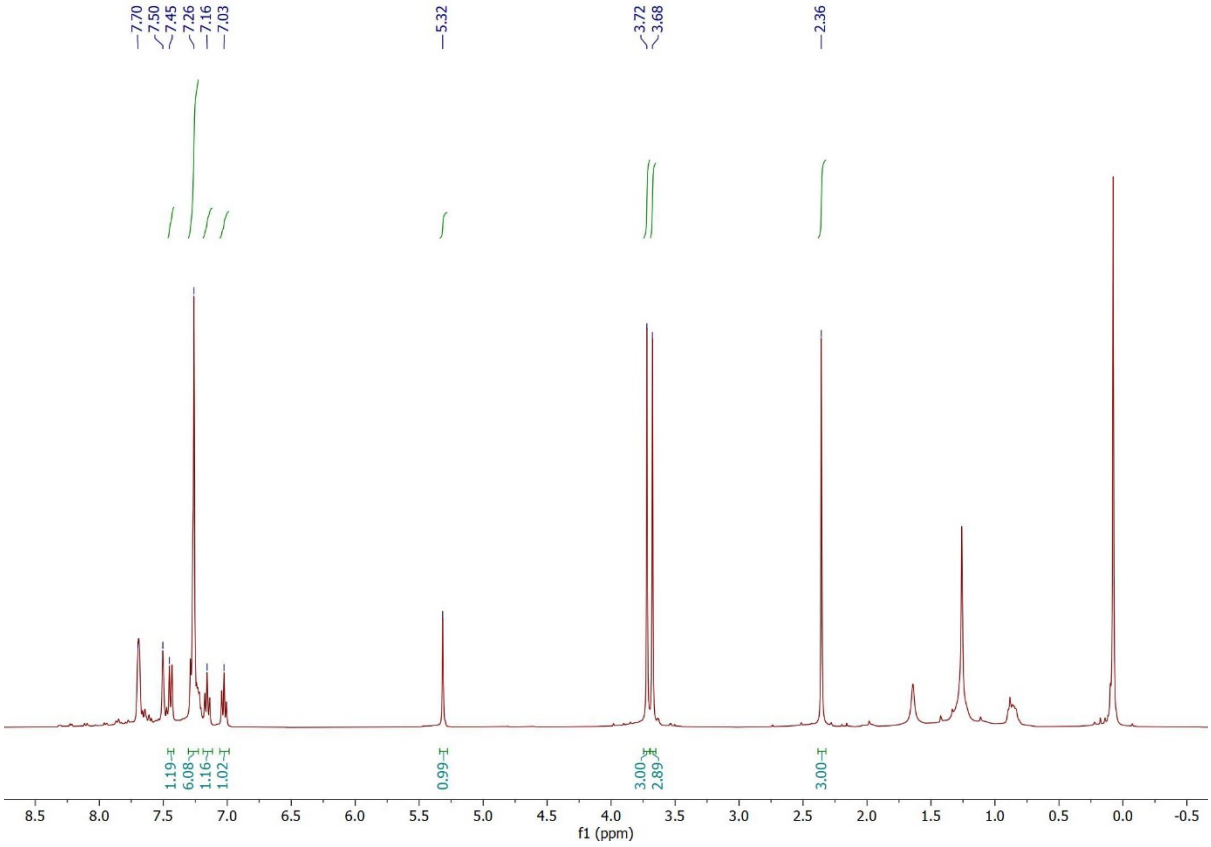
60 mins- ^{1}H NMR (400 MHz, $CDCl_3$) for product:



12.6 Exchange in Product

We also considered the possibility of deuterium exchange in product in reaction conditions by adding D_2O (25 eq) externally and we found that the product does not show any exchange.

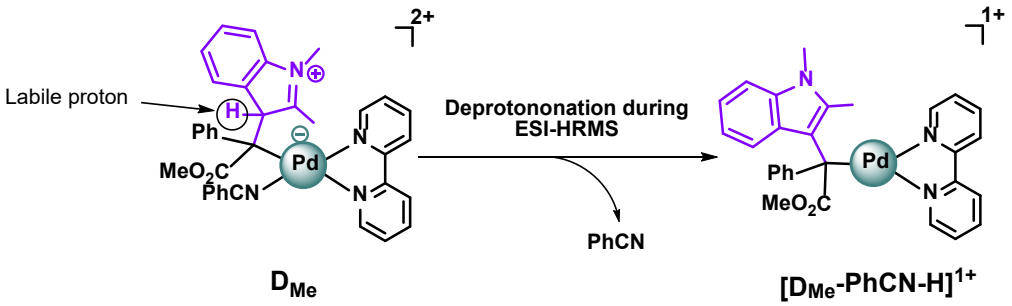
Procedure: Powdered $[Pd(PhCN)_2Cl_2]$ (3.9 mg, 0.01 mmol, 5.0 mol%), 2,2'-bipyridine (1.6 mg, 0.01 mmol, 5.0 mol%), $NaBAr^F$ (21.3 mg, 0.02 mmol, 12.0 mol%) were introduced into an oven-dried Schlenk tube under nitrogen. After chloroform (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under nitrogen for 1.0 h. Indole alkylated product, methyl 2-(1,2-dimethyl-1H-indol-3-yl)-2-phenylacetate (58.6 mg, 0.2 mmol) and D_2O (100 mg, 5.0 mmol, 25 eq) were then introduced. The resulting mixture was stirred at 30°C under nitrogen for 1 h. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction mixture was subjected to ^1H NMR for analysis.



13. ESI-HRMS for $[D_{Me}\text{-PhCN-H}]^+$ species

Procedure: Powdered $[Pd(PhCN)_2Cl_2]$ (7.7 mg, 0.02 mmol), $NaBAr^F$ (42.5 mg, 0.048 mmol), and 2,2'-bipyridine (3.1 mg, 0.02 mmol) were introduced into an oven-dried Schlenk tube under argon. After chloroform (2.0 mL) was injected into the Schlenk tube, the solution was stirred at 30°C under argon for 1 h. Then, 1,2-dimethyl-1*H*-indole (4.4 mg, 0.03 mmol) and methyl-α-diazo-α-phenylacetate (3.5 mg, 0.02 mmol) was introduced in one portion, and the resulting mixture was stirred at 30°C under argon for few minutes. The reaction mixture was then filtered, and the filtrate was concentrated under vacuum. The crude reaction sample was then subjected to ESI-HRMS in positive ion mode in acetonitrile solvent.

From our computational studies and deuterium labelling experiments, Pd–H pathway is found to be feasible, going via intermediate **D** which is the most stable intermediate. We attempted to detect this intermediate using ESI-HRMS, and fortunately we could detect **$[D_{Me}\text{-PhCN-H}]^{+1}$** species. Since **$D_{Me}$** has a labile proton on C3 carbon of indole, it is highly likely to be lost during ESI-HRMS and thus generating **$[D_{Me}\text{-PhCN-H}]^{+1}$**.



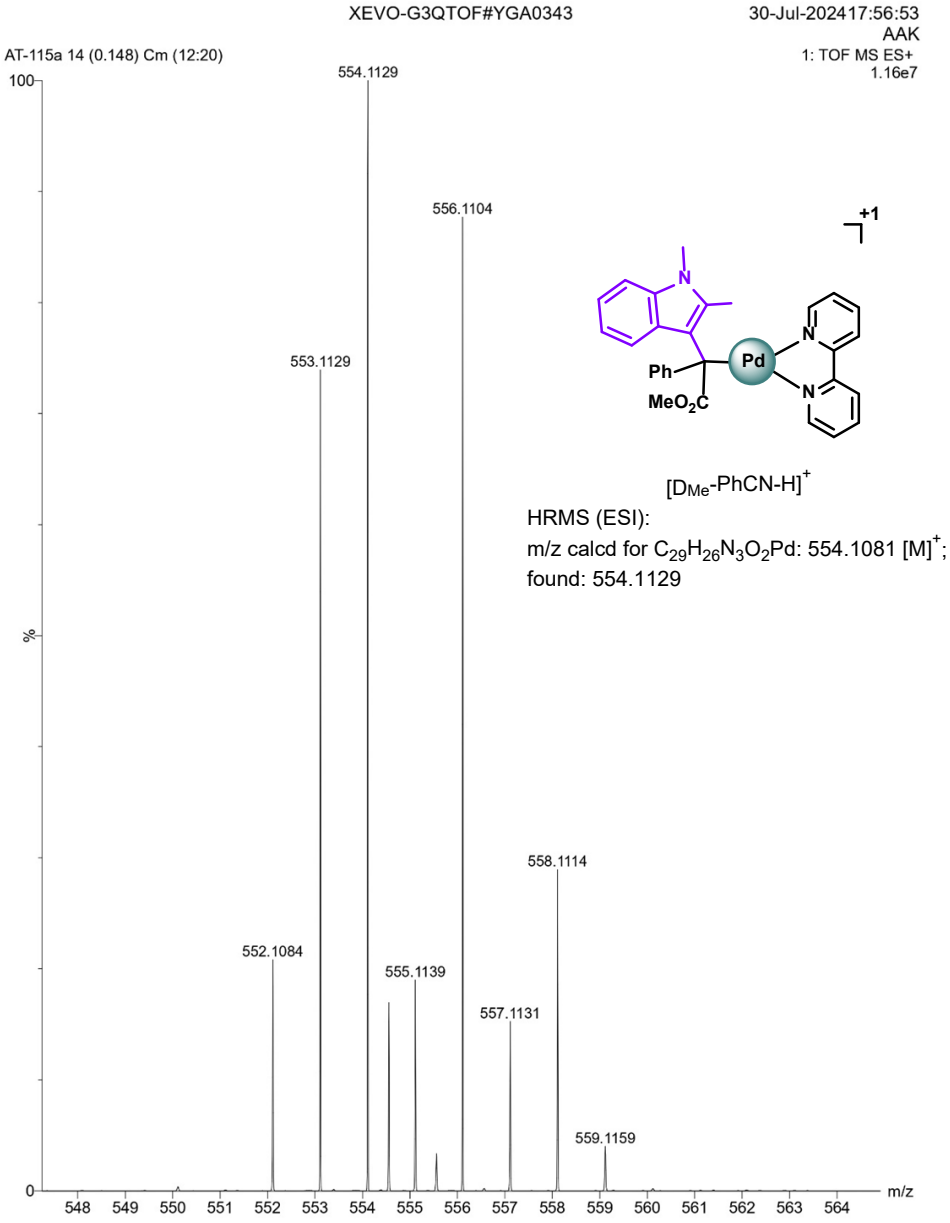


Fig. S14 Experimentally detected $[D_{Me}\text{-PhCN-H}]^+$ species through ESI-HRMS spectrum from the reaction mixture in positive ion mode.

HRMS (ESI): *m*/*z* Calcd for $C_{29}H_{26}N_3O_2Pd$: 554.1081 $[M]^+$; Found: 554.1129 (Δ = 8.6 ppm).

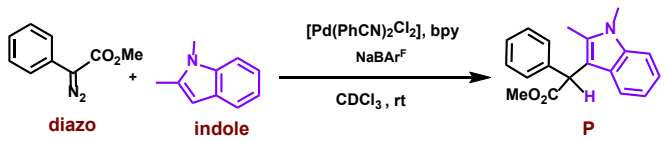
14. Kinetic Study- VTNA

14.1. Kinetic Analysis

Kinetic data was obtained by doing *in situ* experiments using 400 MHz ^{1}H NMR. ^{1}H NMR spectra were analysed with the ester methyl proton signal for product (δ 3.75 ppm, s, 3H), ester

methyl proton signal for diazoester (δ 3.90 ppm, s, 3H) and methyl protons signal for 1,2-dimethylindole (δ 2.46 ppm, s, 3H) relative to the methyl proton signal of mesitylene (δ 2.32 ppm, s, 9H) being used to monitor product formation. T_1 was taken as 5.6s which was found to be the highest for relaxation of proton at C3 position of indole. D_1 was therfore taken as 15s for a pulse of 30°.

14.2. General Procedure of Kinetic Profiling Experiments



Standard reaction

Stock solutions of 1,2-dimethylindole (indole) (0.3 M), methyl-α-diazo-α-phenylacetate (diazo) (0.2 M) and bpy (0.01 M) were prepared in $CDCl_3$ in screw-cap vials. These solutions were stored at –20 °C. Stock solutions of $NaBAr^F$ and $[Pd(PhCN)_2Cl_2]$ catalyst was not prepared due to the insoluble nature of these compounds in $CDCl_3$. Following is the procedure used for kinetic analysis of standard reaction; the same procedure was used for all the reactions unless stated otherwise. In an oven dried round-bottomed flask, $[Pd(PhCN)_2Cl_2]$ catalyst (5 mol%, 0.0042 mmol, 1.61 mg) and $NaBAr^F$ (12 mol%, 0.0101 mmol, 8.95 mg) were measured and subsequently, 0.42 mL of bpy (5 mol%, 0.0042 mmol) from its stock solution was added into the flask under Ar conditions. Extra 0.58 mL of $CDCl_3$ was injected into the flask. The catalyst mixture was stirred for 45 minutes at room-temperature. After the activation, 0.48 mL of indole (0.144 mmol) and 0.42 mL of diazo (0.084 mmol) were injected into the activated catalyst mixture in one portion, extra 0.10 mL of $CDCl_3$ was injected into the flask along with 14 µL mesitylene as an internal standard. Immediately 0.5 mL sample was taken out from the reaction mixture and put into NMR tube for monitoring change in concentrations of reactants and products with time.

14.3. Reproducibility of the Experiments

The reproducibility of the method and reaction was checked on standard reaction.

Table S11 (a) Reaction conditions for the standard reaction. (b) Time course data for the standard reaction

(a)

	[diazo]/ M	[indole] /M	[Pd]	[bpy]	[$NaBAr^F$]
Standard reaction	0.042 M	0.072 M	5 mol%	5 mol%	12 mol%

(b)

SET - A		SET - B	
Time / min	**[P] / M**	**Time / min**	**[P] / M**
0.0	0.000	0.0	0.000
10.3	0.004	10.3	0.004
20.9	0.006	20.8	0.006
30.0	0.008	31.5	0.008
41.6	0.011	42.2	0.011
49.7	0.013	49.3	0.013
61.6	0.017	59.9	0.015
69.7	0.019	70.6	0.018
81.4	0.022	81.2	0.021
89.1	0.023	91.9	0.023
100.8	0.025	102.5	0.025
108.5	0.026	109.6	0.026
120.2	0.028	120.3	0.027
131.8	0.029	130.9	0.029
139.8	0.030	141.6	0.030
151.5	0.030	152.3	0.031
159.2	0.031	159.4	0.031
170.9	0.031	170.0	0.032
179.0	0.031	180.7	0.033
190.6	0.032	191.4	0.033
201.3	0.032	198.7	0.033

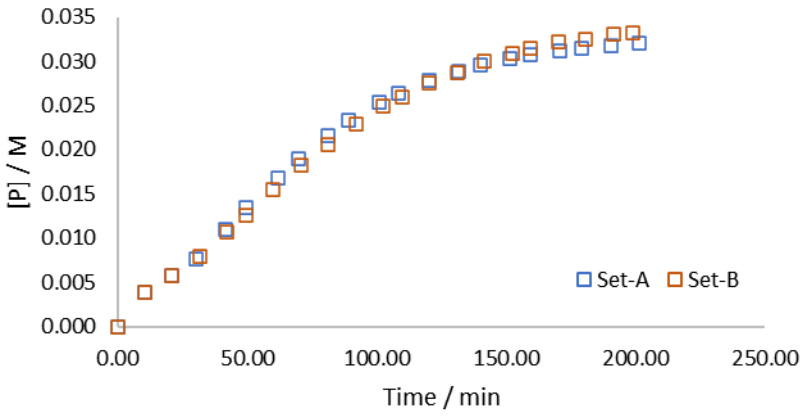


Fig. S15 Repeatability of the standard reaction. Each profile corresponds to a discrete standard reaction set.

14.4. Same Excess Study:

Table S12 (a) Reaction conditions for the same excess (b) Time course data for the model reaction under same excess conditions

(a)

	[diazo] / M	[indole] /M	[Pd]	[bpy]	[$NaBAr^F$]
Standard Reaction	0.042 M	0.072 M	5 mol%	5 mol%	12 mol%
Same Excess	0.026 M	0.056 M	5 mol%	5 mol%	12 mol%

(b)

Standard Reaction	
Time/ min	**[diazo] / M**
0.0	0.042
10.3	0.040
20.9	0.036
30.0	0.032
41.6	0.028
49.7	0.025
61.6	0.021
69.7	0.018
81.4	0.015
89.1	0.013
100.8	0.010
108.5	0.009
120.2	0.007
131.8	0.006
139.8	0.005
151.5	0.004
159.2	0.004
170.9	0.003
179.0	0.003

Same Excess		
Time / min	**[diazo] / M**	**Shifted Time / min**
0.0	0.026	42.0
10.0	0.024	52.3
19.6	0.020	62.9
31.0	0.017	72.0
39.6	0.015	83.6
49.2	0.012	91.7
59.4	0.010	103.6
70.1	0.008	111.7
80.7	0.007	123.4
91.4	0.005	131.1
102.1	0.004	142.8
109.2	0.004	150.5
119.9	0.003	162.2
130.5	0.003	173.8
141.2	0.002	181.8
151.9	0.002	193.5
159.0	0.002	201.2
169.6	0.001	212.9
180.3	0.001	221.0

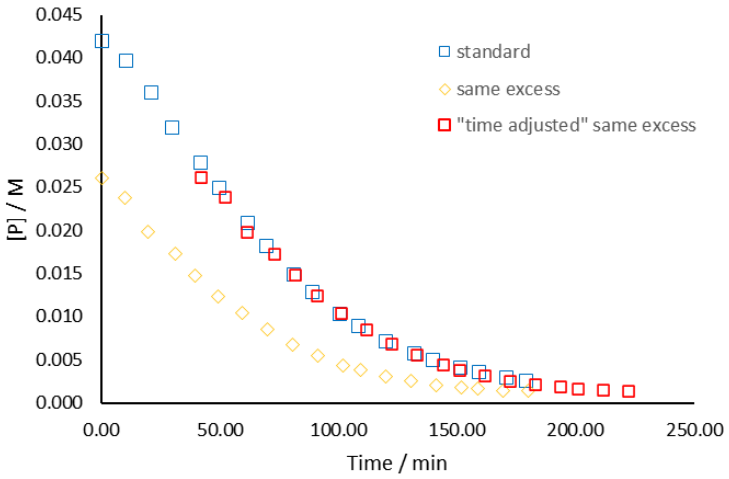


Fig. S16 Variable timescale normalization analysis of the standard reaction under same excess conditions.

14.5. Kinetic Order in Indole:

Table S13 (a) Reaction conditions for the different excess with respect to indole (b) Normalised time data for standard [indole] with exponent value = 0, 1, 2 (c) Normalised time data for different [indole] with exponent value = 0, 1, 2

(a)

	[diazo] / M	[indole] /M	[Pd]	[bpy]	[$NaBAr^F$]
Standard Reaction	0.042 M	0.072 M	5 mol%	5 mol%	12 mol%
Indole Excess	0.042 M	0.040 M	5 mol%	5 mol%	12 mol%

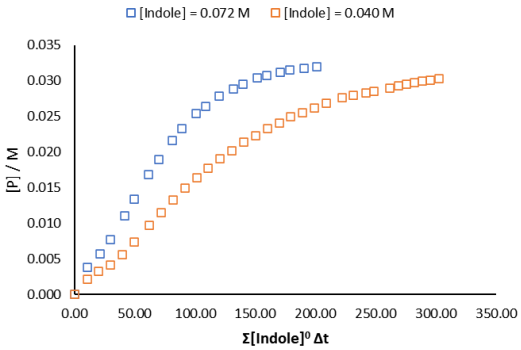
(b)

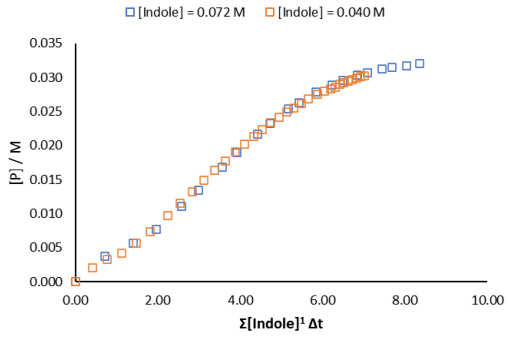
Standard Reaction					
Time / min	**[P] /M**	**[indole] /M**	**Time Axis 0^{th} Order**	**Time Axis 1^{st} Order**	**Time Axis 2^{nd} Order**
0.0	0.000	0.072	0.00	0.00	0.00
10.3	0.004	0.066	10.33	0.72	0.05
20.9	0.006	0.064	20.88	1.41	0.09
30.0	0.008	0.056	30.00	1.95	0.13
41.6	0.011	0.052	41.60	2.58	0.16
49.7	0.013	0.050	49.67	2.99	0.18
61.6	0.017	0.046	61.63	3.56	0.21
69.7	0.019	0.044	69.72	3.93	0.23
81.4	0.022	0.041	81.37	4.42	0.25
89.1	0.023	0.039	89.13	4.72	0.26
100.8	0.025	0.037	100.75	5.16	0.28
108.5	0.026	0.035	108.52	5.44	0.29
120.2	0.028	0.034	120.17	5.84	0.30
131.8	0.029	0.033	131.78	6.23	0.31
139.8	0.030	0.032	139.83	6.49	0.32
151.5	0.030	0.031	151.48	6.86	0.33
159.2	0.031	0.031	159.23	7.10	0.34
170.9	0.031	0.030	170.88	7.45	0.35
179.0	0.031	0.030	178.97	7.69	0.36
190.6	0.032	0.030	190.58	8.04	0.37
201.3	0.032	0.029	201.25	8.35	0.38

(c)

Indole Excess					
Time / min	**[P] /M**	**[indole] /M**	**Time Axis 0^{th} Order**	**Time Axis 1^{st} Order**	**Time Axis 2^{nd} Order**
0.0	0.000	0.040	0.00	0.00	0.00
10.4	0.002	0.038	10.42	0.40	0.02
19.9	0.003	0.037	19.93	0.76	0.03

29.7	0.004	0.036	29.67	1.12	0.04
39.4	0.006	0.035	39.45	1.47	0.06
49.2	0.007	0.034	49.20	1.81	0.07
62.3	0.010	0.032	62.25	2.24	0.08
72.0	0.012	0.031	72.02	2.55	0.09
81.8	0.013	0.029	81.77	2.84	0.10
91.5	0.015	0.028	91.53	3.12	0.11
101.3	0.016	0.026	101.33	3.38	0.11
111.1	0.018	0.025	111.10	3.63	0.12
120.9	0.019	0.024	120.90	3.88	0.13
130.7	0.020	0.023	130.70	4.11	0.13
140.5	0.021	0.022	140.47	4.33	0.14
150.2	0.022	0.021	150.22	4.54	0.14
160.0	0.023	0.020	160.02	4.74	0.15
169.8	0.024	0.020	169.80	4.94	0.15
179.6	0.025	0.019	179.57	5.13	0.15
189.3	0.026	0.018	189.33	5.31	0.16
199.1	0.026	0.018	199.12	5.49	0.16
208.9	0.027	0.017	208.87	5.66	0.16
221.9	0.028	0.017	221.90	5.88	0.17
231.7	0.028	0.016	231.65	6.04	0.17
241.7	0.028	0.016	241.68	6.21	0.17
248.4	0.029	0.016	248.43	6.31	0.17
261.9	0.029	0.015	261.90	6.42	0.18
268.6	0.029	0.015	268.62	6.52	0.18
275.4	0.029	0.015	275.35	6.63	0.18
282.1	0.030	0.015	282.08	6.73	0.18
288.8	0.030	0.015	288.82	6.83	0.18
295.5	0.030	0.014	295.53	6.92	0.18
302.3	0.030	0.014	302.30	7.02	0.18





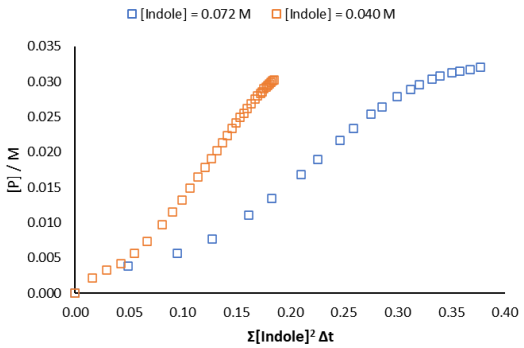


Fig. S17 Variable timescale normalization analysis of the standard reaction under different excess conditions with respect to [indole] demonstrating overlay at order = 1.

14.6. Kinetic Order in Diazo

Table S14 (a) Reaction conditions for the different excess with respect to diazo (b) Normalised time data for standard [diazo] with exponent value = 0, 1, 2 (c) Normalised time data for different [diazo] with exponent value = 0, 1, 2

(a)

	[diazo] / M	[indole] /M	[Pd]	[bpy]	[$NaBAr^F$]
Standard Reaction	0.042 M	0.072 M	5 mol%	5 mol%	12 mol%
Diazo Excess	0.026 M	0.072 M	5 mol%	5 mol%	12 mol%

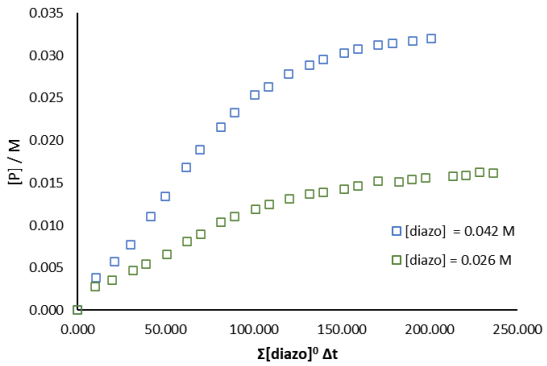
(b)

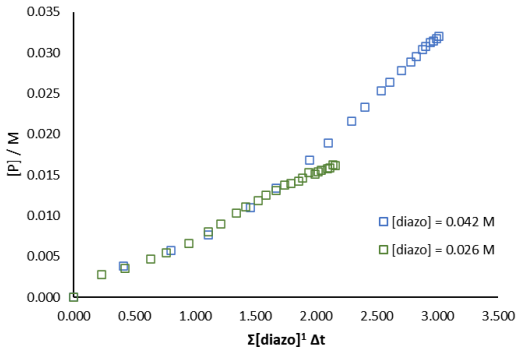
Standard Reaction					
Time / min	**[P] / M**	**[diazo] / M**	**Time Axis 0th Order**	**Time Axis 1st Order**	**Time Axis 2nd Order**
0.00	0.000	0.042	0.00	0.00	0.00E+0
10.33	0.004	0.038	10.33	0.32	9.49E-03
20.88	0.006	0.036	20.88	0.64	1.85E-02
30.00	0.008	0.032	30.00	0.87	2.43E-02
41.60	0.011	0.028	41.60	1.05	2.86E-02
49.67	0.013	0.025	49.67	1.29	3.39E-02
61.63	0.017	0.021	61.63	1.50	3.78E-02
69.72	0.019	0.018	69.72	1.65	4.00E-02
81.37	0.022	0.015	81.37	1.76	4.14E-02
89.13	0.023	0.013	89.13	1.87	4.26E-02
100.75	0.025	0.010	100.75	1.97	4.35E-02
108.52	0.026	0.009	108.52	2.03	4.39E-02
120.17	0.028	0.007	120.17	2.10	4.44E-02
131.78	0.029	0.006	131.78	2.16	4.47E-02
139.83	0.030	0.005	139.83	2.21	4.50E-02
151.48	0.030	0.004	151.48	2.25	4.51E-02
159.23	0.031	0.004	159.23	2.28	4.52E-02
170.88	0.031	0.003	170.88	2.31	4.53E-02

178.97	0.031	0.003	178.97	2.34	4.54E-02
190.58	0.032	0.002	190.58	2.37	4.55E-02
201.25	0.032	0.002	201.25	2.40	4.56E-02

c)

Diazo Excess					
Time / min	**[P] / M**	**[diazo] / M**	**Time Axis 0th Order**	**Time Axis 1st Order**	**Time Axis 2nd Order**
0.00	0.000	0.026	0.00	0.00	0.00E+00
9.92	0.003	0.020	10.50	0.23	5.28E-03
19.72	0.004	0.019	22.53	0.42	9.03E-03
31.32	0.005	0.018	31.33	0.63	1.29E-02
39.05	0.005	0.017	38.43	0.76	1.51E-02
50.67	0.007	0.015	49.38	0.95	1.80E-02
62.28	0.008	0.013	61.30	1.11	2.03E-02
70.02	0.009	0.012	71.63	1.21	2.16E-02
81.62	0.010	0.010	79.97	1.34	2.31E-02
89.38	0.011	0.010	90.65	1.42	2.38E-02
101.02	0.012	0.008	101.32	1.52	2.48E-02
108.77	0.012	0.008	109.07	1.58	2.53E-02
120.37	0.013	0.007	119.73	1.67	2.59E-02
131.97	0.014	0.006	130.37	1.74	2.63E-02
139.72	0.014	0.006	141.05	1.79	2.66E-02
151.77	0.014	0.005	151.70	1.85	2.69E-02
159.40	0.015	0.005	158.80	1.89	2.71E-02
171.02	0.015	0.004	169.43	1.94	2.74E-02
182.60	0.015	0.004	180.10	1.99	2.75E-02
190.28	0.015	0.004	190.77	2.02	2.77E-02
197.95	0.016	0.003	201.45	2.04	2.77E-02
213.33	0.016	0.003	208.55	2.09	2.79E-02
221.03	0.016	0.003	226.82	2.11	2.80E-02
228.72	0.016	0.003	237.97	2.13	2.80E-02
236.38	0.016	0.002	249.15	2.15	2.81E-02





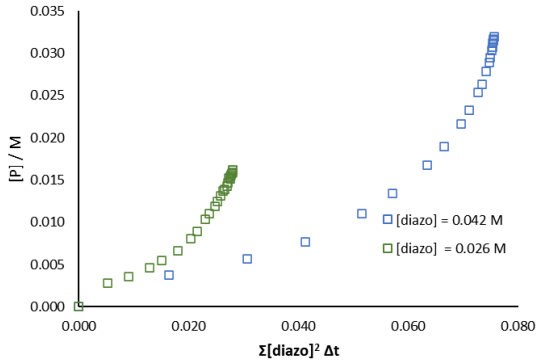


Fig. S18 Variable timescale normalization analysis of the standard reaction under different excess conditions with respect to [diazo] demonstrating overlay at order = 1.

14.7. Kinetic Order in Pd

Table S15 (a) Reaction conditions for the different excess with respect to Pd (b) Normalised time data for standard [Pd] with exponent value = 0, 1, 2 (c) Normalised time data for different [Pd] with exponent value = 0, 1, 2

(a)

	[diazo] / M	[indole] /M	[Pd]	[bpy]	[$NaBAr^F$]
Standard Reaction	0.042 M	0.072 M	5 mol%	5 mol%	12 mol%
Pd Excess	0.042 M	0.072 M	6 mol%	5 mol%	12 mol%

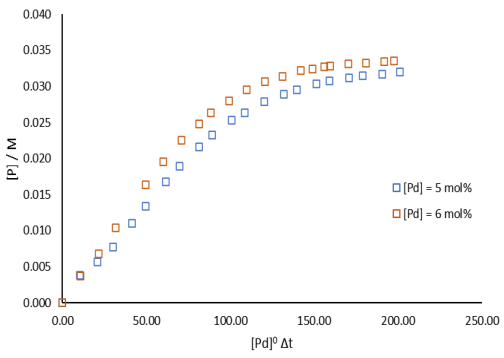
(b)

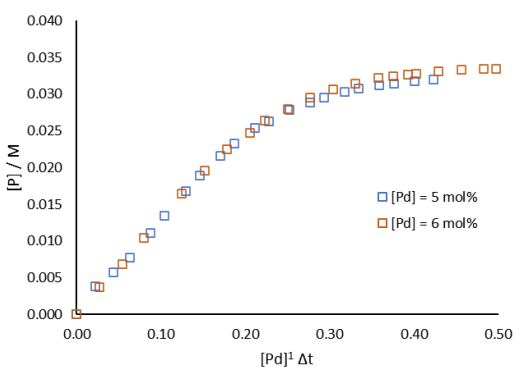
Standard Reaction				
Time / min	**[P] / M**	**Time Axis 0^{th} Order**	**Time Axis 1^{st} Order**	**Time Axis 2^{nd} Order**
0.00	0.000	0.00	0.00	0.00E+00
10.33	0.004	10.33	0.02	4.56E-05
20.88	0.006	20.88	0.04	9.21E-05
30.00	0.008	30.00	0.06	1.32E-04
41.60	0.011	41.60	0.09	1.83E-04
49.67	0.013	49.67	0.10	2.19E-04
61.63	0.017	61.63	0.13	2.72E-04
69.72	0.019	69.72	0.15	3.07E-04
81.37	0.022	81.37	0.17	3.59E-04
89.13	0.023	89.13	0.19	3.93E-04
100.75	0.025	100.75	0.21	4.44E-04
108.52	0.026	108.52	0.23	4.79E-04
120.17	0.028	120.17	0.25	5.30E-04
131.78	0.029	131.78	0.28	5.81E-04
139.83	0.030	139.83	0.29	6.17E-04
151.48	0.030	151.48	0.32	6.68E-04
159.23	0.031	159.23	0.33	7.02E-04
170.88	0.031	170.88	0.36	7.54E-04
178.97	0.031	178.97	0.38	7.89E-04

190.58	0.032	190.58	0.40	8.40E-04
201.25	0.032	201.25	0.42	8.88E-04

(c)

Pd Excess				
Time / min	**[P] / M**	**Time Axis 0th Order**	**Time Axis 1st Order**	**Time Axis 2nd Order**
0.00	0.000	0.00	0.00	0.00E+00
10.63	0.004	10.63	0.03	6.75E-05
21.48	0.007	21.48	0.05	1.36E-04
31.70	0.010	31.70	0.08	2.01E-04
49.50	0.016	49.50	0.12	3.14E-04
60.15	0.020	60.15	0.15	3.82E-04
70.80	0.023	70.80	0.18	4.50E-04
81.45	0.025	81.45	0.21	5.17E-04
88.55	0.026	88.55	0.22	5.62E-04
99.20	0.028	99.20	0.25	6.30E-04
109.88	0.030	109.88	0.28	6.98E-04
120.55	0.031	120.55	0.30	7.66E-04
131.22	0.031	131.22	0.33	8.33E-04
141.87	0.032	141.87	0.36	9.01E-04
148.98	0.032	148.98	0.38	9.46E-04
156.08	0.033	156.08	0.39	9.91E-04
159.65	0.033	159.65	0.40	1.01E-03
170.32	0.033	170.32	0.43	1.08E-03
180.97	0.033	180.97	0.46	1.15E-03
191.63	0.033	191.63	0.48	1.22E-03
197.45	0.033	197.45	0.50	1.25E-03





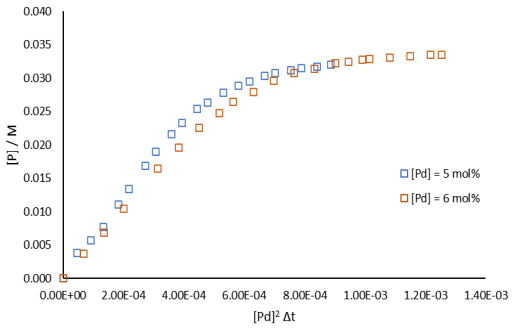


Fig. S19 Variable timescale normalization analysis of the standard reaction under different excess conditions with respect to [Pd] demonstrating overlay order = 1.

15. Microkinetic Modelling

To perform microkinetic modeling, COPASI software was used.[12] The purpose of performing microkinetic modeling was to compare the conventional carbene insertion, conventional cross-coupling, and crossover pathways. Additionally, the study aimed to compare the yield obtained from experimental data with that predicted by COPASI.

15.1. Fitting of experimental data (Parameter Estimation)

The comparison of the conventional carbene insertion, conventional cross-coupling, and crossover pathways was performed by fitting experimental data through parameter estimation in COPASI. The standard reaction data used for this analysis are presented in the Table S16. The initial values for each parameter (activation free energy) in the parameter estimation run were taken from calculations done at $SMD_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p), LANL2DZ(Pd) level of theory, as shown in Table S2. The lower and upper bounds were adjusted accordingly to achieve the best-fit values, ensuring that the estimated values closely aligned with the initial values.

Examples of the best fits identified for each pathway are detailed below. It is important to note that the activation free energy estimated by COPASI may not have physical significance, as the systems could be underestimated.

Table S16 Experimental data used for Parameter Estimation

Time / sec	[P] / M	[indole] / M	[diazo] / M
0	0	0.072	0.042
300	0.0033292	0.06695	0.03727
504	0.0037938	0.06698	0.03797

620	0.0041031	0.06642	0.03769
737	0.0043094	0.0661	0.03739
836	0.0045975	0.06576	0.03707
935	0.0047522	0.06562	0.03678
1035	0.0051224	0.06495	0.03645
1248	0.0057011	0.06439	0.03595
1461	0.0064053	0.06353	0.03514
1675	0.0071863	0.06264	0.03429
1888	0.0079783	0.06171	0.03332
2103	0.0089124	0.06081	0.03233
2317	0.0097553	0.05978	0.03138
2530	0.0107074	0.05873	0.03039
2743	0.0116526	0.05769	0.02932
2956	0.0125426	0.05663	0.02828
3168	0.0135569	0.05558	0.02724
3381	0.0144613	0.05455	0.02611
3594	0.0154191	0.05355	0.02506
3828	0.0163209	0.05252	0.02401
4021	0.0172244	0.0515	0.02297
4233	0.0181731	0.05061	0.02199
4446	0.0190382	0.04961	0.02099
4660	0.0198484	0.04872	0.02004
4873	0.0206296	0.0477	0.0191
5086	0.0214594	0.04693	0.01817
5299	0.0222037	0.04616	0.01733
5512	0.0229375	0.04535	0.0165
5724	0.0235639	0.04458	0.01572
5937	0.0242197	0.04386	0.01492
6151	0.024902	0.04318	0.01421
6363	0.0254291	0.04251	0.01353
6576	0.025987	0.04194	0.01286
6790	0.0265919	0.04143	0.01224
7003	0.027027	0.04083	0.01165
7217	0.0274804	0.0402	0.01103
7430	0.0278551	0.03965	0.01048
7643	0.0283456	0.03927	0.00998
7856	0.028716	0.03888	0.00952
8069	0.0291985	0.03851	0.00908
8282	0.0294544	0.03802	0.00862
8495	0.0299265	0.03766	0.00823
8708	0.0302551	0.03735	0.00783
8921	0.0305295	0.03693	0.00746
9135	0.0308002	0.03661	0.00711
9348	0.0312242	0.03635	0.00678
9561	0.0314742	0.03606	0.00645
9774	0.0315218	0.03564	0.00612
9988	0.0318895	0.03543	0.00586
10202	0.0321569	0.0352	0.00557

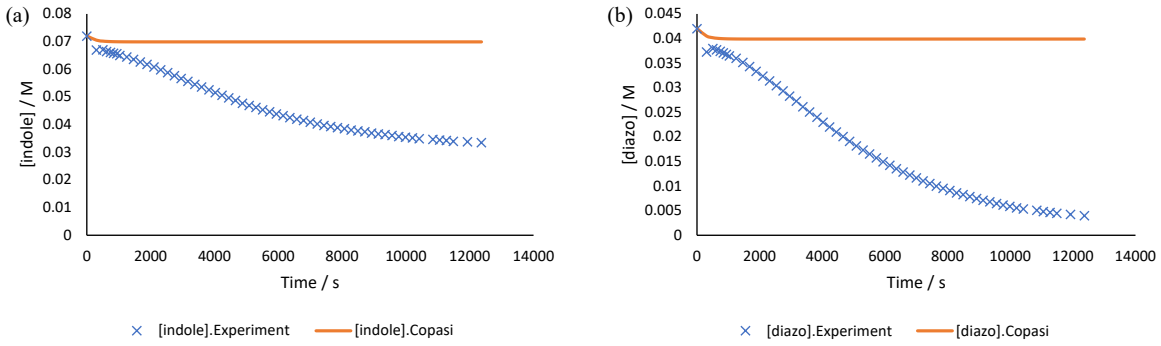
10415	0.0322863	0.03485	0.00531
10843	0.0325019	0.03464	0.00506
11056	0.0326409	0.0344	0.00482
11268	0.0328669	0.03424	0.00461
11482	0.0330758	0.03396	0.00443
11924	0.0332546	0.03377	0.00422
12366	0.033448	0.03348	0.00396

15.1.1. Conventional Carbene insertion

Table S17 Computed kinetic constants (k) for forward (with subscript 'F') and reverse (with subscript 'R') reaction for each step of the reaction for Conventional Carbene Insertion

Rxn, No.	Reaction	Estimated Parameter	
		k_F	k_R
Rxn_1	A + S_1 = B + PhCN	1E-02	6.5869E-08
Rxn_2	B = C + N2	6.30051E+07	8.96685E-08
Rxn_3	C + S_2 = D	54348.9	1.15138E-07
Rxn_4	D = E_a	0.000601478	1.05985E+09
Rxn_5	E_a + PhCN = P + A	4.19451E-05	1.35704E-07

Parameter Estimation Results	
Objective Value	0.07010327922
Root Mean Square	0.02007217998
Standard Deviation	0.0206750821



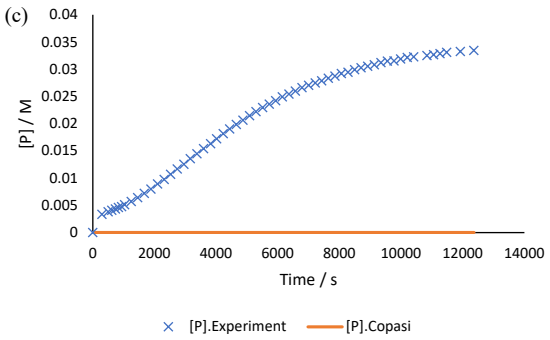


Fig. S20 Comparison of experimental data with COPASI-fitted data for the Conventional Carbene Insertion. (a) Fit for indole (S_2), (b) fit for diazo (S_1), and (c) fit for the product (P).

15.1.2. Conventional Cross-Coupling

Table S18 Computed kinetic constants (k) for forward (with subscript 'F') and reverse (with subscript 'R') reaction for each step of the reaction for Conventional Cross-Coupling

Rxn. No.	Reaction	Estimated	
		k_F	k_R
Rxn_1	$A + S_2 = A_1 + PhCN$	8.76211E+11	1.1521E+09
Rxn_2	$A_1 + S_1 = B_1 + PhCN$	1E-02	0.244364
Rxn_3	$B_1 = C_1 + N2$	6.37833E+10	1E-15
Rxn_4	$C_1 + PhCN = D$	26065	8.85919E-08
Rxn_5	$D = F + PhCN$	1E-2	6.49472E+07
Rxn_6	$F = F_1$	6.719906E+07	1.67062E+08
Rxn_7	$F_1 = P_1$	1.3349E+09	78.8895
Rxn_8	$P_1 + 2\ PhCN = P + A$	1.41355E+10	1.03638E+09

Parameter Estimation Results	
Objective Value	0.04194804211
Root Mean Square	0.01633456404
Standard Deviation	0.01733933821

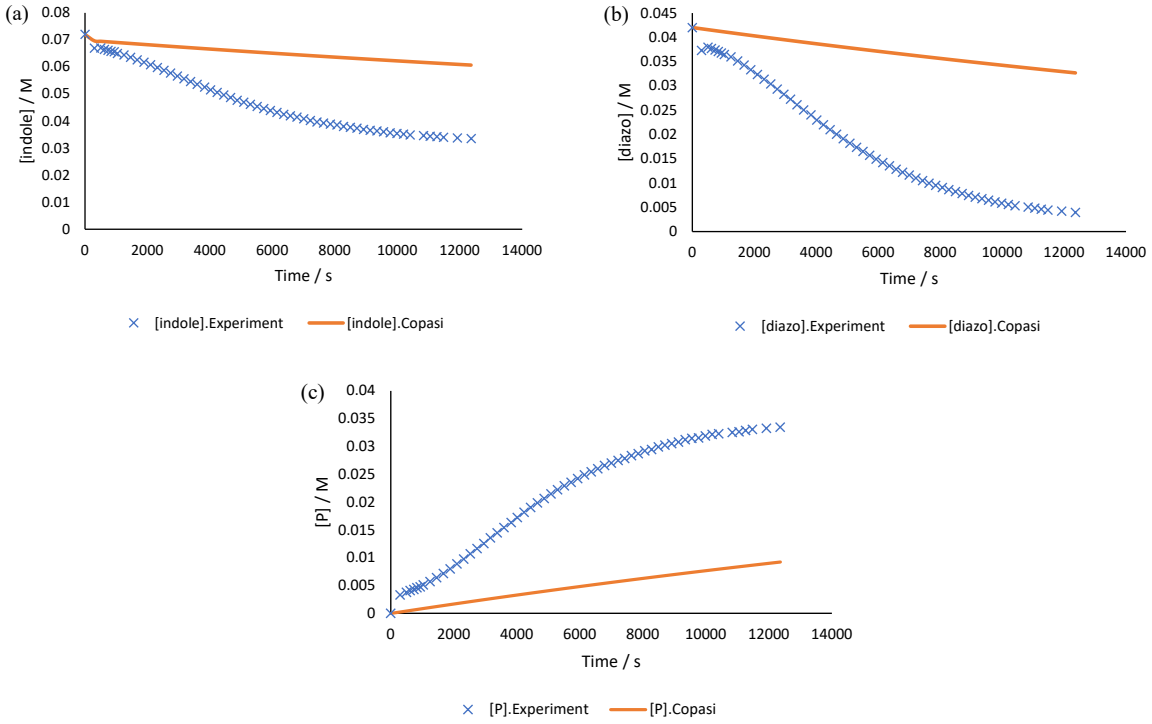


Fig. S21 Comparison of experimental data with COPASI-fitted data for the Conventional Cross-Coupling. (a) Fit for indole (S_2), (b) fit for diazo (S_1), and (c) fit for the product (P).

15.1.3. Crossover Pathway

Table S19 Computed kinetic constants (k) for forward (with subscript 'F') and reverse (with subscript 'R') reaction for each step of the reaction for Crossover Pathway

Rxn, No.	Reaction	Estimated	
		k_F	k_R
Rxn_01	A + S_1 = B + PhCN	0.30975	0.653128
Rxn_02	B = C + N_2	3.96619E+08	8.31378E-09
Rxn_03	C + S_2 = D	119860	9.67898E-08
Rxn_04	D = F + PhCN	0.626834	1.21276E+09
Rxn_05	F = F_1	5.80765E+12	1.45968E+08
Rxn_06	F_1 = P_1	2.79878E+08	28.7905
Rxn_07	P_1 + 2 PhCN = P + A	9.69522E+10	1.06178E+07

Parameter Estimation Results	
Objective Value	0.000218626439
Root Mean Square	0.001120925418
Standard Deviation	0.001168937658

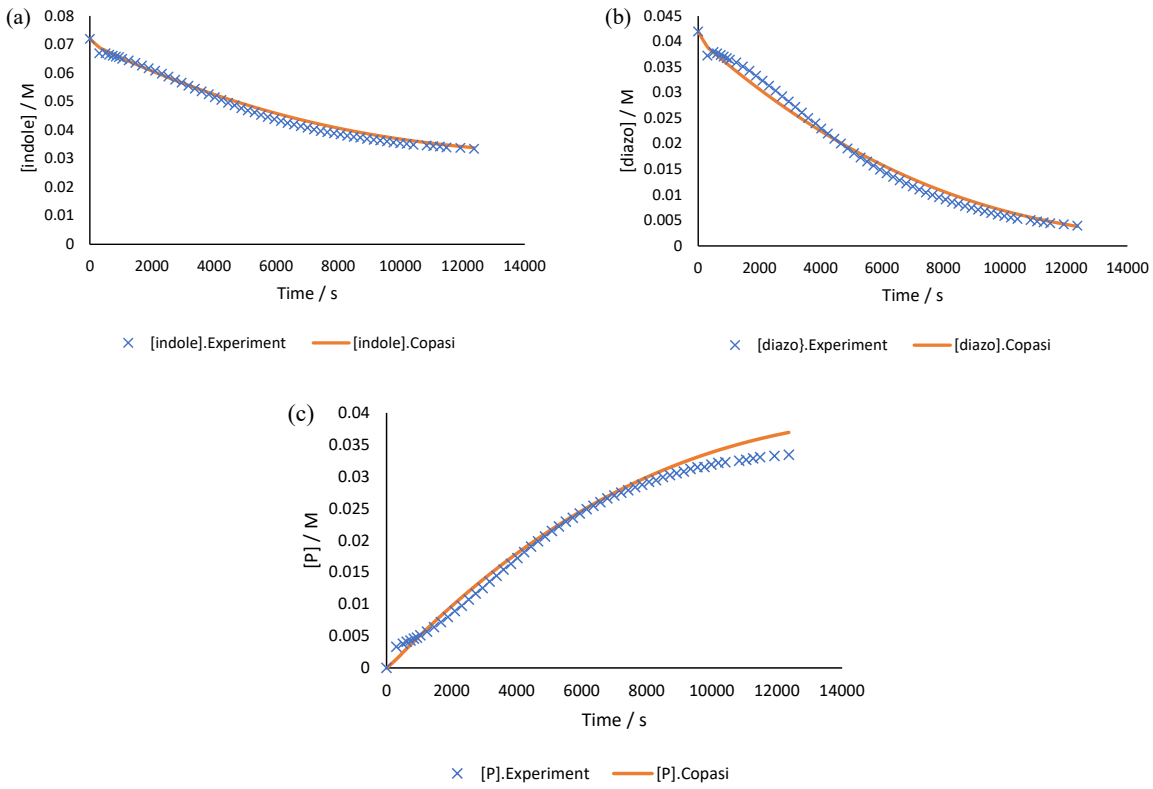


Fig. S22 Comparison of experimental data with COPASI-fitted data for the Crossover Pathway. (a) Fit for indole (S_2), (b) fit for diazo (S_1), and (c) fit for the product (P).

We want to highlight the following points:

1. The kinetic constants presented above may not have physical significance, as the system involves 14 parameters and is likely underestimated.
2. The Parameter Estimation Results reveal that the expected amount of product generated via the crossover pathway is the most significant among all pathways. Additionally, the crossover pathway demonstrates an almost perfect alignment with the experimental data, with only minor deviations observed.

15.2. Comparison of Experimental Data with Kinetic Model Predictions

The reaction was divided into multiple steps (Table S20). The forward and reverse step rate was calculated using Eyring - Polanyi Equation,

$$k = \frac{\kappa k_B T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}}$$

where, κ is the transmission factor, k_B is the Boltzmann constant (in J/K), T is the temperature (in K), h is the Planck constant (in J·s), $\Delta G^{\ddagger}$ is the activation free energy (in J/mol) and R is the ideal gas constant (in J/mol·K). Since the reaction under consideration is homogeneous, the

transmission factor (κ) is taken as 1. The activation free energy ($\Delta G^{\ddagger}$) is calculated computationally for each reaction step.

For reaction steps involving association or dissociation processes in solution, such as formation of intermediates or coordination to metal-species, are governed by diffusion. The diffusion-controlled rate constants can be estimated using the Stokes–Einstein equation with the Smoluchowski formulation,

$$k_{\text{diff}} = \frac{8k_B T}{3\eta}.10^3.N_A$$

where, η is viscosity of the solvent (Pa·s) and N_A is Avogadro's number.

In this study, chloroform ($CHCl_3$) was used as the solvent. The viscosity (η) of $CHCl_3$ at 298 K is 0.542 mPa·s. The diffusion rate constant (k_{diff}) corresponds to an activation free energy of 3.69 kcal/mol, as calculated using the Eyring equation.

To operate COPASI, it was necessary to input the rate constant values and the initial concentrations of each reactant. The initial concentrations were derived from experimental data;

[A] = 0.0021 M

[diazo] = 0.042 M

[indole] = 0.072 M

To compare the yield, we used the estimated activation free energy values as shown in Table S20, estimated using parameter estimation runs. The values presented here are the results of multiple parameter estimation runs conducted to determine the optimal fit.

Table S20 The different steps of the reaction (Scheme 1 and Scheme 9 of the main text) and calculated and estimated activation free energy ($\Delta G^{\ddagger}$) (in kcal/mol) for forward (with subscript 'F') and reverse (with subscript 'R')

Rxn, No.	Reaction	Actual*		Estimated	
		$\Delta G^{\ddagger}_F$	$\Delta G^{\ddagger}_R$	$\Delta G^{\ddagger}_F$	$\Delta G^{\ddagger}_R$
Rxn_01	A + S_1 = B + PhCN	20.1	18.6	18.59	18.74
Rxn_02	B = C + N2	0.4	33.1	0.03	29.1
Rxn_03	C + S_2 = D	7.7	30.5	7.62	28.08
Rxn_04	D = F + PhCN	18.3	3.6	17.73	6.27
Rxn_05	F = F_1	0.1	2.4	0.04	2.02
Rxn_06	F_1 = P_1	0.4	14.6	4.61	14.95
Rxn_07	P_1 + 2 PhCN = P + A	3.69	3.69	0.74	6.25

- The activation free energy barrier were calculated at $SMD_{(DCM)}$/DLPNO-CCSD(T)/def2-TZVP//B3LYP-D3/6-31G(d,p), LANL2DZ(Pd) level of theory, as shown in Table S2.

Table S21 The computed yield of product [P] formed from the crossover pathway, calculated by micro-kinetic modeling

	Experiment	**COPASI**
[P] / M	0.0334480	0.0369145
Yield (%)	79.64	87.89

Table S22 Concentrations of selected species in the solution during the reaction in standard conditions predicted by COPASI

S. No.	**Time / sec**	**[S_1] / M**	**[S_2] / M**	**[P] / M**
1	0	0.042	0.072	0
2	441.643	0.0375887	0.0675887	0.00388368
3	883.286	0.0340515	0.0640515	0.00731508
4	1324.93	0.0310118	0.0610118	0.0102907
5	1766.57	0.0283428	0.0583428	0.0129142
6	2208.21	0.0259707	0.0559707	0.0152515
7	2649.86	0.0238454	0.0538454	0.0173492
8	3091.5	0.0219299	0.0519299	0.0192419
9	3533.14	0.0201958	0.0501958	0.0209568
10	3974.79	0.0186203	0.0486203	0.0225161
11	4416.43	0.0171846	0.0471846	0.0239376
12	4858.07	0.0158734	0.0458734	0.0252366
13	5299.71	0.0146732	0.0446732	0.026426
14	5741.36	0.0135727	0.0435727	0.0275169
15	6183	0.0125622	0.0425622	0.0285189
16	6624.64	0.011633	0.041633	0.0294405
17	7066.29	0.0107776	0.0407776	0.030289
18	7507.93	0.00998932	0.0399893	0.0310712
19	7949.57	0.00926224	0.0392622	0.0317927
20	8391.21	0.00859105	0.0385911	0.0324588
21	8832.86	0.007971	0.037971	0.0330743
22	9274.5	0.00739781	0.0373978	0.0336433
23	9716.14	0.00686762	0.0368676	0.0341697
24	10157.8	0.00637695	0.0363769	0.0346569
25	10599.4	0.00592261	0.0359226	0.0351081
26	11041.1	0.00550175	0.0355017	0.035526
27	11482.7	0.00511172	0.0351117	0.0359134
28	11924.4	0.00475014	0.0347501	0.0362725
29	12366	0.00441481	0.0344148	0.0366055
30	12807.6	0.00410374	0.0341037	0.0369145

Table S20 reports a maximum error of 4.21 kcal/mol in the estimated values. This indicates that the calculated activation free energy approximates the actual activation free energy. However, directly using the actual activation free energy does not reproduce the desired yield. This discrepancy arises because COPASI incorporates activation free energy into its modelling framework but does not account for other factors affecting reaction yield. Nonetheless, the estimated values demonstrate a trend that closely corresponds to the experimental results.

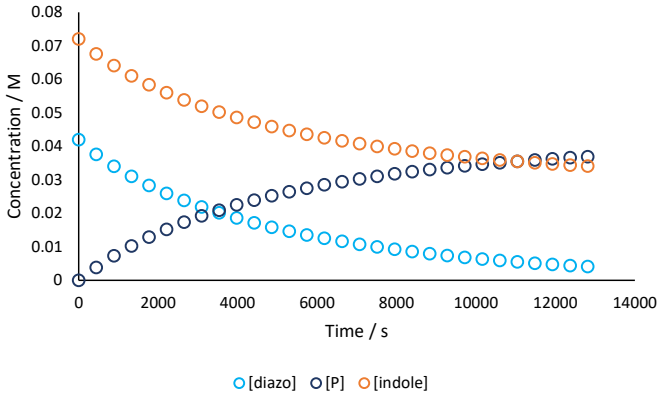


Fig. S23 COPASI time-course simulation for the crossover pathway illustrating the concentration changes of indole (S_2), diazo (S_1), and product (P).

16. Cartesian Coordinates and Electronic Energies of Optimized Geometries

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A

Number of imaginary frequencies : 0 Electronic energy : HF=-1616.5681344
Zero-point correction= 0.493284 (Hartree/Particle)
Thermal correction to Energy= 0.525709
Thermal correction to Enthalpy= 0.526653
Thermal correction to Gibbs Free Energy= 0.423404
Sum of electronic and zero-point Energies= -1616.074850
Sum of electronic and thermal Energies= -1616.042426
Sum of electronic and thermal Enthalpies= -1616.041482
Sum of electronic and thermal Free Energies= -1616.144731

Cartesian Coordinates

46	0.450897	-0.015213	0.014845
7	-1.075672	-1.363956	-0.003559
7	-1.107152	1.293739	0.033206
8	-4.462886	-0.829825	0.984582
8	-4.444051	0.700255	-1.073578
6	-0.943066	-2.695142	0.094785
1	0.054746	-3.099539	-0.001178
6	-2.054707	-3.503687	0.329675
1	-1.927411	-4.579084	0.380124
6	-3.292268	-2.922249	0.577774
1	-4.138312	-3.537572	0.861968
6	-3.417779	-1.524706	0.528625
6	-2.298778	-0.770688	0.101933
6	-2.309399	0.670383	-0.124503
6	-3.434234	1.404996	-0.559387
6	-3.362574	2.805608	-0.530014
1	-4.231062	3.397117	-0.797090
6	-2.150064	3.415793	-0.226985
1	-2.057036	4.495848	-0.220574
6	-1.016791	2.631970	-0.010697
1	-0.034024	3.063019	0.119929
6	-6.583868	-0.797188	2.060739
1	-6.141021	-1.289501	2.929471
1	-7.638033	-1.080145	2.000444
1	-6.524653	0.284466	2.212446
6	-5.865459	-1.211337	0.786258
1	-5.929491	-2.296951	0.659200
6	-6.384280	-0.514961	-0.483943
1	-7.478191	-0.494645	-0.444418
1	-6.109097	-1.090156	-1.374491
6	-5.848700	0.905405	-0.685410
1	-5.856526	1.473255	0.251744
6	-6.571116	1.657182	-1.792563
1	-6.130274	2.642673	-1.962637
1	-7.622012	1.798597	-1.524844
1	-6.523569	1.095119	-2.729343
7	1.897282	1.429174	0.108895
7	1.934615	-1.421457	-0.087419
6	2.809913	2.146262	0.168995
6	2.865829	-2.112867	-0.161941
6	3.908528	3.040987	0.241790
6	4.379481	3.457731	1.504844
6	4.507758	3.500018	-0.950252

6	5.454269	4.337051	1.563814
1	3.907148	3.095392	2.411866
6	5.581228	4.378932	-0.866723
1	4.132915	3.170088	-1.913432
6	6.051798	4.795390	0.383987
1	5.827330	4.666863	2.527491
1	6.051993	4.741098	-1.774381
1	6.890141	5.482597	0.439629
6	3.987293	-2.977166	-0.251774
6	4.430779	-3.405821	-1.520777
6	4.636294	-3.394740	0.929395
6	5.528350	-4.255196	-1.596639
1	3.920291	-3.075379	-2.419265
6	5.731730	-4.244288	0.829037
1	4.281963	-3.056312	1.897380
6	6.175223	-4.672394	-0.427629
1	5.880822	-4.593627	-2.565066
1	6.240686	-4.574570	1.728207
1	7.031057	-5.336462	-0.496409

B

Number of imaginary frequencies : 0 Electronic energy : HF=-2130.8390248
Zero-point correction= 0.633613 (Hartree/Particle)
Thermal correction to Energy= 0.675475
Thermal correction to Enthalpy= 0.676420
Thermal correction to Gibbs Free Energy= 0.556120
Sum of electronic and zero-point Energies= -2130.205412
Sum of electronic and thermal Energies= -2130.163549
Sum of electronic and thermal Enthalpies= -2130.162605
Sum of electronic and thermal Free Energies= -2130.282904

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Cartesian Coordinates

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46	-0.572043	0.432491	-0.631362
7	0.685494	-1.142753	-1.148482
7	1.265268	1.283044	-0.134272
8	4.239461	-1.149038	-1.489419
8	4.052405	-0.620723	1.031896
6	0.322581	-2.257219	-1.797371
1	-0.734365	-2.409581	-1.962264
6	1.280477	-3.164706	-2.245496
1	0.963674	-4.069741	-2.751481
6	2.631005	-2.863038	-2.108968
1	3.382969	-3.514563	-2.539178
6	3.006698	-1.670323	-1.474409
6	1.988831	-0.876314	-0.892173
6	2.239824	0.326179	-0.102198
6	3.373106	0.492554	0.717362
6	3.636672	1.762045	1.248074
1	4.531637	1.930714	1.836813
6	2.702630	2.771425	1.055504
1	2.860489	3.764895	1.458989
6	1.495769	2.481597	0.417557
1	0.701921	3.209711	0.370694
6	6.522325	-1.231956	-2.142718
1	6.214546	-1.180501	-3.189477
1	7.465497	-1.781386	-2.083774
1	6.693142	-0.212133	-1.786201

6	5.461947	-1.934531	-1.309298
1	5.302853	-2.947248	-1.694452
6	5.784439	-2.003701	0.192740
1	6.834476	-2.291415	0.308718
1	5.186225	-2.784404	0.675540
6	5.517470	-0.700528	0.950734
1	5.869818	0.168538	0.384262
6	6.090338	-0.705656	2.359521
1	7.181154	-0.774457	2.322755
1	5.708196	-1.561285	2.923703
1	5.825365	0.206334	2.900636
6	-1.828988	2.156016	-0.007503
6	-1.419585	3.514448	-0.527418
6	-1.023230	3.647165	-1.868240
6	-1.484026	4.644252	0.304835
6	-0.671512	4.898834	-2.367637
1	-0.980672	2.772521	-2.511789
6	-1.119855	5.891382	-0.202284
1	-1.788683	4.548091	1.340433
6	-0.716341	6.020781	-1.534006
1	-0.361336	4.999157	-3.402551
1	-1.159823	6.763209	0.442548
1	-0.439898	6.995429	-1.923287
6	-1.739880	1.837410	1.484126
8	-0.882356	2.325257	2.181471
8	-2.632117	0.907933	1.838480
6	-2.297224	0.126076	3.057723
1	-3.256450	-0.292553	3.360945
1	-1.936082	0.818531	3.818363
6	-1.289722	-0.927449	2.688134
6	-1.718280	-2.153912	2.161611
6	0.085300	-0.669805	2.798378
6	-0.789913	-3.106152	1.740984
1	-2.781827	-2.367731	2.091281
6	1.014980	-1.625224	2.382315
1	0.419284	0.277451	3.210008
6	0.577896	-2.839894	1.848414
1	-1.131160	-4.060395	1.350976
1	2.078127	-1.428409	2.477325
1	1.301976	-3.584958	1.532267
7	-2.262454	-0.662902	-0.948039
6	-3.204986	-1.335271	-0.849070
6	-4.381730	-2.106234	-0.675599
6	-4.720179	-3.120976	-1.592389
6	-5.200268	-1.824072	0.439669
6	-5.882421	-3.854805	-1.381859
1	-4.085334	-3.319515	-2.449423
6	-6.357251	-2.569757	0.630664
1	-4.923089	-1.031975	1.127828
6	-6.695809	-3.581318	-0.276200
1	-6.157987	-4.638295	-2.079545
1	-6.997808	-2.364244	1.481658
1	-7.601679	-4.158756	-0.121302
7	-3.135949	1.914277	-0.469925
7	-4.157623	1.755911	-0.887688

TS(B-C)

Number of imaginary frequencies : 1 Electronic energy : HF=-2130.8362042

Zero-point correction= 0.631789 (Hartree/Particle)
Thermal correction to Energy= 0.673726
Thermal correction to Enthalpy= 0.674670
Thermal correction to Gibbs Free Energy= 0.554855
Sum of electronic and zero-point Energies= -2130.204414
Sum of electronic and thermal Energies= -2130.162477
Sum of electronic and thermal Enthalpies= -2130.161533
Sum of electronic and thermal Free Energies= -2130.281348

Cartesian Coordinates

46	0.561520	-0.377618	-0.745746
7	-0.772145	1.173461	-1.226464
7	-1.212751	-1.199666	0.008682
8	-4.332690	0.950946	-1.449534
8	-3.989107	0.761048	1.117253
6	-0.494273	2.243511	-1.982922
1	0.549114	2.438427	-2.191493
6	-1.515176	3.050238	-2.484285
1	-1.266084	3.922650	-3.077983
6	-2.841963	2.686357	-2.280885
1	-3.641379	3.254700	-2.742312
6	-3.130139	1.537501	-1.529586
6	-2.051869	0.856879	-0.918075
6	-2.214101	-0.274077	-0.003513
6	-3.283276	-0.361012	0.912422
6	-3.452338	-1.545473	1.638525
1	-4.296755	-1.656950	2.309723
6	-2.480487	-2.533947	1.533606
1	-2.560349	-3.457160	2.096249
6	-1.342548	-2.302759	0.762617
1	-0.520579	-3.000506	0.762036
6	-6.649923	0.824523	-1.949408
1	-6.402456	0.645249	-2.998054
1	-7.619565	1.326889	-1.901688
1	-6.736797	-0.143948	-1.448535
6	-5.585975	1.690077	-1.292451
1	-5.513297	2.645431	-1.822948
6	-5.823299	1.954744	0.203505
1	-6.876338	2.219545	0.344558
1	-5.232622	2.815498	0.536303
6	-5.458777	0.780349	1.115558
1	-5.805562	-0.171155	0.697556
6	-5.950996	0.963260	2.542861
1	-7.044045	0.990207	2.564308
1	-5.573270	1.901495	2.959317
1	-5.618720	0.145076	3.187101
6	1.805539	-2.022997	-0.311724
6	1.378047	-3.407094	-0.580983
6	0.586421	-3.692303	-1.713470
6	1.772670	-4.455726	0.276672
6	0.188222	-4.997641	-1.974542
1	0.288068	-2.886340	-2.377670
6	1.353310	-5.757519	0.018272
1	2.382995	-4.247864	1.149313
6	0.567336	-6.029528	-1.106530
1	-0.417436	-5.215664	-2.847880
1	1.647147	-6.561236	0.685255
1	0.251720	-7.048086	-1.309749
6	2.435571	-1.606974	0.999666

8	3.493770	-1.021001	1.091762
8	1.572658	-1.860970	1.982274
6	1.665581	-0.972868	3.171555
1	2.710446	-0.919811	3.478792
1	1.079707	-1.502286	3.922003
6	1.087378	0.365589	2.805669
6	1.922576	1.416166	2.401020
6	-0.303256	0.543870	2.774762
6	1.373605	2.623526	1.965155
1	2.999421	1.283802	2.425837
6	-0.853065	1.748755	2.337298
1	-0.954727	-0.266039	3.092650
6	-0.012991	2.788404	1.926895
1	2.028790	3.436554	1.666769
1	-1.931093	1.876760	2.317349
1	-0.438922	3.731263	1.596943
7	2.214107	0.746705	-1.161110
6	3.106476	1.448794	-0.906849
6	4.216468	2.267203	-0.585459
6	4.334298	3.556783	-1.143928
6	5.181516	1.764939	0.314907
6	5.426390	4.341973	-0.794585
1	3.585842	3.923748	-1.838345
6	6.263990	2.570358	0.650209
1	5.064621	0.770577	0.730915
6	6.386411	3.850829	0.098520
1	5.533933	5.334870	-1.217888
1	7.015419	2.200899	1.339912
1	7.236752	4.470728	0.364657
7	3.150785	-1.843345	-1.343227
7	3.854998	-1.879345	-2.195843

C

Number of imaginary frequencies : 0 Electronic energy : HF=-2021.3448899
Zero-point correction= 0.623892 (Hartree/Particle)
Thermal correction to Energy= 0.664088
Thermal correction to Enthalpy= 0.665032
Thermal correction to Gibbs Free Energy= 0.546970
Sum of electronic and zero-point Energies= -2020.720998
Sum of electronic and thermal Energies= -2020.680802
Sum of electronic and thermal Enthalpies= -2020.679857
Sum of electronic and thermal Free Energies= -2020.797920

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Cartesian Coordinates

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46	-0.594730	0.274903	-0.539541
7	0.849564	-1.184397	-1.057830
7	1.126782	1.329823	-0.094646
8	4.318182	-0.619107	-1.708317
8	4.256549	-0.117195	0.829534
6	0.623900	-2.358603	-1.657571
1	-0.407356	-2.682086	-1.722070
6	1.676100	-3.112183	-2.179352
1	1.473143	-4.071517	-2.642040
6	2.964369	-2.589245	-2.167325
1	3.774346	-3.121085	-2.653320
6	3.191900	-1.335193	-1.579664
6	2.109984	-0.705662	-0.922295

6	2.232701	0.535582	-0.150986
6	3.383861	0.872663	0.593466
6	3.475175	2.155558	1.145258
1	4.373216	2.455842	1.673674
6	2.374313	3.003099	1.064053
1	2.402308	3.996936	1.496129
6	1.192912	2.536229	0.494594
1	0.285056	3.121537	0.522110
6	6.523641	-0.329565	-2.539463
1	6.128858	-0.331649	-3.557914
1	7.545457	-0.717262	-2.561409
1	6.553804	0.705452	-2.186871
6	5.661121	-1.193781	-1.632593
1	5.640494	-2.219572	-2.015384
6	6.111872	-1.207541	-0.162233
1	7.200259	-1.323791	-0.134546
1	5.687088	-2.072816	0.358590
6	5.704221	0.037434	0.630010
1	5.866281	0.951280	0.047743
6	6.384527	0.124334	1.987539
1	7.465756	0.229036	1.861265
1	6.190284	-0.780814	2.570149
1	6.025119	0.983154	2.560331
6	-1.866080	1.721938	-0.001107
6	-2.378590	2.783961	-0.749863
6	-1.984127	2.972320	-2.114504
6	-3.303988	3.710163	-0.161407
6	-2.484534	4.032235	-2.844100
1	-1.287367	2.269109	-2.559499
6	-3.799428	4.763556	-0.904312
1	-3.619964	3.568960	0.867346
6	-3.389816	4.924093	-2.240054
1	-2.188535	4.178921	-3.877150
1	-4.501847	5.463564	-0.464947
1	-3.783385	5.754564	-2.819384
6	-2.286292	1.427082	1.395357
8	-3.288018	0.770095	1.603094
8	-1.381251	1.829683	2.279603
6	-1.247929	0.999150	3.511074
1	-2.245229	0.805196	3.906451
1	-0.692944	1.644089	4.190914
6	-0.503124	-0.248051	3.129344
6	-1.202043	-1.408246	2.765198
6	0.894683	-0.225857	3.023422
6	-0.510208	-2.528468	2.301089
1	-2.284468	-1.428106	2.845633
6	1.586314	-1.344957	2.559869
1	1.439799	0.671769	3.304090
6	0.882160	-2.495890	2.194015
1	-1.056107	-3.429432	2.037971
1	2.668423	-1.319057	2.480196
1	1.419726	-3.371074	1.841420
7	-2.233528	-0.902782	-0.843412
6	-3.237729	-1.476602	-0.737314
6	-4.469743	-2.157847	-0.565852
6	-4.827603	-3.214936	-1.426453
6	-5.313844	-1.749283	0.488682
6	-6.039622	-3.864151	-1.222640
1	-4.167180	-3.511534	-2.234492
6	-6.520594	-2.415108	0.672846

1	-5.014006	-0.928803	1.131330
6	-6.881394	-3.466397	-0.177331
1	-6.330980	-4.678982	-1.876700
1	-7.182435	-2.115262	1.478439
1	-7.825875	-3.979384	-0.025622

TS(C-D)

Number of imaginary frequencies : 1 Electronic energy : HF=-2463.7113175
Zero-point correction= 0.809549 (Hartree/Particle)
Thermal correction to Energy= 0.860534
Thermal correction to Enthalpy= 0.861479
Thermal correction to Gibbs Free Energy= 0.718873
Sum of electronic and zero-point Energies= -2462.901388
Sum of electronic and thermal Energies= -2462.850402
Sum of electronic and thermal Enthalpies= -2462.849458
Sum of electronic and thermal Free Energies= -2462.992063

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Cartesian Coordinates

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46	-0.418579	0.027538	-0.135004
7	-2.060344	1.095775	-1.073315
7	-2.052863	-0.754378	0.938635
8	-5.383717	-0.213693	-1.321301
8	-5.364624	0.607273	1.137262
6	-1.998536	1.904588	-2.139341
1	-1.028864	2.323886	-2.376421
6	-3.126914	2.190056	-2.907345
1	-3.051047	2.876828	-3.743072
6	-4.320619	1.531077	-2.632201
1	-5.187353	1.665171	-3.270432
6	-4.373970	0.640085	-1.551976
6	-3.242491	0.540737	-0.712204
6	-3.238313	-0.201983	0.556514
6	-4.362881	-0.242784	1.416700
6	-4.298976	-1.043794	2.564186
1	-5.148389	-1.118368	3.233710
6	-3.106713	-1.686893	2.869241
1	-3.016345	-2.297603	3.760480
6	-1.988557	-1.486648	2.063879
1	-1.029961	-1.904188	2.335337
6	-7.524185	-0.281639	-2.486301
1	-8.572809	0.027384	-2.447728
1	-7.488074	-1.373742	-2.535926
1	-7.089156	0.115262	-3.407403
6	-6.782140	0.223862	-1.256358
1	-6.791690	1.319009	-1.218757
6	-7.316950	-0.380034	0.046711
1	-7.064077	-1.446144	0.035327
1	-8.410392	-0.316639	0.060347
6	-6.777739	0.282361	1.327375
1	-6.875884	-0.418106	2.163177
6	-7.460057	1.594798	1.687379
1	-7.009520	2.029637	2.582713
1	-8.520867	1.419454	1.885789
1	-7.377879	2.323985	0.876026
6	0.893636	-1.227201	0.778548
6	0.796715	-2.628077	0.519739
6	0.190685	-3.066133	-0.696314

6	1.295226	-3.632233	1.408780
6	0.074177	-4.412934	-0.998970
1	-0.181763	-2.323059	-1.392783
6	1.154284	-4.976881	1.102786
1	1.731384	-3.330996	2.351457
6	0.555745	-5.373994	-0.101560
1	-0.388326	-4.721811	-1.930394
1	1.503683	-5.727342	1.805333
1	0.454044	-6.430078	-0.332699
6	1.358088	-0.657960	2.087069
8	1.343435	-1.272017	3.143192
8	1.691321	0.638017	1.987563
6	1.962504	1.337581	3.253901
1	2.752759	0.802132	3.783655
1	1.052110	1.280625	3.856942
6	2.350299	2.752555	2.935195
6	1.370376	3.696939	2.595014
6	3.691172	3.152246	2.992411
6	1.726796	5.015799	2.313535
1	0.324002	3.402261	2.572185
6	4.050882	4.472947	2.715100
1	4.456659	2.435322	3.279062
6	3.068922	5.405903	2.375282
1	0.959644	5.744496	2.069610
1	5.091325	4.775620	2.781856
1	3.343599	6.438281	2.180383
6	3.771425	-3.167771	-0.939270
6	3.212402	-1.944134	-1.380850
6	2.671774	-1.876865	-2.673581
6	2.722837	-3.010107	-3.486281
6	3.289574	-4.207525	-3.023751
6	3.823913	-4.306681	-1.734457
6	4.051869	-1.680832	0.734546
6	3.338835	-1.019108	-0.289632
1	2.238073	-0.953531	-3.044479
1	2.327914	-2.964978	-4.496152
1	3.325939	-5.070784	-3.680264
1	4.273312	-5.231736	-1.389695
1	3.173639	0.044740	-0.302429
7	4.256315	-2.971918	0.366691
6	4.987298	-3.992639	1.109806
1	4.409572	-4.919737	1.120738
1	5.958435	-4.182540	0.642400
1	5.142258	-3.665928	2.136660
6	4.561764	-1.115978	2.017470
1	4.417956	-0.035406	2.022795
1	4.037244	-1.534650	2.885985
1	5.630743	-1.314868	2.144876
7	1.011379	1.114279	-1.131214
6	1.721879	1.913410	-1.586312
6	2.606794	2.889259	-2.126233
6	2.956114	2.842996	-3.491283
6	3.120907	3.890387	-1.276796
6	3.822695	3.803698	-3.999666
1	2.552707	2.066651	-4.132971
6	3.986326	4.841060	-1.807505
1	2.840669	3.917954	-0.229041
6	4.336044	4.798982	-3.160882
1	4.099234	3.778555	-5.048350
1	4.387990	5.616518	-1.164008

1	5.011888	5.545803	-3.565561

D

Number of imaginary frequencies : 0 Electronic energy : HF=-2463.8956052
Zero-point correction= 0.814503 (Hartree/Particle)
Thermal correction to Energy= 0.864515
Thermal correction to Enthalpy= 0.865459
Thermal correction to Gibbs Free Energy= 0.727167
Sum of electronic and zero-point Energies= -2463.081103
Sum of electronic and thermal Energies= -2463.031090
Sum of electronic and thermal Enthalpies= -2463.030146
Sum of electronic and thermal Free Energies= -2463.168438

Cartesian Coordinates

46	0.055636	0.111830	-0.030706
7	1.497355	1.383416	0.979913
7	1.819321	-0.384757	-1.073651
8	4.873797	0.317835	1.504313
8	4.991792	1.291488	-0.919168
6	1.270423	2.145441	2.059350
1	0.251526	2.481450	2.208669
6	2.296259	2.483736	2.941083
1	2.091139	3.134802	3.783679
6	3.558935	1.923833	2.762392
1	4.353062	2.097382	3.480432
6	3.780735	1.080522	1.666741
6	2.745365	0.927805	0.721438
6	2.915064	0.248756	-0.570030
6	4.092490	0.381485	-1.338735
6	4.179681	-0.309997	-2.553973
1	5.075139	-0.242063	-3.161266
6	3.071052	-1.012800	-3.005133
1	3.089579	-1.529083	-3.958165
6	1.889543	-0.993183	-2.265743
1	0.981311	-1.434459	-2.644972
6	6.905589	0.400580	2.834178
1	7.920090	0.804348	2.897296
1	6.965315	-0.691560	2.841682
1	6.355349	0.718291	3.723846
6	6.223421	0.884275	1.563289
1	6.133475	1.976620	1.560112
6	6.909737	0.383669	0.289227
1	6.722871	-0.694030	0.227128
1	7.993711	0.514700	0.374174
6	6.434009	1.083420	-0.995073
1	6.666724	0.449928	-1.857966
6	7.033828	2.465950	-1.205194
1	6.631722	2.922022	-2.112715
1	8.120083	2.391874	-1.303359
1	6.806580	3.126000	-0.362989
6	-1.228620	-1.439727	-0.785220
6	-0.462860	-2.707274	-1.115011
6	0.408675	-3.274381	-0.167263
6	-0.664213	-3.402996	-2.323047
6	1.048540	-4.488436	-0.411518
1	0.603628	-2.750985	0.761574
6	-0.024884	-4.620196	-2.565549

1	-1.293770	-2.977123	-3.094890
6	0.831660	-5.170564	-1.610944
1	1.723724	-4.897108	0.334121
1	-0.191145	-5.131552	-3.508873
1	1.333508	-6.113513	-1.803942
6	-1.710944	-0.653304	-1.978294
8	-1.109729	-0.593167	-3.037366
8	-2.852381	0.036935	-1.734563
6	-3.329927	0.938249	-2.784647
1	-4.415984	0.831165	-2.768775
1	-2.942607	0.577419	-3.740267
6	-2.920572	2.367404	-2.532998
6	-1.577397	2.704344	-2.307935
6	-3.877711	3.386254	-2.597826
6	-1.205032	4.037854	-2.137749
1	-0.820489	1.926683	-2.295362
6	-3.500708	4.724960	-2.458821
1	-4.920857	3.137363	-2.774467
6	-2.164527	5.053393	-2.221351
1	-0.161879	4.288780	-1.968925
1	-4.250380	5.506760	-2.533212
1	-1.869193	6.092396	-2.112502
6	-2.310376	-3.592926	1.768257
6	-1.895265	-2.266909	1.624411
6	-1.173517	-1.681549	2.660195
6	-0.875316	-2.451851	3.791460
6	-1.288071	-3.785227	3.895810
6	-2.028212	-4.384666	2.872858
6	-3.168661	-2.953214	-0.227724
6	-2.359173	-1.771175	0.269753
1	-0.838596	-0.654102	2.600563
1	-0.313506	-2.004912	4.605291
1	-1.040708	-4.359764	4.781974
1	-2.362173	-5.413079	2.951323
1	-3.021468	-0.905290	0.342939
7	-3.070748	-3.953217	0.611968
6	-3.624244	-5.301620	0.453524
1	-2.797471	-6.015313	0.470390
1	-4.304425	-5.509579	1.282267
1	-4.155331	-5.385764	-0.491184
6	-3.961087	-3.004951	-1.484285
1	-4.046727	-2.008173	-1.911712
1	-3.472852	-3.660402	-2.214393
1	-4.965582	-3.397153	-1.297469
7	-1.540940	1.032880	0.857347
6	-2.402268	1.724875	1.214512
6	-3.452856	2.583609	1.632290
6	-4.270066	2.226182	2.723323
6	-3.655864	3.785763	0.927465
6	-5.295124	3.084527	3.103998
1	-4.095877	1.296423	3.255270
6	-4.688448	4.628537	1.324869
1	-3.017359	4.039757	0.090120
6	-5.503518	4.280918	2.406855
1	-5.932036	2.825555	3.943127
1	-4.857245	5.556381	0.788658
1	-6.306156	4.945338	2.711213

A_1

Number of imaginary frequencies : 0 Electronic energy : HF=-1734.5515209
Zero-point correction= 0.579958 (Hartree/Particle)
Thermal correction to Energy= 0.615765
Thermal correction to Enthalpy= 0.616709
Thermal correction to Gibbs Free Energy= 0.508187
Sum of electronic and zero-point Energies= -1733.971563
Sum of electronic and thermal Energies= -1733.935756
Sum of electronic and thermal Enthalpies= -1733.934811
Sum of electronic and thermal Free Energies= -1734.043334

Cartesian Coordinates

46	0.790924	0.134581	-0.093880
7	-1.101436	1.035919	-0.141555
7	-0.443585	-1.599894	-0.173734
8	-4.176039	-0.515878	-1.127440
8	-3.778314	-1.772554	1.096227
6	-1.385586	2.335893	-0.318152
1	-0.567727	3.031715	-0.244550
6	-2.674814	2.772569	-0.613869
1	-2.859887	3.834658	-0.726881
6	-3.681907	1.844856	-0.842641
1	-4.663082	2.165835	-1.172836
6	-3.385291	0.482128	-0.709242
6	-2.103079	0.113095	-0.234216
6	-1.741019	-1.277890	0.045441
6	-2.639807	-2.234900	0.564426
6	-2.237804	-3.577100	0.587764
1	-2.925851	-4.342015	0.930653
6	-0.933805	-3.898360	0.224581
1	-0.588261	-4.925914	0.242855
6	-0.040380	-2.875681	-0.094778
1	1.005913	-3.070946	-0.288358
6	-6.167742	-1.309632	-2.147123
1	-5.866468	-0.832538	-3.082405
1	-7.259720	-1.340893	-2.108007
1	-5.792046	-2.336794	-2.151463
6	-5.629377	-0.532799	-0.955381
1	-6.011135	0.493215	-0.985081
6	-5.961573	-1.160433	0.408325
1	-7.015187	-1.458627	0.403801
1	-5.843861	-0.419941	1.207090
6	-5.084599	-2.360606	0.775579
1	-4.951775	-3.031359	-0.080828
6	-5.595954	-3.120987	1.989339
1	-6.575065	-3.558752	1.775369
1	-5.695575	-2.448784	2.846254
1	-4.914530	-3.929350	2.267077
6	1.407530	4.007531	0.505708
6	1.748643	3.108007	-0.519554
6	1.628067	3.509708	-1.850504
6	1.163526	4.801047	-2.113150
6	0.820556	5.678003	-1.071344
6	0.938284	5.295131	0.268656
6	2.101529	2.126663	1.551622
6	2.145396	1.846217	0.121165
1	1.880195	2.833433	-2.661025
1	1.067755	5.136125	-3.140614
1	0.466517	6.675883	-1.307770

1	0.681919	5.976773	1.072214
7	1.623653	3.353681	1.749231
6	1.358375	4.010334	3.029787
1	1.991670	4.896448	3.118886
1	0.308965	4.312796	3.069105
1	1.567792	3.331170	3.853391
6	2.551228	1.232232	2.657266
1	3.302326	1.730908	3.279150
1	1.716635	0.945097	3.306254
1	2.986814	0.323388	2.242823
7	2.511114	-0.980872	-0.154574
6	3.479508	-1.616277	-0.261938
6	4.656980	-2.398943	-0.394263
6	5.146608	-3.112199	0.719960
6	5.316315	-2.449824	-1.640337
6	6.299968	-3.874573	0.576905
1	4.627877	-3.063944	1.671776
6	6.468137	-3.218852	-1.760596
1	4.926274	-1.896983	-2.488436
6	6.957610	-3.927397	-0.657535
1	6.688251	-4.428043	1.425183
1	6.985362	-3.267373	-2.712828
1	7.857708	-4.525172	-0.760452
1	3.039164	1.343135	-0.239140

B_1

Number of imaginary frequencies : 0 Electronic energy : HF=-2248.8136647
Zero-point correction= 0.720446 (Hartree/Particle)
Thermal correction to Energy= 0.765637
Thermal correction to Enthalpy= 0.766581
Thermal correction to Gibbs Free Energy= 0.641952
Sum of electronic and zero-point Energies= -2248.093219
Sum of electronic and thermal Energies= -2248.048028
Sum of electronic and thermal Enthalpies= -2248.047084
Sum of electronic and thermal Free Energies= -2248.171713

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Cartesian Coordinates

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46	1.142801	0.075270	0.191997
7	0.086653	-1.774407	0.335846
7	-0.855265	0.750773	0.890598
8	-3.128506	-2.384442	1.807700
8	-3.795333	-0.942188	-0.260446
6	0.646510	-2.994256	0.398206
1	1.699199	-3.064223	0.174695
6	-0.082613	-4.116444	0.777944
1	0.403697	-5.085286	0.803285
6	-1.400138	-3.970119	1.197225
1	-1.954050	-4.819814	1.579636
6	-1.969976	-2.692150	1.203287
6	-1.218045	-1.611407	0.675659
6	-1.745320	-0.243995	0.632970
6	-3.086889	0.040592	0.323148
6	-3.560954	1.342132	0.525541
1	-4.598648	1.581403	0.324536
6	-2.660175	2.320702	0.919669
1	-2.980605	3.344790	1.072050
6	-1.305735	2.002192	1.038237

1	-0.572024	2.765715	1.243361
6	-5.092910	-2.980872	2.999171
1	-4.475644	-3.263122	3.854988
1	-6.001745	-3.588176	3.009584
1	-5.376391	-1.930940	3.115263
6	-4.334113	-3.204802	1.700017
1	-4.050312	-4.259920	1.620762
6	-5.109757	-2.792208	0.438039
1	-6.130413	-3.180979	0.518024
1	-4.662664	-3.252559	-0.450142
6	-5.145789	-1.281258	0.192044
1	-5.340932	-0.736206	1.122367
6	-6.136408	-0.875593	-0.888834
1	-5.919970	-1.405400	-1.821358
1	-6.082383	0.198615	-1.084483
1	-7.157564	-1.118238	-0.581958
6	2.102858	2.103333	0.362042
6	1.763329	2.832190	1.647191
6	1.664654	2.113528	2.848795
6	1.618922	4.229232	1.652900
6	1.388672	2.781944	4.039861
1	1.787758	1.034308	2.847272
6	1.333386	4.889558	2.847059
1	1.708305	4.792903	0.731105
6	1.217293	4.169010	4.039137
1	1.306078	2.222034	4.965653
1	1.211760	5.967883	2.847582
1	1.000235	4.688786	4.966827
6	1.711840	2.608944	-1.023772
8	2.373001	2.352055	-2.013201
8	0.567560	3.274152	-0.970598
6	-0.057520	3.706353	-2.235711
1	0.651200	3.509390	-3.042100
1	-0.196169	4.783013	-2.129612
6	-1.362814	2.983870	-2.424478
6	-1.389003	1.583997	-2.500460
6	-2.556056	3.698304	-2.566348
6	-2.585929	0.910545	-2.727900
1	-0.467345	1.024750	-2.375695
6	-3.757670	3.024529	-2.804479
1	-2.548048	4.783334	-2.507747
6	-3.773885	1.632128	-2.887206
1	-2.604111	-0.174095	-2.770063
1	-4.675856	3.589862	-2.929805
1	-4.704689	1.107649	-3.078989
7	3.497809	1.948170	0.358794
7	4.603974	1.816051	0.430012
6	3.641601	-2.828496	-1.005901
6	3.714330	-1.621288	-0.288860
6	4.493702	-1.574773	0.868323
6	5.176539	-2.727186	1.264584
6	5.084492	-3.918111	0.528227
6	4.305769	-3.991039	-0.629891
6	2.347034	-1.369911	-2.151475
6	2.843747	-0.645733	-0.981685
1	4.573690	-0.666554	1.455995
1	5.792738	-2.701979	2.157189
1	5.629577	-4.795832	0.858581
1	4.237033	-4.909002	-1.203292
1	3.248239	0.316346	-1.287824

7	2.786110	-2.622388	-2.126153
6	2.492017	-3.688893	-3.083735
1	3.421142	-4.019229	-3.554158
1	2.038203	-4.529615	-2.553054
1	1.802876	-3.331693	-3.845737
6	1.532528	-0.788455	-3.253755
1	1.923062	-1.071694	-4.235554
1	0.492122	-1.128491	-3.194349
1	1.549932	0.299257	-3.174716

C_1

Number of imaginary frequencies : 0 Electronic energy : HF=-2139.201817
Zero-point correction= 0.709037 (Hartree/Particle)
Thermal correction to Energy= 0.753173
Thermal correction to Enthalpy= 0.754118
Thermal correction to Gibbs Free Energy= 0.627278
Sum of electronic and zero-point Energies= -2138.492780
Sum of electronic and thermal Energies= -2138.448644
Sum of electronic and thermal Enthalpies= -2138.447699
Sum of electronic and thermal Free Energies= -2138.574539

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Cartesian Coordinates

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46	0.627499	-0.370068	0.318728
7	-1.108804	-1.344737	-0.617108
7	-1.021602	0.734793	1.177957
8	-4.477381	-1.185110	0.615990
8	-4.220594	1.206702	-0.364144
6	-1.121269	-2.513604	-1.274598
1	-0.170093	-2.889969	-1.621388
6	-2.294080	-3.237753	-1.477345
1	-2.261421	-4.170882	-2.028777
6	-3.479473	-2.793381	-0.905533
1	-4.381158	-3.390916	-0.978447
6	-3.471064	-1.599585	-0.173213
6	-2.273596	-0.843217	-0.132846
6	-2.193082	0.455072	0.553591
6	-3.247986	1.395779	0.540822
6	-3.159406	2.508313	1.386515
1	-3.973030	3.224091	1.434192
6	-1.992359	2.707421	2.116284
1	-1.886004	3.563235	2.773705
6	-0.921851	1.832421	1.946191
1	0.031723	2.017772	2.421348
6	-6.660792	-1.450645	1.527110
1	-6.322739	-2.348187	2.050367
1	-7.726847	-1.559449	1.310186
1	-6.531938	-0.596275	2.198073
6	-5.885654	-1.263133	0.230394
1	-6.034998	-2.139059	-0.409489
6	-6.262973	0.005715	-0.554967
1	-7.354621	0.095928	-0.559699
1	-5.951244	-0.088650	-1.601242
6	-5.642857	1.298207	-0.013629
1	-5.718497	1.345969	1.078499
6	-6.234816	2.547679	-0.651477
1	-7.298126	2.628016	-0.407713
1	-6.132753	2.509945	-1.739882

1	-5.737269	3.453210	-0.293955
6	2.006230	0.488610	1.440262
6	2.367377	0.077262	2.742924
6	1.735058	-1.052922	3.351256
6	3.365777	0.781938	3.490508
6	2.076702	-1.446477	4.631418
1	0.976769	-1.589816	2.790243
6	3.707057	0.373152	4.766739
1	3.866090	1.636787	3.048145
6	3.063112	-0.736273	5.337133
1	1.590688	-2.299791	5.092223
1	4.468300	0.905674	5.326660
1	3.332821	-1.051712	6.340934
6	2.722530	1.640642	0.813823
8	3.722874	1.427282	0.150648
8	2.149181	2.810053	1.049950
6	2.747170	4.012051	0.400230
1	3.831287	3.929460	0.482710
1	2.386750	4.819603	1.037729
6	2.297890	4.160800	-1.024579
6	3.199043	3.949543	-2.076946
6	0.979879	4.545268	-1.314332
6	2.789788	4.126227	-3.400483
1	4.223372	3.661690	-1.857794
6	0.568283	4.708803	-2.636228
1	0.282423	4.734395	-0.502011
6	1.474423	4.502089	-3.680961
1	3.500897	3.986211	-4.208975
1	-0.448716	5.021182	-2.852821
1	1.159766	4.652321	-4.709260
6	2.170952	-3.288360	-1.956087
6	2.385080	-2.768718	-0.667495
6	2.633554	-3.654791	0.382850
6	2.646593	-5.025307	0.114976
6	2.414388	-5.516917	-1.178566
6	2.173199	-4.649953	-2.246555
6	2.118133	-1.036406	-2.190691
6	2.319190	-1.294532	-0.768070
1	2.822262	-3.289187	1.387317
1	2.847178	-5.725730	0.919151
1	2.435144	-6.586806	-1.356923
1	2.015835	-5.031017	-3.249912
7	1.999651	-2.190934	-2.845858
6	1.786514	-2.373636	-4.282680
1	2.661073	-2.859824	-4.722600
1	0.908269	-3.003233	-4.444628
1	1.627364	-1.410349	-4.762120
6	2.114109	0.294073	-2.864008
1	2.798767	0.306069	-3.718053
1	1.115901	0.554307	-3.234469
1	2.429824	1.068096	-2.165284
1	3.149981	-0.717963	-0.362449

TS(C_1-D)

Number of imaginary frequencies : 1 Electronic energy : HF=-2139.3108182
Zero-point correction= 0.710308 (Hartree/Particle)
Thermal correction to Energy= 0.752697
Thermal correction to Enthalpy= 0.753642

Thermal correction to Gibbs Free Energy= 0.634989
Sum of electronic and zero-point Energies= -2138.597584
Sum of electronic and thermal Energies= -2138.555194
Sum of electronic and thermal Enthalpies= -2138.554250
Sum of electronic and thermal Free Energies= -2138.672903

Cartesian Coordinates

46	0.535166	0.006922	-0.476487
7	-1.203385	-0.881192	-1.414935
7	-0.891260	0.353953	0.997675
8	-4.030983	-2.145560	0.369151
8	-4.438374	0.398002	0.633276
6	-1.267814	-1.556417	-2.570193
1	-0.430161	-1.443371	-3.250204
6	-2.361025	-2.363396	-2.884377
1	-2.398782	-2.875780	-3.839287
6	-3.359653	-2.554072	-1.934638
1	-4.167801	-3.251146	-2.124197
6	-3.276928	-1.878814	-0.708191
6	-2.229863	-0.942073	-0.533477
6	-2.135636	-0.042363	0.625328
6	-3.265959	0.496777	1.277430
6	-3.078271	1.209103	2.467699
1	-3.936490	1.583655	3.014569
6	-1.783254	1.497385	2.884486
1	-1.601169	2.076149	3.782930
6	-0.705453	1.111205	2.089610
1	0.305873	1.426057	2.310365
6	-5.741847	-3.343567	1.494850
1	-5.132772	-4.248311	1.434286
1	-6.795796	-3.633400	1.502376
1	-5.514182	-2.841107	2.439339
6	-5.462759	-2.434259	0.307789
1	-5.688067	-2.968560	-0.621262
6	-6.241424	-1.108697	0.334914
1	-7.281337	-1.323591	0.602060
1	-6.257036	-0.656263	-0.662873
6	-5.665054	-0.062533	1.292846
1	-5.384424	-0.512321	2.251785
6	-6.592550	1.125825	1.497618
1	-6.129656	1.888396	2.129320
1	-7.520120	0.803155	1.978770
1	-6.842778	1.584022	0.536349
6	2.141001	0.823195	0.336481
6	2.862150	0.379649	1.498679
6	2.701537	-0.945519	1.977014
6	3.781105	1.237657	2.163787
6	3.430836	-1.395306	3.071757
1	1.997543	-1.606679	1.484060
6	4.508522	0.777871	3.250926
1	3.891096	2.264669	1.835598
6	4.337595	-0.539212	3.705441
1	3.294266	-2.409064	3.433127
1	5.200816	1.441444	3.758890
1	4.904155	-0.890479	4.562572
6	1.941116	2.285888	0.062139
8	1.664569	3.042541	0.974177
8	1.898218	2.590610	-1.242142
6	1.108571	3.792559	-1.604464

1	1.457935	4.030005	-2.609236
1	1.364566	4.599585	-0.917390
6	-0.347266	3.422303	-1.561942
6	-0.900772	2.658020	-2.599487
6	-1.137658	3.758045	-0.455308
6	-2.225153	2.226820	-2.528658
1	-0.295457	2.413335	-3.469137
6	-2.466003	3.334314	-0.391278
1	-0.708919	4.344602	0.351050
6	-3.009299	2.563620	-1.421914
1	-2.649837	1.644516	-3.340678
1	-3.077747	3.606286	0.462900
1	-4.037684	2.223868	-1.357621
6	4.182811	-1.902104	-0.560676
6	2.940619	-1.684772	-1.188077
6	2.070449	-2.770980	-1.360366
6	2.465633	-4.022001	-0.894292
6	3.704418	-4.204570	-0.252402
6	4.590154	-3.142807	-0.077820
6	4.183331	0.276552	-1.170565
6	2.872222	-0.251574	-1.490045
1	1.110455	-2.649735	-1.849212
1	1.810271	-4.875246	-1.033708
1	3.981461	-5.192016	0.101375
1	5.549737	-3.284556	0.406144
1	2.315478	0.190391	-2.314510
7	4.897812	-0.685348	-0.575025
6	6.232689	-0.564356	0.011016
1	6.166032	-0.763193	1.083841
1	6.902236	-1.289471	-0.457014
1	6.623494	0.438652	-0.142577
6	4.747477	1.621976	-1.470151
1	4.951772	2.180257	-0.548519
1	5.692770	1.523431	-2.013171
1	4.051436	2.200531	-2.071348

CPA

Number of imaginary frequencies : 0 Electronic energy : HF=-1299.2297736
Zero-point correction= 0.289975 (Hartree/Particle)
Thermal correction to Energy= 0.306771
Thermal correction to Enthalpy= 0.307715
Thermal correction to Gibbs Free Energy= 0.246904
Sum of electronic and zero-point Energies= -1298.939798
Sum of electronic and thermal Energies= -1298.923003
Sum of electronic and thermal Enthalpies= -1298.922058
Sum of electronic and thermal Free Energies= -1298.982870

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Cartesian Coordinates

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8	0.637565	1.365597	1.139766
8	-0.583680	1.381547	-1.106146
8	-0.977059	3.319694	0.666844
8	1.210045	3.029844	-0.738680
1	1.149064	3.992815	-0.668559
6	-0.036335	-1.457211	-0.004181
6	1.300260	-0.747430	0.139680
6	1.634880	0.478435	0.705578

6	2.968173	0.874722	0.819535
6	3.980826	0.045179	0.338237
1	5.016476	0.359679	0.425019
6	3.663470	-1.161672	-0.293549
1	4.447073	-1.785432	-0.714470
6	2.328542	-1.540005	-0.397786
6	1.744243	-2.749685	-1.094992
1	1.854654	-3.651474	-0.478110
1	2.232502	-2.957528	-2.052431
6	0.258670	-2.356898	-1.249437
1	-0.418105	-3.213330	-1.313334
1	0.126325	-1.754737	-2.154540
6	-1.347646	-0.704184	-0.142599
6	-1.632319	0.538792	-0.695493
6	-2.945454	1.000147	-0.791062
6	-3.989066	0.206227	-0.314112
1	-5.010110	0.568755	-0.383849
6	-3.721284	-1.023198	0.297374
1	-4.529456	-1.616395	0.716046
6	-2.403448	-1.460599	0.390890
6	-1.861659	-2.695902	1.077728
1	-2.002946	-3.588748	0.454097
1	-2.355815	-2.894209	2.034095
6	-0.362543	-2.355708	1.234770
1	0.283963	-3.235696	1.292700
1	-0.210053	-1.765057	2.144235
15	-0.027858	2.372999	0.055058
1	3.187439	1.840763	1.259911
1	-3.123972	1.986084	-1.204462

E_g

Number of imaginary frequencies : 0 Electronic energy : HF=-2463.8698882
Zero-point correction= 0.813709 (Hartree/Particle)
Thermal correction to Energy= 0.864292
Thermal correction to Enthalpy= 0.865236
Thermal correction to Gibbs Free Energy= 0.726504
Sum of electronic and zero-point Energies= -2463.056179
Sum of electronic and thermal Energies= -2463.005596
Sum of electronic and thermal Enthalpies= -2463.004652
Sum of electronic and thermal Free Energies= -2463.143384

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Cartesian Coordinates

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46	0.592291	-0.505306	0.075210
7	2.352498	-1.769691	0.376611
7	2.097030	0.953034	0.328852
8	5.552093	-0.772496	-0.878977
8	5.464543	0.427875	1.443957
6	2.394906	-3.103810	0.260017
1	1.474427	-3.638778	0.454864
6	3.571466	-3.759622	-0.100503
1	3.588835	-4.842528	-0.154903
6	4.693455	-3.013994	-0.451020
1	5.585464	-3.508114	-0.818667
6	4.635676	-1.616080	-0.372178
6	3.463875	-1.030109	0.157364
6	3.335314	0.398120	0.465030
6	4.400540	1.132154	1.028376

6	4.236543	2.506450	1.237618
1	5.056329	3.098461	1.628868
6	2.983964	3.064769	1.018563
1	2.797448	4.115245	1.210223
6	1.923838	2.250885	0.621761
1	0.920338	2.638604	0.559592
6	7.607102	-0.237377	-1.930698
1	7.400731	0.834506	-1.860360
1	7.201242	-0.602252	-2.877012
1	8.690661	-0.381059	-1.938586
6	6.991876	-0.992984	-0.762384
1	7.205866	-2.062000	-0.870298
6	7.472791	-0.515139	0.617189
1	8.562198	-0.409194	0.583953
1	7.250535	-1.269973	1.379526
6	6.837245	0.796345	1.088102
1	6.791056	1.530796	0.275749
6	7.530183	1.379707	2.310765
1	8.562769	1.646731	2.068468
1	7.541585	0.649932	3.125228
1	7.020915	2.278952	2.666674
6	-2.505798	0.187669	-0.195584
6	-3.613260	-0.097138	-1.141966
6	-4.427629	-1.235832	-1.029386
6	-3.851186	0.793964	-2.206620
6	-5.448176	-1.473568	-1.950093
1	-4.263260	-1.932763	-0.217500
6	-4.868241	0.551821	-3.128606
1	-3.259046	1.701578	-2.288471
6	-5.671111	-0.584857	-3.004459
1	-6.068414	-2.358777	-1.846235
1	-5.044403	1.257187	-3.935147
1	-6.465839	-0.773097	-3.719220
6	-2.644141	0.100202	1.147123
8	-1.623904	0.472575	1.974731
8	-3.746645	-0.389895	1.746341
6	-4.468680	0.524460	2.663088
1	-4.006751	0.465857	3.654498
1	-5.460119	0.071490	2.717957
6	-4.509010	1.939827	2.160431
6	-3.959261	2.978055	2.922192
6	-5.077088	2.227782	0.911057
6	-3.989604	4.293014	2.449895
1	-3.518975	2.762511	3.892503
6	-5.085932	3.535212	0.429591
1	-5.498770	1.425219	0.313989
6	-4.546614	4.570675	1.200027
1	-3.582865	5.095355	3.057939
1	-5.524633	3.748681	-0.540145
1	-4.571283	5.591328	0.830562
6	-0.247977	2.546119	-1.829332
6	-0.972627	2.176231	-0.682127
6	-1.354773	3.153615	0.239815
6	-0.943450	4.470039	0.012024
6	-0.170119	4.807983	-1.110255
6	0.189123	3.845708	-2.061001
6	-0.745953	0.353928	-2.087761
6	-1.249426	0.738099	-0.769731
1	-1.952866	2.896076	1.104775
1	-1.239423	5.244906	0.711268

1	0.135834	5.838325	-1.259381
1	0.758299	4.116081	-2.943636
1	-1.749995	0.056148	2.839656
7	-0.123315	1.404309	-2.649549
6	0.618217	1.420867	-3.906541
1	0.510642	0.468356	-4.420745
1	0.228625	2.216162	-4.546505
1	1.677621	1.606939	-3.706857
6	-0.967563	-0.926645	-2.825093
1	-0.025736	-1.423118	-3.077967
1	-1.571598	-1.599538	-2.222165
1	-1.514498	-0.723597	-3.751815
7	-0.666764	-2.134321	0.138949
6	-1.386647	-3.019554	0.356456
6	-2.299526	-4.071642	0.639574
6	-2.123399	-5.335852	0.044154
6	-3.373888	-3.821947	1.519196
6	-3.030103	-6.349965	0.333224
1	-1.293498	-5.510412	-0.632683
6	-4.268782	-4.850726	1.793329
1	-3.500904	-2.836581	1.956080
6	-4.097747	-6.108563	1.204696
1	-2.906950	-7.327965	-0.119636
1	-5.101149	-4.673832	2.466257
1	-4.801052	-6.905322	1.425279

E_h

Number of imaginary frequencies : 0 Electronic energy : HF=-2463.8609881
Zero-point correction= 0.813289 (Hartree/Particle)
Thermal correction to Energy= 0.864073
Thermal correction to Enthalpy= 0.865017
Thermal correction to Gibbs Free Energy= 0.725105
Sum of electronic and zero-point Energies= -2463.047699
Sum of electronic and thermal Energies= -2462.996915
Sum of electronic and thermal Enthalpies= -2462.995971
Sum of electronic and thermal Free Energies= -2463.135883

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Cartesian Coordinates

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46	-0.180572	-0.301666	-0.258698
7	1.244173	-1.794832	-0.927811
7	1.445246	0.062094	1.057697
8	4.785964	-1.281529	-0.809443
8	4.255450	-2.097906	1.622769
6	1.092952	-2.559193	-2.018278
1	0.076105	-2.747729	-2.340180
6	2.198620	-3.074412	-2.693667
1	2.052361	-3.714011	-3.557050
6	3.480065	-2.710079	-2.288314
1	4.345844	-3.032185	-2.855685
6	3.633790	-1.880670	-1.170400
6	2.477031	-1.511561	-0.449447
6	2.495743	-0.772351	0.817994
6	3.457437	-1.034342	1.814962
6	3.434083	-0.272973	2.990334
1	4.185812	-0.432222	3.755129
6	2.382601	0.611662	3.188272
1	2.296985	1.184455	4.104511

6	1.376340	0.713155	2.227301
1	0.499275	1.318126	2.401588
6	7.108667	-0.856686	-0.996721
1	6.921940	-0.318054	-1.929017
1	8.113546	-1.284535	-1.038910
1	7.073417	-0.139538	-0.171299
6	6.080213	-1.961294	-0.805282
1	6.128271	-2.653825	-1.652624
6	6.238944	-2.746230	0.506430
1	7.299399	-2.985645	0.637606
1	5.703537	-3.700015	0.446077
6	5.712642	-2.016416	1.746263
1	5.993892	-0.956970	1.734588
6	6.146641	-2.681583	3.044495
1	5.712203	-2.182929	3.914545
1	7.235480	-2.645610	3.141795
1	5.830649	-3.728476	3.058721
6	-1.581837	1.642206	0.080049
6	-0.887864	2.592388	1.015291
6	0.388349	3.150049	0.774889
6	-1.549231	2.959129	2.204817
6	0.953360	4.056014	1.666747
1	0.967061	2.844781	-0.083348
6	-0.968746	3.851491	3.106061
1	-2.529025	2.551417	2.419672
6	0.280048	4.414201	2.837838
1	1.932881	4.470148	1.448537
1	-1.504325	4.116877	4.012057
1	0.724359	5.119357	3.533248
6	-1.410585	1.872187	-1.332478
8	-2.184859	1.243197	-2.214194
8	-0.568384	2.763527	-1.771071
6	0.243060	2.577055	-3.019482
1	-0.098974	3.354688	-3.704123
1	0.030014	1.584080	-3.425938
6	1.671357	2.728458	-2.613880
6	2.221700	4.009136	-2.469290
6	2.425985	1.600978	-2.262446
6	3.515712	4.160364	-1.973664
1	1.635200	4.884085	-2.735593
6	3.720875	1.752513	-1.765919
1	2.000162	0.607805	-2.381201
6	4.261641	3.032651	-1.618374
1	3.942429	5.152660	-1.868792
1	4.305849	0.880548	-1.496122
1	5.270527	3.152550	-1.235375
6	-4.472930	-0.178242	1.595715
6	-3.079721	0.074521	1.533186
6	-2.222160	-0.656436	2.372988
6	-2.762332	-1.618523	3.221395
6	-4.150023	-1.858228	3.258296
6	-5.024656	-1.140081	2.446207
6	-4.148565	1.416235	0.032812
6	-2.884288	1.074381	0.509673
1	-1.154503	-0.463807	2.380573
1	-2.108240	-2.181661	3.879565
1	-4.545406	-2.605806	3.938359
1	-6.092942	-1.325999	2.472593
1	-2.086676	1.627601	-3.098585
7	-5.099037	0.653349	0.680849

6	-6.530446	0.614549	0.417957
1	-6.800814	-0.330317	-0.065172
1	-7.085297	0.709542	1.354917
1	-6.817042	1.436011	-0.236418
6	-4.546918	2.479524	-0.940549
1	-4.890895	2.061701	-1.893898
1	-5.354079	3.098346	-0.537068
1	-3.710913	3.150639	-1.142807
7	-1.762058	-1.255571	-1.175912
6	-2.833398	-1.699359	-1.239801
6	-4.154516	-2.217182	-1.290667
6	-5.015156	-1.843730	-2.341921
6	-4.593148	-3.067980	-0.257588
6	-6.315356	-2.336528	-2.357865
1	-4.660067	-1.183557	-3.126110
6	-5.897396	-3.551370	-0.292188
1	-3.927015	-3.317480	0.560543
6	-6.753084	-3.191266	-1.338256
1	-6.986833	-2.063275	-3.165001
1	-6.247272	-4.207663	0.497538
1	-7.767213	-3.577852	-1.360922

TS(A_1-B_1)

Number of imaginary frequencies : 1 Electronic energy : HF=-2248.8025965
Zero-point correction= 0.719539 (Hartree/Particle)
Thermal correction to Energy= 0.764569
Thermal correction to Enthalpy= 0.765513
Thermal correction to Gibbs Free Energy= 0.639016
Sum of electronic and zero-point Energies= -2248.076683
Sum of electronic and thermal Energies= -2248.031653
Sum of electronic and thermal Enthalpies= -2248.030709
Sum of electronic and thermal Free Energies= -2248.157205

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Cartesian Coordinates

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46	1.053536	0.002750	-0.062174
7	0.207831	-1.879977	0.224972
7	-0.941017	0.569278	0.503580
8	-2.966800	-2.698613	1.662884
8	-3.773077	-1.399764	-0.426142
6	0.868811	-3.042910	0.327604
1	1.926996	-3.031686	0.121504
6	0.223751	-4.209304	0.727596
1	0.786587	-5.134267	0.782996
6	-1.105509	-4.158148	1.129948
1	-1.591449	-5.037942	1.535819
6	-1.782197	-2.933401	1.082831
6	-1.120335	-1.813319	0.515965
6	-1.760425	-0.506245	0.370362
6	-3.126050	-0.338046	0.078303
6	-3.684062	0.939778	0.217972
1	-4.744198	1.090538	0.049060
6	-2.845054	2.007136	0.503213
1	-3.232824	3.014496	0.595968
6	-1.465938	1.797111	0.571800
1	-0.785438	2.626844	0.685720
6	-4.840665	-3.436635	2.922684
1	-4.179259	-3.641383	3.767536

1	-5.690817	-4.122026	2.971841
1	-5.214640	-2.413638	3.022028
6	-4.099603	-3.624820	1.607878
1	-3.725264	-4.651915	1.541200
6	-4.940283	-3.307353	0.359809
1	-5.928521	-3.762291	0.484413
1	-4.489643	-3.763327	-0.528611
6	-5.088817	-1.811048	0.070690
1	-5.296493	-1.250223	0.988966
6	-6.129996	-1.510494	-0.996825
1	-5.899159	-2.054127	-1.917565
1	-6.158888	-0.442113	-1.227785
1	-7.123871	-1.813164	-0.655489
6	1.908418	2.894795	0.680702
6	1.189179	3.500191	1.833580
6	1.008602	2.739700	3.000986
6	0.694154	4.812431	1.772802
6	0.341906	3.284951	4.095853
1	1.383385	1.720006	3.043186
6	0.011907	5.344212	2.867057
1	0.841628	5.405551	0.878358
6	-0.161967	4.587003	4.028175
1	0.210386	2.694713	4.997106
1	-0.368976	6.359337	2.817477
1	-0.684234	5.011554	4.879601
6	1.540480	2.915184	-0.747114
8	2.074664	2.181038	-1.587321
8	0.563943	3.772866	-1.009082
6	0.075837	3.867561	-2.402754
1	0.902988	3.605625	-3.063249
1	-0.163127	4.924979	-2.512845
6	-1.128799	2.994427	-2.621322
6	-0.983318	1.606702	-2.778029
6	-2.407987	3.557542	-2.693586
6	-2.098277	0.799280	-2.995482
1	0.009954	1.172067	-2.745173
6	-3.524335	2.751318	-2.929582
1	-2.531211	4.631722	-2.584769
6	-3.371399	1.372007	-3.077892
1	-1.978816	-0.273550	-3.116659
1	-4.508760	3.202662	-3.005427
1	-4.236866	0.743647	-3.265449
7	3.132218	2.437758	0.919731
7	4.173947	2.063197	1.166368
6	4.038701	-2.623261	-0.636574
6	3.792499	-1.460116	0.115238
6	4.252806	-1.391327	1.431561
6	4.941576	-2.489859	1.953664
6	5.169908	-3.639175	1.182487
6	4.719231	-3.727706	-0.140219
6	2.927059	-1.225495	-2.027079
6	3.022568	-0.543775	-0.737279
1	4.090672	-0.501767	2.030166
1	5.315170	-2.451673	2.971488
1	5.714912	-4.472671	1.612755
1	4.908141	-4.611895	-0.739138
1	3.307035	0.504646	-0.818347
7	3.474641	-2.432319	-1.932708
6	3.559993	-3.454961	-2.976243
1	4.609442	-3.628902	-3.226705

1	3.120730	-4.383826	-2.604578
1	3.020595	-3.132806	-3.864275
6	2.346417	-0.665555	-3.278767
1	3.019842	-0.812535	-4.128786
1	1.392631	-1.149310	-3.521272
1	2.172812	0.402100	-3.147436

$TS(A\text{-}B)_R$

Number of imaginary frequencies : 1 Electronic energy : HF=-2130.8222546
Zero-point correction= 0.633138 (Hartree/Particle)
Thermal correction to Energy= 0.674532
Thermal correction to Enthalpy= 0.675477
Thermal correction to Gibbs Free Energy= 0.556030
Sum of electronic and zero-point Energies= -2130.189117
Sum of electronic and thermal Energies= -2130.147722
Sum of electronic and thermal Enthalpies= -2130.146778
Sum of electronic and thermal Free Energies= -2130.266225

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Cartesian Coordinates

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46	-0.551736	0.042858	0.327313
7	0.633902	-1.643803	-0.138961
7	1.273845	0.780670	0.804149
8	4.099640	-1.541186	-0.981358
8	4.296739	-0.966899	1.524524
6	0.210312	-2.759181	-0.747420
1	-0.858169	-2.928353	-0.774353
6	1.122578	-3.643081	-1.324032
1	0.763458	-4.557237	-1.783473
6	2.470669	-3.303836	-1.373426
1	3.172429	-3.931945	-1.910422
6	2.901490	-2.105080	-0.785028
6	1.956411	-1.345052	-0.054556
6	2.276558	-0.136700	0.699792
6	3.512403	0.098638	1.338079
6	3.780239	1.390433	1.815440
1	4.743943	1.614173	2.259209
6	2.777967	2.351724	1.760735
1	2.946929	3.357055	2.129273
6	1.506560	2.003111	1.300756
1	0.680663	2.704883	1.302755
6	6.243159	-1.571935	-2.006904
1	5.763780	-1.571621	-2.988605
1	7.204642	-2.085126	-2.090541
1	6.429914	-0.534307	-1.715153
6	5.366541	-2.278114	-0.984319
1	5.183638	-3.309664	-1.302949
6	5.940943	-2.277834	0.442810
1	7.010424	-2.505057	0.384981
1	5.479422	-3.071862	1.039616
6	5.731042	-0.966054	1.204406
1	5.931705	-0.097195	0.567267
6	6.531544	-0.897307	2.495808
1	7.602539	-0.911628	2.274857
1	6.297290	-1.752579	3.135690
1	6.312574	0.016604	3.053849
6	-1.104616	2.195941	-1.267193
6	0.248970	2.478054	-1.815775

6	0.918337	1.484812	-2.552225
6	0.878211	3.708965	-1.576988
6	2.203980	1.714422	-3.032007
1	0.437513	0.527303	-2.737663
6	2.171286	3.926551	-2.056593
1	0.367813	4.482827	-1.018178
6	2.837400	2.936104	-2.779643
1	2.712675	0.941884	-3.599977
1	2.651280	4.882554	-1.872998
1	3.839433	3.117086	-3.155196
6	-1.737003	2.884492	-0.120088
8	-3.032157	2.546502	0.013092
8	-1.115705	3.598866	0.647132
6	-3.579262	2.650185	1.370967
1	-4.656346	2.729516	1.229752
1	-3.199498	3.561266	1.836418
6	-3.190641	1.401384	2.123767
6	-4.123512	0.400490	2.389426
6	-1.846207	1.204084	2.520511
6	-3.737868	-0.780011	3.040113
1	-5.161693	0.541021	2.102015
6	-1.460411	0.009485	3.155154
1	-1.151118	2.033405	2.459913
6	-2.408428	-0.988310	3.406514
1	-4.486884	-1.531440	3.271095
1	-0.438779	-0.107385	3.504081
1	-2.117125	-1.900036	3.917797
7	-2.318576	-0.794691	-0.188321
6	-3.385153	-1.189963	-0.423154
6	-4.686951	-1.678698	-0.705128
6	-5.299197	-2.569022	0.201613
6	-5.347648	-1.264901	-1.879975
6	-6.577098	-3.039551	-0.075870
1	-4.773650	-2.875926	1.099145
6	-6.626489	-1.746639	-2.136933
1	-4.861455	-0.583175	-2.569141
6	-7.238211	-2.629178	-1.239697
1	-7.059844	-3.726204	0.611342
1	-7.147321	-1.436458	-3.036486
1	-8.236351	-3.000761	-1.448874
7	-1.969783	1.587291	-2.095719
7	-2.679323	1.045975	-2.785744

$TS(A-B)_S$

Number of imaginary frequencies : 1 Electronic energy : HF=-2130.8223243
Zero-point correction= 0.633264 (Hartree/Particle)
Thermal correction to Energy= 0.674637
Thermal correction to Enthalpy= 0.675581
Thermal correction to Gibbs Free Energy= 0.556689
Sum of electronic and zero-point Energies= -2130.189061
Sum of electronic and thermal Energies= -2130.147687
Sum of electronic and thermal Enthalpies= -2130.146743
Sum of electronic and thermal Free Energies= -2130.265635

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Cartesian Coordinates

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46	0.325370	-0.436932	0.387571
7	-1.453158	-1.104698	-0.289272

7	-0.903786	1.138816	1.049002
8	-4.750814	-0.158255	0.689194
8	-4.028523	2.065848	-0.399473
6	-1.638736	-2.305716	-0.851725
1	-0.751030	-2.878909	-1.084845
6	-2.925864	-2.788945	-1.084983
1	-3.052207	-3.753923	-1.562467
6	-4.024081	-2.068478	-0.631876
1	-5.022598	-2.481305	-0.719828
6	-3.823278	-0.830808	0.002082
6	-2.509351	-0.309460	0.047430
6	-2.159837	1.018938	0.543600
6	-2.992451	2.154935	0.441042
6	-2.606589	3.320819	1.119065
1	-3.253435	4.190880	1.108133
6	-1.360825	3.366520	1.737165
1	-1.026874	4.261818	2.249653
6	-0.497543	2.274624	1.628922
1	0.519422	2.299258	1.998068
6	-6.964025	-0.005607	1.545063
1	-6.804245	-0.933637	2.098634
1	-8.027411	0.077720	1.305906
1	-6.688924	0.831684	2.192915
6	-6.145299	0.001321	0.263756
1	-6.430851	-0.849296	-0.363823
6	-6.262185	1.301187	-0.550663
1	-7.313796	1.605404	-0.565134
1	-5.967632	1.127744	-1.591317
6	-5.398377	2.452065	-0.026723
1	-5.440692	2.519548	1.066088
6	-5.738119	3.785659	-0.674342
1	-5.067616	4.578982	-0.334474
1	-6.761283	4.076074	-0.419679
1	-5.658620	3.712735	-1.762588
6	1.611316	-0.561373	-2.019229
6	2.049347	0.856340	-2.121808
6	3.412262	1.188928	-2.130433
6	1.084856	1.877319	-2.192824
6	3.796229	2.529170	-2.184693
1	4.162315	0.410763	-2.088739
6	1.478488	3.210363	-2.262632
1	0.026199	1.628958	-2.187700
6	2.837537	3.541427	-2.250837
1	4.852634	2.777969	-2.186792
1	0.727008	3.990965	-2.327282
1	3.144770	4.580911	-2.303732
6	2.438718	-1.697397	-1.549780
8	3.485683	-1.560268	-0.948321
8	1.834002	-2.879448	-1.799793
6	2.209315	-3.993384	-0.918744
1	3.273474	-3.919659	-0.690078
1	2.017626	-4.891699	-1.504443
6	1.331796	-3.898577	0.303406
6	1.546886	-2.856789	1.233776
6	0.247884	-4.755983	0.487139
6	0.663059	-2.676428	2.312626
1	2.460770	-2.275956	1.176051
6	-0.627568	-4.577900	1.569627
1	0.081852	-5.572739	-0.210285
6	-0.434455	-3.532163	2.470816

1	0.869737	-1.910542	3.054086
1	-1.455833	-5.266115	1.707057
1	-1.107262	-3.403745	3.312473
7	2.074959	0.321445	1.087123
6	3.158244	0.722218	1.210735
6	4.491148	1.183761	1.351800
6	5.526518	0.456417	0.727546
6	4.758783	2.353443	2.090885
6	6.833011	0.915534	0.851466
1	5.290268	-0.437532	0.162545
6	6.072809	2.792887	2.200695
1	3.950158	2.897980	2.566966
6	7.105196	2.076964	1.583366
1	7.641864	0.367475	0.379926
1	6.295586	3.690202	2.768009
1	8.128870	2.425950	1.675784
7	0.577533	-0.915954	-2.803212
7	-0.319966	-1.190051	-3.429997

TS_{dimer}

Number of imaginary frequencies : 1 Electronic energy : HF=-2860.1292859
Zero-point correction= 0.865487 (Hartree/Particle)
Thermal correction to Energy= 0.921960
Thermal correction to Enthalpy= 0.922904
Thermal correction to Gibbs Free Energy= 0.768612
Sum of electronic and zero-point Energies= -2859.263799
Sum of electronic and thermal Energies= -2859.207326
Sum of electronic and thermal Enthalpies= -2859.206382
Sum of electronic and thermal Free Energies= -2859.360674

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Cartesian Coordinates

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6	0.830840	1.211235	0.191786
6	0.739006	0.784464	1.635254
8	0.515291	1.562114	2.542147
6	1.141293	2.584610	-0.171827
6	0.800552	3.051609	-1.468849
6	1.784092	3.487629	0.718224
6	1.097783	4.350607	-1.863978
1	0.278006	2.390317	-2.153113
6	2.059911	4.788331	0.319320
1	2.048110	3.158079	1.713696
6	1.727519	5.222445	-0.970792
1	0.829139	4.688460	-2.859491
1	2.535893	5.471957	1.015251
1	1.949852	6.241042	-1.273787
8	0.746208	-0.548741	1.741109
6	0.347976	-1.152532	3.007721
1	-0.229770	-0.416023	3.571915
1	1.255857	-1.385608	3.569533
6	2.786508	0.209330	-0.354410
6	3.689512	1.243229	0.321582
8	3.806860	1.258555	1.525770
8	4.241006	2.057757	-0.559607
6	5.212681	3.066102	-0.039909
1	5.164862	3.847615	-0.797857
1	4.819257	3.436219	0.907223
7	2.632274	0.476457	-1.684523

7	2.402355	0.796171	-2.733755
6	3.118985	-1.223385	-0.059558
6	3.344227	-2.137138	-1.104407
6	3.743283	-3.442080	-0.829291
6	3.923170	-3.857196	0.490844
6	3.719006	-2.949088	1.531592
6	3.329889	-1.638020	1.266119
1	3.215478	-0.933083	2.075929
1	3.881898	-3.254641	2.560354
1	4.235949	-4.873959	0.705035
1	3.912724	-4.131984	-1.649420
1	3.227436	-1.837575	-2.141471
6	6.575381	2.460711	0.091457
6	7.441653	2.436241	-1.009829
6	6.982725	1.894057	1.307434
6	8.702961	1.853011	-0.897426
1	7.131418	2.882657	-1.951390
6	8.245099	1.311983	1.418471
1	6.308000	1.910029	2.157843
6	9.104771	1.290982	0.317299
1	9.374662	1.844892	-1.750099
1	8.561733	0.883034	2.364109
1	10.090359	0.844603	0.407368
46	-0.836641	0.385988	-0.670529
7	-2.750870	-0.415610	-1.310362
7	-2.150649	1.795715	0.210862
8	-5.778791	0.066332	0.532852
8	-5.572209	2.353008	-0.680634
6	-2.974165	-1.585295	-1.925125
1	-2.140615	-2.027015	-2.453754
6	-4.221619	-2.204400	-1.881865
1	-4.379935	-3.135382	-2.414667
6	-5.229251	-1.654012	-1.095772
1	-6.173695	-2.171773	-0.973222
6	-4.989133	-0.447891	-0.424158
6	-3.757032	0.210437	-0.657042
6	-3.447677	1.542505	-0.122982
6	-4.430303	2.548730	-0.006243
6	-4.121659	3.709876	0.712051
1	-4.874654	4.476480	0.858070
6	-2.826798	3.871765	1.187579
1	-2.544187	4.752570	1.752772
6	-1.852746	2.924794	0.875013
1	-0.827174	3.068931	1.173954
6	-7.722423	0.096165	1.889724
1	-7.349138	-0.781019	2.423086
1	-8.815137	0.081332	1.915899
1	-7.375255	0.988866	2.417719
6	-7.237776	0.087045	0.447778
1	-7.586833	-0.826247	-0.046343
6	-7.678106	1.309826	-0.373015
1	-8.743596	1.483720	-0.189585
1	-7.568390	1.107729	-1.444203
6	-6.884898	2.584484	-0.071829
1	-6.741262	2.714301	1.006955
6	-7.502804	3.828811	-0.691209
1	-6.879660	4.709497	-0.515091
1	-8.489878	4.016188	-0.259068
1	-7.614451	3.700844	-1.771610
7	0.146744	-1.231914	-1.432498

6	0.302251	-2.378826	-1.538199
6	0.486198	-3.782117	-1.609696
6	0.643924	-4.427779	-2.851561
6	0.518668	-4.499136	-0.397963
6	0.838921	-5.804489	-2.870372
1	0.619086	-3.856387	-3.773788
6	0.707753	-5.875292	-0.441223
1	0.408942	-3.977315	0.544535
6	0.869829	-6.524885	-1.669633
1	0.965231	-6.318434	-3.817326
1	0.729029	-6.439379	0.485041
1	1.020763	-7.599642	-1.694459
6	-0.448706	-2.387089	2.681135
6	-0.073454	-3.638748	3.179631
6	-1.593333	-2.286426	1.875900
6	-0.837992	-4.773594	2.888823
1	0.811396	-3.727840	3.804050
6	-2.343178	-3.419467	1.566541
1	-1.897158	-1.314782	1.496258
6	-1.968774	-4.667068	2.077358
1	-0.548651	-5.737301	3.296675
1	-3.224780	-3.328559	0.938613
1	-2.558519	-5.549158	1.848231

$TS(E_a\text{-}P)_{CPA}$

Number of imaginary frequencies : 1 Electronic energy : HF=-3763.1340553
Zero-point correction= 1.099504 (Hartree/Particle)
Thermal correction to Energy= 1.167534
Thermal correction to Enthalpy= 1.168478
Thermal correction to Gibbs Free Energy= 0.990251
Sum of electronic and zero-point Energies= -3762.034551
Sum of electronic and thermal Energies= -3761.966521
Sum of electronic and thermal Enthalpies= -3761.965577
Sum of electronic and thermal Free Energies= -3762.143805

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Cartesian Coordinates

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6	2.375479	-1.470984	-0.964305
6	1.141140	-2.131270	-1.354975
6	0.711105	-3.325590	-0.707262
6	0.259349	-1.523545	-2.300140
6	-0.529064	-3.854974	-0.948457
1	1.407164	-3.826915	-0.043758
6	-1.001884	-2.016068	-2.503079
1	0.589144	-0.637240	-2.829336
6	-1.490668	-3.157141	-1.762763
1	-0.814630	-4.802647	-0.502728
1	-1.652686	-1.523346	-3.217434
1	-2.282374	-3.765458	-2.199076
6	3.303847	-0.940259	-2.002290
8	4.233186	-0.167171	-1.731476
8	3.068069	-1.357816	-3.238459
6	4.057982	-0.983245	-4.267990
1	4.242669	0.090308	-4.202069
1	3.537182	-1.215736	-5.197577
6	5.313888	-1.792004	-4.092540
6	6.488764	-1.198285	-3.617949
6	5.293141	-3.169578	-4.350886

6	7.632561	-1.970530	-3.409850
1	6.499829	-0.135034	-3.399803
6	6.432185	-3.944070	-4.132341
1	4.382810	-3.633265	-4.722503
6	7.603920	-3.344174	-3.661725
1	8.544059	-1.501523	-3.051919
1	6.411424	-5.009580	-4.339770
1	8.494192	-3.944698	-3.501314
6	3.378803	-1.989138	2.585461
6	2.412175	-1.614097	1.617022
6	1.175291	-1.103907	2.044977
6	0.936245	-0.982172	3.411225
6	1.904627	-1.368375	4.358009
6	3.137776	-1.879554	3.958773
6	4.287699	-2.349177	0.546659
6	3.009908	-1.840088	0.321517
1	0.425419	-0.804531	1.320838
1	-0.014932	-0.588369	3.758285
1	1.688206	-1.268770	5.416558
1	3.882346	-2.170525	4.692259
7	4.509581	-2.423095	1.907854
6	5.720999	-2.892115	2.564877
1	5.934134	-2.256645	3.427422
1	5.616573	-3.928781	2.903351
1	6.565747	-2.825620	1.880356
6	5.315233	-2.789449	-0.445383
1	6.095072	-2.034354	-0.593740
1	5.798245	-3.720421	-0.135201
1	4.861364	-2.969489	-1.420929
8	2.146836	2.494912	1.573376
8	2.565235	3.083123	-0.909516
8	3.903899	1.246956	0.390794
8	1.445394	0.907686	-0.398007
1	1.843831	-0.236066	-0.637178
6	1.931455	5.536438	0.905281
6	0.850361	4.532847	1.274161
6	0.916256	3.197148	1.648159
6	-0.216046	2.486953	2.043667
6	-1.453857	3.129468	2.045817
1	-2.338797	2.581456	2.352077
6	-1.562290	4.456831	1.617628
1	-2.531903	4.945180	1.577470
6	-0.416089	5.142745	1.226756
6	-0.297329	6.543918	0.669298
1	-0.352895	7.288260	1.473720
1	-1.095012	6.782681	-0.040603
6	1.103116	6.525122	0.018651
1	1.568471	7.511303	-0.046078
1	1.036462	6.118139	-0.995897
6	3.231238	5.125949	0.233702
6	3.531557	4.093804	-0.643507
6	4.789350	3.965803	-1.227692
6	5.780235	4.897325	-0.914162
1	6.762541	4.806322	-1.366416
6	5.525583	5.914896	0.011527
1	6.312290	6.608802	0.291810
6	4.261847	6.013472	0.586945
6	3.779194	6.971490	1.653695
1	3.563858	7.958667	1.225459
1	4.518584	7.123403	2.445342

6	2.490911	6.285415	2.160970
1	1.763899	6.980666	2.588126
1	2.741748	5.546642	2.929482
1	4.171421	0.636492	-0.375044
15	2.498094	1.879087	0.143379
1	-0.104383	1.447862	2.328393
1	4.980141	3.132905	-1.895970
46	-2.838023	-2.050794	-0.363223
7	-4.084151	-0.719099	0.773175
7	-4.211355	-1.474548	-1.851179
8	-5.962905	1.971931	-0.648014
8	-7.451757	-0.066284	-1.281057
6	-3.852520	-0.289728	2.019502
1	-3.160666	-0.873591	2.613690
6	-4.471383	0.859807	2.510007
1	-4.299041	1.168283	3.535323
6	-5.247302	1.637251	1.655326
1	-5.657073	2.581266	1.995737
6	-5.441965	1.215264	0.333065
6	-4.929219	-0.047893	-0.042871
6	-5.191108	-0.677252	-1.344582
6	-6.435192	-0.559260	-2.002559
6	-6.559204	-1.062697	-3.302495
1	-7.489552	-0.942005	-3.845978
6	-5.497936	-1.777889	-3.846009
1	-5.564176	-2.206451	-4.839684
6	-4.363409	-2.013046	-3.072106
1	-3.568067	-2.648244	-3.437809
6	-6.959136	3.951812	-1.485736
1	-6.015934	4.478133	-1.322145
1	-7.779827	4.667970	-1.393312
1	-6.956422	3.557801	-2.506064
6	-7.126710	2.834284	-0.466874
1	-7.113043	3.258683	0.543093
6	-8.408265	2.004658	-0.651124
1	-9.243678	2.692204	-0.820087
1	-8.635077	1.447465	0.264469
6	-8.337617	0.983485	-1.790238
1	-7.872091	1.415947	-2.683379
6	-9.692239	0.375250	-2.122050
1	-9.604588	-0.396881	-2.890702
1	-10.373094	1.147619	-2.491017
1	-10.132882	-0.080303	-1.230775
7	-1.842047	-2.721031	1.314484
6	-1.400851	-3.351822	2.185652
6	-0.870892	-4.158929	3.228596
6	0.524144	-4.296625	3.364163
6	-1.757026	-4.826641	4.098808
6	1.023002	-5.109841	4.375481
1	1.190187	-3.760212	2.699710
6	-1.236294	-5.633672	5.103678
1	-2.829281	-4.711601	3.978861
6	0.149429	-5.775157	5.241118
1	2.095977	-5.215697	4.493830
1	-1.907287	-6.153384	5.779273
1	0.548397	-6.406286	6.029068

$TS(E_{free}\text{-}P)_{CPA}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2471.0458639
Zero-point correction= 0.704935 (Hartree/Particle)
Thermal correction to Energy= 0.746524
Thermal correction to Enthalpy= 0.747468
Thermal correction to Gibbs Free Energy= 0.627487
Sum of electronic and zero-point Energies= -2470.325706
Sum of electronic and thermal Energies= -2470.284117
Sum of electronic and thermal Enthalpies= -2470.283173
Sum of electronic and thermal Free Energies= -2470.403154

Cartesian Coordinates

6	2.144332	0.785878	0.586496
6	2.758316	1.797953	1.516811
6	3.692073	2.734687	1.053432
6	2.366409	1.854009	2.863828
6	4.232876	3.689527	1.915411
1	3.983668	2.713045	0.007949
6	2.910357	2.802630	3.727569
1	1.623439	1.149707	3.227328
6	3.847788	3.725914	3.256764
1	4.955426	4.407550	1.536680
1	2.592688	2.829892	4.766423
1	4.265897	4.471725	3.927026
6	2.347607	-0.590951	0.884961
8	1.812001	-1.579033	0.238439
8	3.084610	-0.915250	1.942388
6	3.344776	-2.326090	2.191640
1	2.407392	-2.885491	2.171670
1	3.748141	-2.325875	3.206178
6	4.340275	-2.858991	1.191182
6	3.975424	-3.834510	0.258758
6	5.633885	-2.322025	1.153494
6	4.894811	-4.279540	-0.692626
1	2.962719	-4.225983	0.265212
6	6.550385	-2.757776	0.197128
1	5.912172	-1.549795	1.865821
6	6.182092	-3.739928	-0.726646
1	4.602355	-5.037744	-1.413228
1	7.549939	-2.333627	0.172467
1	6.895721	-4.080999	-1.471141
6	1.458712	2.237025	-2.791986
6	1.289111	2.245239	-1.383266
6	0.504429	3.246726	-0.791230
6	-0.088859	4.204379	-1.607677
6	0.081436	4.174594	-3.006579
6	0.858696	3.194587	-3.617190
6	2.686941	0.543984	-1.933128
6	2.061781	1.148758	-0.857563
1	0.370209	3.265942	0.284959
1	-0.689704	4.992651	-1.162392
1	-0.393659	4.935332	-3.619179
1	1.000798	3.187421	-4.693490
7	2.290626	1.177744	-3.108870
6	2.715819	0.840837	-4.451402
1	3.604273	1.407250	-4.759791
1	2.938438	-0.225483	-4.517973
1	1.905578	1.056014	-5.152394
6	3.652822	-0.597029	-1.950090
1	3.162428	-1.560644	-2.135165

1	4.428022	-0.457560	-2.709892
1	4.156298	-0.681921	-0.984470
8	-2.309560	0.509087	-0.788489
8	-1.997543	-1.198793	1.100279
8	-0.284498	-0.985943	-0.865554
8	-0.456724	0.762517	1.053036
1	0.742505	0.782345	0.892931
6	-4.943620	-0.781219	0.259626
6	-4.411913	0.634713	0.416936
6	-3.277974	1.254976	-0.098562
6	-3.054803	2.618428	0.091717
6	-3.967423	3.368494	0.833692
1	-3.788230	4.428925	0.984932
6	-5.079516	2.754001	1.418773
1	-5.763016	3.326835	2.039568
6	-5.285555	1.393033	1.213948
6	-6.365953	0.505544	1.794009
1	-7.314986	0.635563	1.256581
1	-6.565593	0.722600	2.848362
6	-5.787468	-0.908927	1.570606
1	-6.549919	-1.689895	1.500763
1	-5.113907	-1.168258	2.394291
6	-4.032025	-1.978116	0.051032
6	-2.730333	-2.215791	0.477564
6	-2.111756	-3.443716	0.236398
6	-2.802485	-4.441900	-0.450984
1	-2.316987	-5.394476	-0.641614
6	-4.092281	-4.202797	-0.938052
1	-4.610395	-4.961184	-1.518523
6	-4.689195	-2.969165	-0.695562
6	-6.023057	-2.449162	-1.187519
1	-6.849491	-2.850191	-0.585445
1	-6.223411	-2.726379	-2.227481
6	-5.876389	-0.923772	-0.988664
1	-6.829732	-0.404323	-0.857589
1	-5.369436	-0.484325	-1.854180
1	0.953551	-1.297454	-0.347967
15	-1.161413	-0.216007	0.095672
1	-2.159603	3.057781	-0.330631
1	-1.086360	-3.580824	0.561348

$TS(B_1\text{-}C_1)$

Number of imaginary frequencies : 1 Electronic energy : HF=-2248.8121807
Zero-point correction= 0.718721 (Hartree/Particle)
Thermal correction to Energy= 0.763931
Thermal correction to Enthalpy= 0.764875
Thermal correction to Gibbs Free Energy= 0.640977
Sum of electronic and zero-point Energies= -2248.093445
Sum of electronic and thermal Energies= -2248.048236
Sum of electronic and thermal Enthalpies= -2248.047291
Sum of electronic and thermal Free Energies= -2248.171190

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Cartesian Coordinates

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46	-0.979191	-0.023347	-0.410065
7	0.533589	-1.529921	-0.649303
7	0.801570	1.195234	-0.951678
8	3.884910	-1.139510	-1.879325

8	4.005424	0.240197	0.332522
6	0.325912	-2.840164	-0.856328
1	-0.681653	-3.203332	-0.727122
6	1.348274	-3.692861	-1.262809
1	1.139553	-4.746912	-1.408823
6	2.602718	-3.169660	-1.552099
1	3.385988	-3.803691	-1.951517
6	2.811109	-1.793256	-1.405251
6	1.765392	-1.004449	-0.863817
6	1.903497	0.447248	-0.686753
6	3.106691	1.045328	-0.261558
6	3.242750	2.433086	-0.379811
1	4.174604	2.915972	-0.106001
6	2.143018	3.173675	-0.799327
1	2.202564	4.251621	-0.899785
6	0.923452	2.529673	-1.013774
1	0.027930	3.092732	-1.227066
6	6.015704	-1.099293	-2.926466
1	5.556450	-1.450947	-3.853027
1	7.051009	-1.448783	-2.896140
1	6.019680	-0.005694	-2.942433
6	5.253264	-1.629441	-1.721786
1	5.252752	-2.724638	-1.744243
6	5.801729	-1.151324	-0.367359
1	6.891288	-1.261207	-0.377192
1	5.425142	-1.787787	0.441221
6	5.429561	0.291536	-0.016503
1	5.541320	0.948180	-0.886373
6	6.200014	0.836638	1.175705
1	7.267577	0.891922	0.945088
1	6.067430	0.186585	2.045569
1	5.854025	1.838984	1.441890
6	-2.291304	1.614678	-0.364428
6	-2.279999	2.563396	-1.501750
6	-2.017637	2.087073	-2.802688
6	-2.560286	3.932302	-1.308089
6	-2.010083	2.964243	-3.881527
1	-1.811475	1.031778	-2.955518
6	-2.538517	4.806676	-2.390627
1	-2.769972	4.310669	-0.313668
6	-2.265673	4.324841	-3.675555
1	-1.804335	2.593629	-4.880267
1	-2.742904	5.861081	-2.236449
1	-2.256632	5.009640	-4.517768
6	-2.238047	2.073972	1.079460
8	-2.950515	1.622030	1.955011
8	-1.244188	2.944354	1.241974
6	-0.888445	3.282774	2.632014
1	-1.806432	3.467969	3.191988
1	-0.334228	4.215718	2.515938
6	-0.051165	2.198905	3.259590
6	-0.359184	1.704247	4.531408
6	1.073356	1.706424	2.584254
6	0.459018	0.739265	5.126017
1	-1.231463	2.076831	5.061123
6	1.880343	0.729098	3.165829
1	1.321798	2.108593	1.610586
6	1.575704	0.248785	4.444743
1	0.224524	0.374712	6.121330
1	2.753092	0.363376	2.632024

1	2.213097	-0.495074	4.913474
7	-3.901150	1.083402	-0.412389
7	-4.910984	0.769083	-0.742342
6	-2.667147	-3.567788	0.372999
6	-3.018591	-2.351638	-0.237612
6	-3.747409	-2.385536	-1.427114
6	-4.111707	-3.625875	-1.957493
6	-3.749058	-4.823475	-1.323385
6	-3.009539	-4.815143	-0.137559
6	-1.800075	-1.956331	1.704987
6	-2.444340	-1.261782	0.587340
1	-4.022777	-1.472378	-1.943615
1	-4.685460	-3.665396	-2.877493
1	-4.047764	-5.771690	-1.757336
1	-2.729012	-5.739551	0.355375
7	-1.915100	-3.269113	1.545473
6	-1.378397	-4.319729	2.410235
1	-2.201820	-4.912527	2.815559
1	-0.724652	-4.967432	1.820679
1	-0.807476	-3.879809	3.224793
6	-1.166186	-1.302830	2.877110
1	-1.449527	-1.785891	3.815973
1	-0.073436	-1.324696	2.801056
1	-1.464706	-0.255492	2.917366
1	-3.114113	-0.500183	0.982659

$TS(E_{free}-P)_{2wat}$

Number of imaginary frequencies : 1 Electronic energy : HF=-1324.6535186
Zero-point correction= 0.465734 (Hartree/Particle)
Thermal correction to Energy= 0.493207
Thermal correction to Enthalpy= 0.494151
Thermal correction to Gibbs Free Energy= 0.407145
Sum of electronic and zero-point Energies= -1324.181272
Sum of electronic and thermal Energies= -1324.153799
Sum of electronic and thermal Enthalpies= -1324.152855
Sum of electronic and thermal Free Energies= -1324.239861

Cartesian Coordinates

6	-0.081081	0.616808	-0.580458
6	0.058496	2.076712	-0.296388
6	-1.060352	2.925062	-0.384210
6	1.268943	2.648514	0.144178
6	-0.971437	4.280577	-0.066741
1	-2.009544	2.507162	-0.704322
6	1.360579	4.002829	0.454050
1	2.145024	2.017650	0.242274
6	0.240289	4.832164	0.350707
1	-1.855712	4.907549	-0.148464
1	2.310503	4.411897	0.789590
1	0.310682	5.887311	0.599199
6	0.858910	-0.119595	-1.353502
8	0.788983	-1.357448	-1.613456
8	1.976863	0.558510	-1.759106
6	3.147356	-0.257921	-1.971998
1	3.879408	0.430441	-2.400985
1	2.930923	-1.053349	-2.688359
6	3.630587	-0.823207	-0.654479

6	4.213708	0.026611	0.296224
6	3.396446	-2.161696	-0.314342
6	4.549559	-0.448413	1.566774
1	4.391484	1.068045	0.041529
6	3.738582	-2.643544	0.951440
1	2.905978	-2.808974	-1.032865
6	4.311085	-1.787377	1.897242
1	4.993936	0.222232	2.296272
1	3.540088	-3.680418	1.205432
1	4.565950	-2.157926	2.885684
6	-3.418076	-0.846827	0.328382
6	-2.229714	-0.158519	0.702011
6	-2.040498	0.192767	2.050084
6	-3.018950	-0.143728	2.978724
6	-4.190959	-0.822516	2.587737
6	-4.408619	-1.179865	1.259850
6	-2.178034	-0.522314	-1.534082
6	-1.442480	0.022789	-0.496991
1	-1.144242	0.723952	2.352073
1	-2.883827	0.125500	4.022252
1	-4.941849	-1.066233	3.333740
1	-5.320240	-1.689128	0.962478
1	0.633511	-0.038720	0.766327
7	-3.355745	-1.080492	-1.034464
6	-4.410464	-1.700020	-1.810108
1	-3.994573	-2.153445	-2.711336
1	-4.879648	-2.492910	-1.221492
1	-5.184873	-0.979658	-2.103408
6	-1.826696	-0.586866	-2.982929
1	-1.368650	-1.547731	-3.247862
1	-2.697119	-0.421646	-3.626046
1	-1.089036	0.186748	-3.205802
8	0.963058	-0.679870	1.580397
8	-0.032534	-2.573844	0.452216
1	0.199775	-2.188524	-0.476455
1	0.544791	-1.655974	1.167986
1	-0.981667	-2.402441	0.564439
1	1.935102	-0.701280	1.571925

TS(C_R-C_S)

Number of imaginary frequencies : 1 Electronic energy : HF=-2021.2952382
Zero-point correction= 0.623459 (Hartree/Particle)
Thermal correction to Energy= 0.662936
Thermal correction to Enthalpy= 0.663880
Thermal correction to Gibbs Free Energy= 0.546451
Sum of electronic and zero-point Energies= -2020.671779
Sum of electronic and thermal Energies= -2020.632302
Sum of electronic and thermal Enthalpies= -2020.631358
Sum of electronic and thermal Free Energies= -2020.748787

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Cartesian Coordinates

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46	-0.348346	0.216008	-0.455911
7	-2.023150	1.500301	-0.224776
7	-1.932724	-1.132906	-0.690568
8	-5.520720	0.793704	-0.465401
8	-4.934588	-1.027045	1.226247
6	-2.003372	2.839750	-0.220116

1	-1.036908	3.316376	-0.306718
6	-3.181885	3.578466	-0.125675
1	-3.136206	4.661477	-0.107680
6	-4.403532	2.917684	-0.137231
1	-5.330767	3.478694	-0.166941
6	-4.427443	1.516168	-0.191540
6	-3.193324	0.822661	-0.113354
6	-3.075500	-0.635729	-0.131314
6	-4.080160	-1.518424	0.326935
6	-4.061103	-2.842745	-0.132211
1	-4.856802	-3.526169	0.143077
6	-2.999122	-3.259531	-0.927409
1	-2.966105	-4.263059	-1.335956
6	-1.923836	-2.397085	-1.137327
1	-1.055759	-2.699530	-1.698554
6	-7.843621	0.788824	-0.988799
1	-7.646574	1.443303	-1.840956
1	-8.856562	0.983628	-0.626751
1	-7.794193	-0.247591	-1.335364
6	-6.838348	1.041912	0.123941
1	-6.898179	2.085680	0.449381
6	-7.003654	0.116303	1.342552
1	-8.071505	0.016256	1.562713
1	-6.535642	0.561414	2.227055
6	-6.382101	-1.269896	1.154968
1	-6.607271	-1.672864	0.160927
6	-6.771670	-2.253065	2.247547
1	-6.256051	-3.209081	2.123872
1	-7.848830	-2.439844	2.218764
1	-6.514522	-1.851410	3.231608
6	1.343421	-0.922504	-0.309951
6	1.974656	-2.040158	-0.939478
6	3.368894	-1.939106	-1.257725
6	1.321724	-3.277681	-1.196054
6	4.025693	-2.987373	-1.882028
1	3.901413	-1.020084	-1.059500
6	2.010265	-4.339062	-1.757410
1	0.323038	-3.432072	-0.819694
6	3.354813	-4.189914	-2.129681
1	5.072582	-2.877831	-2.143163
1	1.512795	-5.293492	-1.894223
1	3.882336	-5.020263	-2.588911
6	2.141762	-0.426714	0.855864
8	1.722857	-0.870909	1.909280
8	3.201753	0.328453	0.650284
6	4.243018	0.352434	1.732377
1	3.728953	0.323730	2.693401
1	4.722589	1.319522	1.584433
6	5.161180	-0.808123	1.508895
6	4.881067	-2.050697	2.096354
6	6.247415	-0.684974	0.630565
6	5.681390	-3.156258	1.807818
1	4.038957	-2.146341	2.775669
6	7.046071	-1.791757	0.342546
1	6.471613	0.279050	0.180412
6	6.760957	-3.028557	0.929760
1	5.469969	-4.113139	2.274639
1	7.896305	-1.688284	-0.324540
1	7.389401	-3.887402	0.714783
7	0.941749	1.825573	-0.387648

6	1.783367	2.625831	-0.371990
6	2.818779	3.592772	-0.309654
6	3.316235	4.170271	-1.494970
6	3.343683	3.945604	0.951920
6	4.344577	5.102619	-1.407999
1	2.900274	3.889006	-2.456678
6	4.372425	4.878441	1.015456
1	2.941643	3.496435	1.854122
6	4.870172	5.454344	-0.159727
1	4.736353	5.557175	-2.311640
1	4.783505	5.163016	1.978250
1	5.671153	6.184549	-0.101394

TS(D-F)

Number of imaginary frequencies : 1 Electronic energy : HF=-2139.3088573
Zero-point correction= 0.707025 (Hartree/Particle)
Thermal correction to Energy= 0.749557
Thermal correction to Enthalpy= 0.750502
Thermal correction to Gibbs Free Energy= 0.630395
Sum of electronic and zero-point Energies= -2138.600580
Sum of electronic and thermal Energies= -2138.558048
Sum of electronic and thermal Enthalpies= -2138.557103
Sum of electronic and thermal Free Energies= -2138.677210

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Cartesian Coordinates

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46	0.766266	-0.741652	-0.148941
7	-0.750362	-2.156499	-0.626222
7	-0.949650	0.131158	0.858837
8	-4.008023	-2.493484	0.822068
8	-4.288793	-0.201241	-0.367170
6	-0.556286	-3.370899	-1.170216
1	0.429971	-3.578367	-1.564761
6	-1.574893	-4.318176	-1.213393
1	-1.394208	-5.282363	-1.675184
6	-2.791746	-4.039680	-0.599448
1	-3.562741	-4.799610	-0.543130
6	-2.984272	-2.791265	0.005872
6	-1.962056	-1.818021	-0.119849
6	-2.091521	-0.451655	0.410386
6	-3.309224	0.253380	0.432150
6	-3.383883	1.434354	1.181727
1	-4.320384	1.974707	1.250331
6	-2.227613	1.929223	1.770369
1	-2.244700	2.848390	2.343836
6	-1.013157	1.283961	1.535158
1	-0.075836	1.699799	1.876282
6	-6.030131	-3.074316	1.921357
1	-5.491851	-3.839562	2.485151
1	-7.069471	-3.392788	1.805931
1	-6.014249	-2.148072	2.502934
6	-5.393270	-2.874498	0.554332
1	-5.411524	-3.819755	0.001315
6	-6.058106	-1.777000	-0.293681
1	-7.144459	-1.896892	-0.225085
1	-5.790237	-1.897498	-1.349187
6	-5.663890	-0.353327	0.109406
1	-5.661918	-0.238027	1.199246

6	-6.530166	0.712292	-0.545566
1	-6.172400	1.714561	-0.295966
1	-7.566400	0.622645	-0.207806
1	-6.509683	0.602842	-1.633948
6	2.298521	0.736222	0.215443
6	2.532685	1.022150	1.664383
6	2.058974	0.189035	2.694940
6	3.234758	2.193312	2.007524
6	2.290682	0.512432	4.030326
1	1.481096	-0.698019	2.451578
6	3.475944	2.504783	3.344264
1	3.615620	2.847542	1.229209
6	3.004193	1.668124	4.358652
1	1.909365	-0.135182	4.813326
1	4.032595	3.402665	3.592508
1	3.186804	1.917588	5.398931
6	2.036128	2.007568	-0.587214
8	0.821976	2.486196	-0.359475
8	2.879504	2.501409	-1.310365
6	0.398891	3.699955	-1.077049
1	0.885746	3.693100	-2.055643
1	0.765628	4.560577	-0.512560
6	-1.099542	3.663663	-1.169828
6	-1.877563	4.654153	-0.562320
6	-1.730454	2.635053	-1.884324
6	-3.269623	4.629056	-0.682440
1	-1.396878	5.455798	-0.007970
6	-3.118525	2.600399	-1.994431
1	-1.130210	1.861460	-2.357638
6	-3.889865	3.603905	-1.397890
1	-3.864722	5.412971	-0.224475
1	-3.600659	1.796887	-2.541783
1	-4.970419	3.591907	-1.504004
6	5.063435	-1.251470	-0.951136
6	4.114452	-1.118460	0.071108
6	4.400469	-1.638233	1.329453
6	5.638490	-2.263557	1.524958
6	6.574348	-2.370367	0.490836
6	6.298564	-1.858534	-0.781996
6	3.333815	-0.179148	-1.958702
6	2.981398	-0.331766	-0.497732
1	3.689529	-1.573511	2.141028
1	5.872532	-2.677344	2.500039
1	7.525852	-2.858258	0.672702
1	7.021477	-1.937012	-1.585983
1	1.906356	-1.525819	-0.899214
7	4.531836	-0.679654	-2.146638
6	5.278308	-0.721611	-3.409926
1	5.466217	-1.764214	-3.676482
1	4.716761	-0.230093	-4.200012
1	6.229267	-0.204180	-3.266219
6	2.474210	0.316895	-3.071299
1	2.906080	1.210648	-3.528979
1	2.371409	-0.461836	-3.834784
1	1.477412	0.564622	-2.709776

F

Number of imaginary frequencies : 0 Electronic energy : HF=-2139.3135772

Zero-point correction= 0.708915 (Hartree/Particle)
Thermal correction to Energy= 0.752117
Thermal correction to Enthalpy= 0.753061
Thermal correction to Gibbs Free Energy= 0.631359
Sum of electronic and zero-point Energies= -2138.604662
Sum of electronic and thermal Energies= -2138.561461
Sum of electronic and thermal Enthalpies= -2138.560516
Sum of electronic and thermal Free Energies= -2138.682219

Cartesian Coordinates

46	0.901157	-0.744185	-0.324643
7	-0.605860	-2.120213	-0.742556
7	-0.822344	0.134438	0.845075
8	-3.765637	-2.578383	0.876930
8	-4.165035	-0.319272	-0.362709
6	-0.409034	-3.318636	-1.328826
1	0.553018	-3.489586	-1.790071
6	-1.402190	-4.291186	-1.330128
1	-1.221485	-5.238056	-1.826418
6	-2.587587	-4.063871	-0.638577
1	-3.332531	-4.846964	-0.557357
6	-2.778253	-2.835333	0.004123
6	-1.793910	-1.827747	-0.156041
6	-1.949551	-0.474196	0.395998
6	-3.193212	0.186043	0.416876
6	-3.306882	1.375515	1.145448
1	-4.259374	1.888187	1.205189
6	-2.164468	1.912188	1.722878
1	-2.206834	2.840338	2.280747
6	-0.932967	1.294077	1.503057
1	-0.016437	1.746943	1.851255
6	-5.735574	-3.153887	2.066043
1	-5.160273	-3.880934	2.643603
1	-6.769864	-3.501443	2.000051
1	-5.723176	-2.202909	2.606120
6	-5.149782	-3.001596	0.670467
1	-5.162413	-3.972728	0.163991
6	-5.868863	-1.962942	-0.205324
1	-6.948342	-2.123182	-0.113991
1	-5.612936	-2.113150	-1.260093
6	-5.526415	-0.510711	0.138499
1	-5.515740	-0.354785	1.223171
6	-6.444471	0.494116	-0.541022
1	-6.125597	1.517942	-0.330244
1	-7.471888	0.372960	-0.186582
1	-6.432449	0.347933	-1.625241
6	2.427978	1.033344	0.344155
6	2.391127	1.196366	1.812916
6	2.016775	0.149829	2.681888
6	2.689244	2.461926	2.363071
6	1.955929	0.357841	4.055152
1	1.723608	-0.811886	2.272623
6	2.648458	2.655722	3.741902
1	2.992007	3.279450	1.717850
6	2.279917	1.609147	4.590839
1	1.648040	-0.452421	4.708005
1	2.905363	3.626627	4.152566
1	2.237740	1.768041	5.663589
6	2.060266	2.302677	-0.419471

8	0.749277	2.433329	-0.573688
8	2.912205	3.079349	-0.788894
6	0.266844	3.644612	-1.265574
1	0.743084	3.662817	-2.250784
1	0.610923	4.515765	-0.703766
6	-1.228328	3.550116	-1.342296
6	-2.031057	4.529257	-0.748174
6	-1.831929	2.488126	-2.030918
6	-3.422252	4.460597	-0.857532
1	-1.570759	5.356541	-0.214560
6	-3.219300	2.410713	-2.129219
1	-1.212461	1.723444	-2.493243
6	-4.015976	3.403286	-1.548345
1	-4.037460	5.235975	-0.411815
1	-3.680640	1.582428	-2.656829
1	-5.096113	3.358516	-1.648413
6	4.927969	-1.315702	-0.919851
6	4.148309	-0.921544	0.180196
6	4.500805	-1.400807	1.443454
6	5.594903	-2.264768	1.556032
6	6.336941	-2.657092	0.436844
6	6.014354	-2.174949	-0.834635
6	3.395694	0.095103	-1.813720
6	3.136621	0.031112	-0.342781
1	3.952619	-1.119456	2.330017
1	5.870660	-2.639052	2.536206
1	7.177045	-3.333046	0.554204
1	6.598330	-2.456251	-1.703397
1	1.756824	-1.537891	-1.308754
7	4.437061	-0.668110	-2.084909
6	5.064736	-0.882146	-3.393687
1	4.946496	-1.929615	-3.681645
1	4.617166	-0.236940	-4.144457
1	6.127444	-0.645635	-3.310300
6	2.677930	0.871766	-2.868526
1	3.238271	1.779938	-3.115624
1	2.556370	0.272651	-3.773475
1	1.683274	1.160766	-2.536071

TS(F-F_1)

Number of imaginary frequencies : 1 Electronic energy : HF=-2139.3003889
Zero-point correction= 0.706834 (Hartree/Particle)
Thermal correction to Energy= 0.749854
Thermal correction to Enthalpy= 0.750798
Thermal correction to Gibbs Free Energy= 0.629164
Sum of electronic and zero-point Energies= -2138.593555
Sum of electronic and thermal Energies= -2138.550535
Sum of electronic and thermal Enthalpies= -2138.549591
Sum of electronic and thermal Free Energies= -2138.671225

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Cartesian Coordinates

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46	0.879351	-0.447240	-0.087650
7	-0.589639	-1.987313	-0.506628
7	-0.971366	0.252179	1.078703
8	-3.790415	-2.556249	0.989980
8	-4.208672	-0.320925	-0.337933
6	-0.296055	-3.187814	-1.036779

1	0.691343	-3.304636	-1.466925
6	-1.224287	-4.223918	-1.027074
1	-0.970788	-5.179052	-1.473345
6	-2.453327	-4.035286	-0.399665
1	-3.158102	-4.855249	-0.321140
6	-2.744872	-2.795370	0.182543
6	-1.803948	-1.746639	0.036260
6	-2.043682	-0.390713	0.563242
6	-3.299429	0.236761	0.482115
6	-3.477931	1.455892	1.147616
1	-4.442164	1.949501	1.124181
6	-2.383858	2.051876	1.764627
1	-2.482672	3.006684	2.267740
6	-1.130817	1.447421	1.661128
1	-0.235701	1.922180	2.043510
6	-5.808581	-3.176464	2.071805
1	-5.245575	-3.871884	2.698331
1	-6.825103	-3.560145	1.951983
1	-5.859822	-2.215124	2.590811
6	-5.145150	-3.031291	0.710771
1	-5.093243	-4.011878	0.224857
6	-5.846559	-2.036847	-0.229321
1	-6.922576	-2.238706	-0.199973
1	-5.521261	-2.198177	-1.263148
6	-5.584436	-0.563651	0.098580
1	-5.636255	-0.383921	1.178382
6	-6.507335	0.385681	-0.651086
1	-6.241255	1.427049	-0.451306
1	-7.545775	0.231140	-0.345059
1	-6.434405	0.214591	-1.729244
6	2.435376	1.027573	0.196993
6	2.773158	1.247630	1.646284
6	2.094574	0.610108	2.696603
6	3.815007	2.142393	1.943029
6	2.464681	0.845925	4.021348
1	1.264738	-0.064403	2.495961
6	4.184696	2.368595	3.268592
1	4.335649	2.649767	1.137124
6	3.512987	1.722740	4.309130
1	1.930767	0.348778	4.824895
1	4.998354	3.052860	3.486547
1	3.800854	1.905547	5.339321
6	2.112615	2.345504	-0.493267
8	0.821594	2.640183	-0.358804
8	2.954585	3.016069	-1.047652
6	0.311600	3.868029	-0.981070
1	0.857783	4.019888	-1.916838
1	0.537679	4.703058	-0.313495
6	-1.165683	3.678213	-1.189623
6	-2.076230	4.636196	-0.733539
6	-1.642070	2.548534	-1.870309
6	-3.444676	4.476933	-0.969444
1	-1.717915	5.515396	-0.204769
6	-3.006542	2.380112	-2.093755
1	-0.939397	1.795853	-2.220572
6	-3.910705	3.350074	-1.647700
1	-4.141881	5.234732	-0.625825
1	-3.368982	1.496422	-2.609180
1	-4.972758	3.229520	-1.838527
6	4.444552	-1.759889	-1.149559

6	3.829413	-1.164648	-0.036671
6	4.094302	-1.678835	1.236300
6	4.959187	-2.772895	1.344335
6	5.552284	-3.351135	0.215643
6	5.304464	-2.845132	-1.065524
6	3.207848	-0.069371	-2.025834
6	3.001919	-0.054265	-0.554183
1	3.652108	-1.244567	2.122498
1	5.178173	-3.177631	2.326743
1	6.220622	-4.197534	0.332197
1	5.774217	-3.282560	-1.939155
1	0.630453	-0.159559	-1.526939
7	4.047608	-1.050472	-2.316053
6	4.577208	-1.412964	-3.635779
1	4.256028	-2.426938	-3.885758
1	4.230936	-0.717148	-4.394762
1	5.667966	-1.378470	-3.592288
6	2.665096	0.853904	-3.065569
1	3.396658	1.640814	-3.280894
1	2.433939	0.319699	-3.989299
1	1.755470	1.345949	-2.728760

F_1

Number of imaginary frequencies : 0 Electronic energy : HF=-2139.3160869
Zero-point correction= 0.709416 (Hartree/Particle)
Thermal correction to Energy= 0.752517
Thermal correction to Enthalpy= 0.753461
Thermal correction to Gibbs Free Energy= 0.630365
Sum of electronic and zero-point Energies= -2138.606671
Sum of electronic and thermal Energies= -2138.563570
Sum of electronic and thermal Enthalpies= -2138.562626
Sum of electronic and thermal Free Energies= -2138.685722

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Cartesian Coordinates

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46	0.334544	0.121955	0.016908
7	-1.460158	-1.164086	-0.476631
7	-1.217490	1.476122	0.343603
8	-4.627498	-0.481368	1.058177
8	-4.589849	1.308537	-0.834986
6	-1.543458	-2.483563	-0.702344
1	-0.646612	-2.976117	-1.049891
6	-2.723276	-3.196257	-0.491255
1	-2.757178	-4.257712	-0.710712
6	-3.823260	-2.549165	0.059895
1	-4.718525	-3.105226	0.313346
6	-3.736337	-1.177270	0.331996
6	-2.561551	-0.491459	-0.059931
6	-2.442017	0.972679	0.046746
6	-3.521901	1.841854	-0.225455
6	-3.372410	3.205568	0.053400
1	-4.203694	3.884051	-0.103816
6	-2.131642	3.676752	0.471010
1	-1.977711	4.729778	0.678832
6	-1.056861	2.795984	0.556573
1	-0.056035	3.136163	0.782933
6	-6.641360	-0.235033	2.284963
1	-6.213217	-0.841631	3.086163

1	-7.726402	-0.367357	2.289952
1	-6.419363	0.814733	2.496773
6	-6.073475	-0.657165	0.938303
1	-6.299114	-1.715202	0.766308
6	-6.587602	0.170897	-0.250237
1	-7.675097	0.263613	-0.160909
1	-6.389606	-0.352746	-1.192088
6	-5.957089	1.561221	-0.367292
1	-5.894909	2.051121	0.611081
6	-6.665890	2.451543	-1.376400
1	-6.154259	3.411330	-1.486269
1	-7.692256	2.646774	-1.053041
1	-6.696511	1.967058	-2.356445
6	2.582061	-0.789450	0.664280
6	2.388454	-1.565651	1.888557
6	1.163821	-2.205935	2.195043
6	3.453563	-1.666449	2.814520
6	1.014976	-2.918312	3.376025
1	0.324501	-2.119144	1.512956
6	3.309487	-2.413030	3.978053
1	4.404618	-1.187851	2.608994
6	2.090285	-3.032501	4.267337
1	0.062801	-3.383164	3.609663
1	4.143604	-2.502643	4.665749
1	1.973373	-3.595594	5.187855
6	3.653346	0.297600	0.746065
8	3.441826	1.130820	1.756648
8	4.582099	0.317844	-0.031964
6	4.306917	2.327694	1.811046
1	5.341103	2.021256	1.647045
1	4.177231	2.680163	2.834214
6	3.826718	3.317289	0.785821
6	2.610865	3.989529	0.987485
6	4.545537	3.533013	-0.395612
6	2.118325	4.859066	0.013937
1	2.070119	3.847734	1.920519
6	4.053912	4.408471	-1.367638
1	5.484496	3.011442	-0.553829
6	2.838199	5.066135	-1.167635
1	1.191621	5.399306	0.185174
1	4.625153	4.584854	-2.273843
1	2.463510	5.755566	-1.917909
6	1.745606	-2.487080	-2.489382
6	1.824848	-2.546870	-1.088788
6	1.709861	-3.794961	-0.468840
6	1.470584	-4.921043	-1.262285
6	1.343744	-4.821434	-2.653673
6	1.492993	-3.589680	-3.296207
6	2.279875	-0.369222	-1.864233
6	2.127008	-1.172789	-0.626068
1	1.793144	-3.903582	0.603368
1	1.382619	-5.892207	-0.786721
1	1.150143	-5.710924	-3.243585
1	1.435835	-3.512396	-4.375910
1	1.289502	1.202902	0.495815
7	2.016831	-1.160937	-2.900943
6	2.011485	-0.792705	-4.319303
1	1.009259	-0.947860	-4.726580
1	2.301651	0.245959	-4.447711
1	2.722120	-1.429691	-4.850873

6	2.655546	1.063422	-2.079747
1	3.643772	1.114299	-2.548939
1	1.928795	1.554095	-2.732758
1	2.706283	1.634411	-1.160258

$TS(F_1-P_1)$

Number of imaginary frequencies : 1 Electronic energy : HF=-2139.3102924
Zero-point correction= 0.708240 (Hartree/Particle)
Thermal correction to Energy= 0.750613
Thermal correction to Enthalpy= 0.751557
Thermal correction to Gibbs Free Energy= 0.631095
Sum of electronic and zero-point Energies= -2138.606653
Sum of electronic and thermal Energies= -2138.564280
Sum of electronic and thermal Enthalpies= -2138.563336
Sum of electronic and thermal Free Energies= -2138.683798

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Cartesian Coordinates

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46	0.375281	-0.031310	0.102091
7	-1.243256	-1.460998	-0.317294
7	-1.290951	1.159010	0.523988
8	-4.495592	-1.152178	1.153932
8	-4.622816	0.685219	-0.692795
6	-1.150752	-2.784758	-0.513870
1	-0.186917	-3.167756	-0.820972
6	-2.239595	-3.632015	-0.314281
1	-2.136547	-4.694287	-0.506069
6	-3.425179	-3.114881	0.196136
1	-4.250376	-3.773441	0.441958
6	-3.513630	-1.739604	0.451589
6	-2.423034	-0.919283	0.077624
6	-2.459978	0.546561	0.204142
6	-3.615171	1.310019	-0.066081
6	-3.595089	2.680086	0.226798
1	-4.485448	3.278739	0.068802
6	-2.406820	3.261975	0.655795
1	-2.347839	4.323642	0.865928
6	-1.253984	2.484911	0.747181
1	-0.293756	2.922209	0.985985
6	-6.543728	-1.191427	2.350710
1	-6.060923	-1.778139	3.135466
1	-7.606212	-1.447379	2.328194
1	-6.447965	-0.132845	2.608623
6	-5.910217	-1.487413	0.999798
1	-6.009322	-2.555449	0.777596
6	-6.496229	-0.669999	-0.162952
1	-7.588176	-0.691105	-0.083182
1	-6.238695	-1.133580	-1.121675
6	-6.008791	0.780571	-0.220463
1	-5.995152	1.234049	0.777135
6	-6.805451	1.634363	-1.195230
1	-6.395113	2.645145	-1.264992
1	-7.846030	1.710902	-0.867429
1	-6.787740	1.189142	-2.194053
6	2.761197	-0.135338	0.353180
6	3.115462	-0.599665	1.713844
6	2.174718	-1.157359	2.599345
6	4.458546	-0.485420	2.123982

6	2.567855	-1.599861	3.858077
1	1.130269	-1.220535	2.304599
6	4.852732	-0.960050	3.372029
1	5.200566	-0.052564	1.460159
6	3.910090	-1.511260	4.243565
1	1.829801	-2.007118	4.541366
1	5.893781	-0.887410	3.668701
1	4.216677	-1.859793	5.224556
6	3.507919	1.131358	-0.092403
8	3.416604	2.074471	0.835366
8	4.102404	1.195509	-1.146551
6	3.856550	3.439024	0.478127
1	4.675522	3.364675	-0.238322
1	4.216837	3.851909	1.419995
6	2.665091	4.178059	-0.063914
6	1.794534	4.849150	0.805534
6	2.381561	4.149805	-1.437122
6	0.655351	5.485706	0.307751
1	2.020559	4.891348	1.867823
6	1.235442	4.774595	-1.932488
1	3.073461	3.655607	-2.113451
6	0.370548	5.441704	-1.060192
1	0.004610	6.033062	0.983652
1	1.031507	4.766662	-2.998964
1	-0.507150	5.948502	-1.449671
6	2.157762	-2.895335	-1.984555
6	2.285544	-2.488451	-0.646378
6	2.452561	-3.467607	0.335899
6	2.476163	-4.810670	-0.053830
6	2.334836	-5.187306	-1.395011
6	2.175470	-4.222457	-2.393958
6	2.046665	-0.629420	-2.076940
6	2.234447	-1.007154	-0.651840
1	2.549989	-3.207472	1.380318
1	2.605717	-5.576551	0.703597
1	2.356472	-6.237287	-1.666582
1	2.079452	-4.506595	-3.435674
1	1.285699	1.101581	0.616420
7	2.009946	-1.741361	-2.796747
6	1.818288	-1.850242	-4.246039
1	0.865450	-2.345971	-4.448723
1	1.828843	-0.867144	-4.708361
1	2.633615	-2.446382	-4.661049
6	1.822889	0.706601	-2.710782
1	2.675815	0.970272	-3.343848
1	0.917925	0.678944	-3.325383
1	1.705433	1.496836	-1.974583

P_1

Number of imaginary frequencies : 0 Electronic energy : HF=-2139.3369886
Zero-point correction= 0.711357 (Hartree/Particle)
Thermal correction to Energy= 0.754003
Thermal correction to Enthalpy= 0.754947
Thermal correction to Gibbs Free Energy= 0.633607
Sum of electronic and zero-point Energies= -2138.625631
Sum of electronic and thermal Energies= -2138.582986
Sum of electronic and thermal Enthalpies= -2138.582042
Sum of electronic and thermal Free Energies= -2138.703382

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Cartesian Coordinates

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46	0.000414	-0.180399	0.405636
7	-1.567372	-0.795375	-0.820664
7	-1.628747	0.727702	1.421223
8	-5.040645	-0.889087	0.012420
8	-4.713954	1.676198	-0.112697
6	-1.476955	-1.715988	-1.791486
1	-0.482913	-2.006007	-2.105255
6	-2.618935	-2.294239	-2.341367
1	-2.519437	-3.020059	-3.140549
6	-3.866546	-1.994252	-1.805363
1	-4.752292	-2.509903	-2.158409
6	-3.955963	-1.075612	-0.749601
6	-2.778712	-0.397695	-0.349000
6	-2.761920	0.649996	0.679404
6	-3.808662	1.576411	0.868923
6	-3.766386	2.401307	2.002305
1	-4.583126	3.085723	2.203418
6	-2.640991	2.373077	2.819871
1	-2.571521	3.011266	3.693680
6	-1.560236	1.562974	2.467741
1	-0.629973	1.577528	3.024328
6	-7.291561	-1.396703	0.577606
1	-6.993266	-2.423464	0.801109
1	-8.333509	-1.400912	0.247057
1	-7.223711	-0.812578	1.499827
6	-6.406446	-0.808625	-0.510380
1	-6.483586	-1.418192	-1.417019
6	-6.719733	0.657533	-0.853033
1	-7.806551	0.770004	-0.924572
1	-6.308141	0.915836	-1.834845
6	-6.159053	1.671246	0.148677
1	-6.313336	1.337400	1.181034
6	-6.707753	3.074378	-0.059841
1	-6.241764	3.789711	0.622691
1	-7.786659	3.087435	0.118707
1	-6.520977	3.408414	-1.084340
6	2.309035	-0.348860	0.964938
6	2.672150	-1.388403	2.015604
6	1.763792	-1.728884	3.024157
6	3.914300	-2.033856	1.946105
6	2.084744	-2.723345	3.949722
1	0.802995	-1.222423	3.090462
6	4.230830	-3.024305	2.875189
1	4.620419	-1.767017	1.167091
6	3.318277	-3.373592	3.874340
1	1.376572	-2.983112	4.729973
1	5.192372	-3.524177	2.817248
1	3.570194	-4.144702	4.595193
6	3.427903	0.704488	0.831833
8	3.172807	1.777899	1.569799
8	4.401271	0.507885	0.139408
6	4.156838	2.884876	1.475759
1	5.154714	2.461104	1.598028
1	3.906093	3.505034	2.336250
6	3.990997	3.605471	0.167584
6	2.874506	4.428224	-0.037531
6	4.907344	3.414640	-0.874403

6	2.668181	5.042014	-1.273799
1	2.172924	4.595812	0.776288
6	4.707552	4.038067	-2.108328
1	5.768237	2.772365	-0.718947
6	3.584956	4.845836	-2.311225
1	1.808816	5.688819	-1.422107
1	5.431939	3.902137	-2.905643
1	3.435160	5.337405	-3.267719
6	2.002002	-2.324529	-2.173670
6	1.855263	-2.306452	-0.775738
6	1.709313	-3.519169	-0.094275
6	1.729595	-4.703747	-0.836360
6	1.883174	-4.692804	-2.229263
6	2.020199	-3.489102	-2.929890
6	2.036988	-0.128153	-1.616504
6	1.847001	-0.890925	-0.368439
1	1.582349	-3.545805	0.980167
1	1.625988	-5.652731	-0.320936
1	1.899312	-5.629716	-2.775878
1	2.141195	-3.478051	-4.007395
1	1.443337	0.278488	1.453369
7	2.105139	-0.980392	-2.629913
6	2.273840	-0.655592	-4.047913
1	1.393936	-0.985348	-4.606090
1	2.410652	0.415245	-4.176738
1	3.156761	-1.177242	-4.423942
6	2.106602	1.349227	-1.794130
1	3.111996	1.662585	-2.097188
1	1.394855	1.684646	-2.553952
1	1.878764	1.876562	-0.868906

TS(F-F_2)

Number of imaginary frequencies : 1 Electronic energy : HF=-2139.3021939
Zero-point correction= 0.709239 (Hartree/Particle)
Thermal correction to Energy= 0.751953
Thermal correction to Enthalpy= 0.752897
Thermal correction to Gibbs Free Energy= 0.630126
Sum of electronic and zero-point Energies= -2138.592955
Sum of electronic and thermal Energies= -2138.550241
Sum of electronic and thermal Enthalpies= -2138.549296
Sum of electronic and thermal Free Energies= -2138.672068

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Cartesian Coordinates

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46	0.404474	0.672148	0.284572
7	2.248795	1.126692	1.068580
7	1.604513	-1.059107	-0.514449
8	5.063260	-1.036858	1.494542
8	5.123758	-0.673084	-1.081545
6	2.471048	2.080884	1.993884
1	1.683126	2.801577	2.157418
6	3.665489	2.121147	2.705286
1	3.827286	2.911570	3.429569
6	4.605067	1.110874	2.531071
1	5.497018	1.081593	3.146066
6	4.355403	0.098257	1.596535
6	3.196566	0.195469	0.786330
6	2.907881	-0.753123	-0.303206

6	3.926928	-1.280645	-1.124445
6	3.600584	-2.321977	-2.002527
1	4.372035	-2.778243	-2.613293
6	2.272105	-2.718684	-2.105922
1	1.983280	-3.522524	-2.774164
6	1.293527	-2.031356	-1.384071
1	0.241705	-2.264229	-1.481058
6	6.844806	-2.478685	2.103435
1	6.365079	-2.642610	3.070961
1	7.925361	-2.588468	2.227025
1	6.494304	-3.251825	1.413881
6	6.522164	-1.087433	1.579746
1	6.871198	-0.339050	2.299383
6	7.118474	-0.779660	0.196958
1	8.165340	-1.101098	0.194105
1	7.116904	0.300704	0.014437
6	6.370583	-1.434104	-0.968023
1	6.114054	-2.474347	-0.737323
6	7.126669	-1.341860	-2.284780
1	6.539387	-1.758020	-3.107565
1	8.067257	-1.896336	-2.221499
1	7.353826	-0.298350	-2.521036
6	-2.655052	0.474156	-0.213738
6	-3.265440	0.350529	1.109038
6	-2.689870	0.965722	2.245559
6	-4.388647	-0.492886	1.284818
6	-3.226167	0.750249	3.507827
1	-1.801818	1.577191	2.132622
6	-4.934840	-0.678519	2.549494
1	-4.853082	-0.973753	0.433805
6	-4.355551	-0.064321	3.663206
1	-2.763176	1.209347	4.375256
1	-5.805575	-1.315516	2.662033
1	-4.774699	-0.224143	4.651626
6	-2.592531	-0.858660	-0.924947
8	-3.649386	-1.077940	-1.683615
8	-1.657874	-1.612334	-0.723057
6	-3.901985	-2.490230	-2.122956
1	-2.940290	-2.936424	-2.378028
1	-4.510652	-2.357867	-3.016510
6	-4.616728	-3.210637	-1.022194
6	-6.011604	-3.112951	-0.913856
6	-3.891228	-3.900910	-0.040073
6	-6.673556	-3.695614	0.167111
1	-6.577667	-2.584150	-1.676345
6	-4.555135	-4.485151	1.038483
1	-2.810810	-3.970797	-0.121010
6	-5.944640	-4.380088	1.144635
1	-7.754342	-3.627283	0.240804
1	-3.991525	-5.026595	1.791747
1	-6.461102	-4.842275	1.980369
6	-1.628009	3.807182	-1.336632
6	-2.271182	3.027257	-0.362028
6	-2.953943	3.681523	0.667551
6	-2.932662	5.078014	0.706847
6	-2.245224	5.827555	-0.256458
6	-1.583193	5.196096	-1.311530
6	-1.401092	1.673467	-2.070717
6	-2.111928	1.619292	-0.782241
1	-3.499194	3.131535	1.422172

1	-3.464861	5.591443	1.500708
1	-2.242276	6.910593	-0.196679
1	-1.082863	5.772942	-2.080808
1	-0.113533	1.987649	0.832043
7	-1.110408	2.945109	-2.335260
6	-0.382982	3.493872	-3.482758
1	0.426190	4.125314	-3.110104
1	0.039747	2.701444	-4.092921
1	-1.065445	4.097078	-4.086486
6	-1.108618	0.549528	-3.010152
1	-0.510369	-0.227825	-2.532397
1	-2.052720	0.093504	-3.325522
1	-0.584211	0.880842	-3.903619

F_2

Number of imaginary frequencies : 0 Electronic energy : HF=-2139.3328268
Zero-point correction= 0.709910 (Hartree/Particle)
Thermal correction to Energy= 0.752950
Thermal correction to Enthalpy= 0.753894
Thermal correction to Gibbs Free Energy= 0.629550
Sum of electronic and zero-point Energies= -2138.622917
Sum of electronic and thermal Energies= -2138.579877
Sum of electronic and thermal Enthalpies= -2138.578933
Sum of electronic and thermal Free Energies= -2138.703277

Cartesian Coordinates

46	0.409212	0.439648	-0.244750
7	1.883467	1.579836	0.613677
7	2.186471	-0.710005	-0.876688
8	5.237520	0.593643	1.383573
8	5.404043	0.823725	-1.206245
6	1.677358	2.592936	1.474555
1	0.671567	2.984117	1.531928
6	2.713343	3.098248	2.254988
1	2.521830	3.929732	2.923852
6	3.962102	2.487313	2.219998
1	4.749990	2.812510	2.889509
6	4.168907	1.407655	1.351973
6	3.126455	1.044068	0.467341
6	3.288344	0.016112	-0.576494
6	4.485259	-0.150648	-1.304744
6	4.587524	-1.246740	-2.171470
1	5.512638	-1.426339	-2.708121
6	3.470128	-2.049125	-2.382199
1	3.511617	-2.891258	-3.064093
6	2.267689	-1.712894	-1.758580
1	1.345647	-2.242470	-1.970129
6	7.342562	-0.083999	2.237240
1	6.860658	-0.347104	3.181615
1	8.377325	0.203130	2.441666
1	7.349108	-0.971989	1.598709
6	6.606628	1.067267	1.567943
1	6.606103	1.934969	2.236609
6	7.189495	1.476595	0.205418
1	8.279010	1.534533	0.299746
1	6.840368	2.477292	-0.072117
6	6.815310	0.537061	-0.944784

1	6.898515	-0.513051	-0.641771
6	7.619537	0.802153	-2.208974
1	7.287797	0.162895	-3.031255
1	8.680852	0.606488	-2.031123
1	7.505316	1.844377	-2.520370
6	-3.028912	-0.057380	-0.069482
6	-2.928421	-0.474637	1.332021
6	-2.649310	0.485406	2.329016
6	-2.991408	-1.840159	1.683625
6	-2.456853	0.086501	3.645722
1	-2.560865	1.530079	2.052387
6	-2.815926	-2.226449	3.008787
1	-3.210677	-2.591501	0.934633
6	-2.545659	-1.268616	3.989868
1	-2.232312	0.827466	4.406185
1	-2.885103	-3.277015	3.270017
1	-2.400131	-1.574532	5.021113
6	-2.227290	-0.967305	-0.964378
8	-2.958605	-1.901894	-1.511290
8	-0.999304	-0.896012	-1.097685
6	-2.269620	-3.113782	-2.082560
1	-1.370291	-2.772271	-2.594848
1	-3.001564	-3.480573	-2.800473
6	-2.004476	-4.073092	-0.964922
6	-3.002907	-4.977589	-0.575098
6	-0.805858	-4.010568	-0.238235
6	-2.806160	-5.807760	0.528531
1	-3.932045	-5.032201	-1.136137
6	-0.609703	-4.842657	0.863244
1	-0.033841	-3.305207	-0.527155
6	-1.610172	-5.738950	1.249231
1	-3.578607	-6.512200	0.820009
1	0.322414	-4.795834	1.417564
1	-1.454264	-6.391414	2.102826
6	-5.160366	2.806522	-0.806724
6	-4.741623	1.846865	0.129097
6	-5.389455	1.795886	1.366610
6	-6.402152	2.721930	1.631924
6	-6.776741	3.686908	0.688527
6	-6.160391	3.739115	-0.564792
6	-3.601567	1.576424	-1.898650
6	-3.722012	1.026759	-0.546120
1	-5.120696	1.059724	2.112637
1	-6.908641	2.690806	2.590818
1	-7.562729	4.395936	0.925236
1	-6.465876	4.467374	-1.307293
1	-0.691803	1.424986	0.164407
7	-4.427319	2.610919	-2.009191
6	-4.646801	3.487590	-3.162568
1	-4.443224	4.518660	-2.865142
1	-3.997714	3.215789	-3.989619
1	-5.689226	3.400281	-3.477937
6	-2.678805	1.119400	-2.975197
1	-1.646384	1.134291	-2.612044
1	-2.920867	0.091306	-3.262374
1	-2.733527	1.735271	-3.870521

P

Number of imaginary frequencies : 0 Electronic energy : HF=-1171.809055
Zero-point correction= 0.420433 (Hartree/Particle)
Thermal correction to Energy= 0.444437
Thermal correction to Enthalpy= 0.445381
Thermal correction to Gibbs Free Energy= 0.365339
Sum of electronic and zero-point Energies= -1171.388622
Sum of electronic and thermal Energies= -1171.364618
Sum of electronic and thermal Enthalpies= -1171.363674
Sum of electronic and thermal Free Energies= -1171.443716

Cartesian Coordinates

6	-1.507567	-0.023211	-0.901961
6	-2.911400	-0.141687	-0.320270
6	-3.873176	0.858130	-0.515974
6	-3.285899	-1.307798	0.360106
6	-5.173932	0.697192	-0.035683
1	-3.602446	1.775557	-1.026159
6	-4.586775	-1.471448	0.836547
1	-2.546820	-2.086594	0.520298
6	-5.536993	-0.467263	0.642476
1	-5.903190	1.487669	-0.189976
1	-4.856168	-2.383834	1.361591
1	-6.549033	-0.589920	1.017799
6	-0.982706	1.403962	-1.038341
8	-1.248220	2.340463	-0.313358
8	-0.053163	1.455607	-2.022047
6	0.914538	2.531019	-1.898699
1	0.395329	3.482369	-1.760839
1	1.431835	2.532077	-2.860522
6	1.855214	2.238215	-0.754769
6	1.851477	3.027157	0.400276
6	2.690136	1.114997	-0.816139
6	2.695065	2.717508	1.469200
1	1.172416	3.871844	0.465697
6	3.527263	0.799089	0.252649
1	2.659993	0.469636	-1.689078
6	3.537726	1.605947	1.394180
1	2.690437	3.339858	2.359621
1	4.156899	-0.083401	0.196605
1	4.198969	1.367920	2.223293
6	1.463944	-1.950133	0.377971
6	0.576125	-1.611019	-0.679011
6	0.823416	-2.116417	-1.964805
6	1.928980	-2.936355	-2.167240
6	2.795270	-3.264199	-1.104774
6	2.575011	-2.775748	0.180792
6	-0.086866	-0.530862	1.204175
6	-0.411625	-0.727095	-0.125282
1	0.170831	-1.856363	-2.793420
1	2.132790	-3.328489	-3.159398
1	3.652769	-3.903817	-1.292243
1	3.252708	-3.017806	0.993773
7	1.027205	-1.299963	1.517806
6	1.725871	-1.314682	2.786941
1	2.096572	-2.322825	2.991111
1	2.569891	-0.615741	2.783425
1	1.043182	-1.036353	3.590539
6	-0.728209	0.359259	2.218006
1	-1.160361	-0.212023	3.049064

1	0.002626	1.064017	2.631344
1	-1.521374	0.943565	1.754086
1	-1.516575	-0.453511	-1.910261

S_1

Number of imaginary frequencies : 0 Electronic energy : HF=-838.7637978
Zero-point correction= 0.240204 (Hartree/Particle)
Thermal correction to Energy= 0.256078
Thermal correction to Enthalpy= 0.257023
Thermal correction to Gibbs Free Energy= 0.193068
Sum of electronic and zero-point Energies= -838.523594
Sum of electronic and thermal Energies= -838.507719
Sum of electronic and thermal Enthalpies= -838.506775
Sum of electronic and thermal Free Energies= -838.570730

Cartesian Coordinates

6	-1.305489	0.741948	-0.196570
6	-2.588635	0.048317	0.043968
6	-2.793487	-1.273726	-0.391682
6	-3.636413	0.703517	0.719395
6	-4.011973	-1.908402	-0.152940
1	-2.000058	-1.792023	-0.911834
6	-4.847978	0.058683	0.951831
1	-3.512371	1.724391	1.068891
6	-5.045471	-1.253308	0.517109
1	-4.148991	-2.929439	-0.497890
1	-5.639667	0.587019	1.475276
1	-5.990766	-1.755811	0.698512
6	-0.122277	0.210705	-0.888476
8	-0.035162	-0.909168	-1.360893
8	0.867096	1.136429	-0.940939
6	2.124873	0.710928	-1.539105
1	2.557471	1.636038	-1.925015
1	1.906930	0.034702	-2.368310
6	3.028441	0.065944	-0.519404
6	3.942499	0.841550	0.203867
6	2.944892	-1.309863	-0.264153
6	4.765239	0.254800	1.166105
1	4.010031	1.909473	0.010562
6	3.766589	-1.896879	0.698229
1	2.222798	-1.905259	-0.813339
6	4.678010	-1.116694	1.414190
1	5.473213	0.865407	1.719124
1	3.696456	-2.963946	0.889062
1	5.318670	-1.575961	2.161680
7	-1.178617	1.974965	0.252269
7	-1.098827	3.036778	0.652553

S_2

Number of imaginary frequencies : 0 Electronic energy : HF=-442.4720156
Zero-point correction= 0.185591 (Hartree/Particle)
Thermal correction to Energy= 0.195258
Thermal correction to Enthalpy= 0.196202
Thermal correction to Gibbs Free Energy= 0.150026
Sum of electronic and zero-point Energies= -442.286425

Sum of electronic and thermal Energies= -442.276758
Sum of electronic and thermal Enthalpies= -442.275814
Sum of electronic and thermal Free Energies= -442.321990

Cartesian Coordinates

6	-0.548847	-0.961699	0.000000
6	-0.306924	0.440175	-0.000013
6	-1.343161	1.379043	-0.000007
6	-2.648556	0.894518	-0.000002
6	-2.911912	-0.490152	0.000004
6	-1.876589	-1.419058	0.000005
6	0.737072	-1.596169	0.000008
6	1.691830	-0.608651	-0.000004
1	-1.140191	2.445871	-0.000002
1	-3.477753	1.596111	0.000001
1	-3.942303	-0.834126	0.000009
1	-2.088996	-2.484719	0.000013
1	0.940034	-2.658065	0.000015
7	1.062382	0.635027	-0.000028
6	1.689611	1.939608	0.000025
1	1.398769	2.511988	-0.888647
1	1.399236	2.511736	0.889017
1	2.774282	1.831928	-0.000282
6	3.180043	-0.743849	-0.000003
1	3.637993	-0.283044	0.884316
1	3.448858	-1.802360	0.000033
1	3.637990	-0.283108	-0.884357

N_2

Number of imaginary frequencies : 0 Electronic energy : HF=-109.5207183
Zero-point correction= 0.005599 (Hartree/Particle)
Thermal correction to Energy= 0.007960
Thermal correction to Enthalpy= 0.008904
Thermal correction to Gibbs Free Energy= -0.012850
Sum of electronic and zero-point Energies= -109.515119
Sum of electronic and thermal Energies= -109.512758
Sum of electronic and thermal Enthalpies= -109.511814
Sum of electronic and thermal Free Energies= -109.533568

Cartesian Coordinates

7	0.000000	0.000000	0.552651
7	0.000000	0.000000	-0.552651

PhCN

Number of imaginary frequencies : 0 Electronic energy : HF=-324.4992479
Zero-point correction= 0.099335 (Hartree/Particle)
Thermal correction to Energy= 0.105437
Thermal correction to Enthalpy= 0.106382
Thermal correction to Gibbs Free Energy= 0.069055
Sum of electronic and zero-point Energies= -324.399912
Sum of electronic and thermal Energies= -324.393810
Sum of electronic and thermal Enthalpies= -324.392866
Sum of electronic and thermal Free Energies= -324.430193

Cartesian Coordinates

6	-1.483700	1.211319	0.000000
6	-0.090965	1.217961	0.000000
6	0.610096	-0.000112	0.000001
6	-0.091110	-1.218054	0.000000
6	-1.483860	-1.211212	0.000000
6	-2.180652	0.000091	0.000000
1	-2.025541	2.152032	0.000000
1	0.459485	2.152877	0.000000
1	0.459177	-2.153067	0.000000
1	-2.025823	-2.151856	-0.000001
1	-3.266579	0.000149	-0.000001
6	2.044471	-0.000032	0.000000
7	3.207658	0.000014	0.000000

H_2O

Number of imaginary frequencies : 0 Electronic energy : HF=-76.418168
Zero-point correction= 0.021381 (Hartree/Particle)
Thermal correction to Energy= 0.024216
Thermal correction to Enthalpy= 0.025161
Thermal correction to Gibbs Free Energy= 0.003727
Sum of electronic and zero-point Energies= -76.396787
Sum of electronic and thermal Energies= -76.393952
Sum of electronic and thermal Enthalpies= -76.393007
Sum of electronic and thermal Free Energies= -76.414441

Cartesian Coordinates

8	0.000000	-0.000000	0.118840
1	-0.000000	-0.760114	-0.475358
1	0.000000	0.760114	-0.475358

TS($D-E_a$)

Number of imaginary frequencies : 1 Electronic energy : HF=-2463.8661469
Zero-point correction= 0.809378 (Hartree/Particle)
Thermal correction to Energy= 0.859273
Thermal correction to Enthalpy= 0.860217
Thermal correction to Gibbs Free Energy= 0.721795
Sum of electronic and zero-point Energies= -2463.056712
Sum of electronic and thermal Energies= -2463.006817
Sum of electronic and thermal Enthalpies= -2463.005873
Sum of electronic and thermal Free Energies= -2463.144295

Cartesian Coordinates

46	0.109711	0.083232	0.066348
7	1.619667	-1.370888	0.610920
7	1.858591	1.305082	0.107396
8	5.041113	-1.124522	-0.409278
8	4.973918	0.459035	1.672486
6	1.432518	-2.695312	0.683640
1	0.416342	-3.040754	0.815889
6	2.500648	-3.582366	0.559928
1	2.326745	-4.648326	0.655705
6	3.765025	-3.095560	0.242657

1	4.584809	-3.779797	0.055918
6	3.949216	-1.712727	0.110429
6	2.859066	-0.866763	0.415487
6	2.959017	0.594621	0.480284
6	4.090146	1.236846	1.025652
6	4.162854	2.633484	0.972802
1	5.040710	3.147369	1.348203
6	3.061111	3.335956	0.502399
1	3.059401	4.419560	0.472483
6	1.909405	2.643598	0.130026
1	1.013050	3.171530	-0.156230
6	7.237400	-1.120848	-1.297780
1	6.852357	-1.574424	-2.213932
1	8.275203	-1.436255	-1.162250
1	7.218819	-0.034235	-1.421203
6	6.402921	-1.551479	-0.100713
1	6.431790	-2.643327	-0.013647
6	6.845485	-0.923693	1.230846
1	7.935526	-1.000368	1.302493
1	6.431175	-1.488347	2.073414
6	6.413199	0.534211	1.413920
1	6.563234	1.111545	0.494376
6	7.097305	1.206393	2.595426
1	6.725587	2.223332	2.744866
1	8.176813	1.259468	2.427701
1	6.915276	0.639200	3.512684
6	-1.361606	1.399937	-0.950147
6	-0.654580	2.521022	-1.656857
6	0.270665	2.293871	-2.697017
6	-0.870471	3.854322	-1.251223
6	0.922892	3.355498	-3.318094
1	0.494719	1.282613	-3.008374
6	-0.215294	4.916142	-1.877183
1	-1.536386	4.067525	-0.423008
6	0.681396	4.672959	-2.917638
1	1.627348	3.152522	-4.118747
1	-0.405223	5.931977	-1.544751
1	1.190346	5.496846	-3.407466
6	-1.935390	0.311399	-1.812484
8	-3.066074	-0.153108	-1.466177
8	-1.299624	-0.131816	-2.852652
6	-1.829302	-1.322104	-3.573155
1	-1.336935	-1.241405	-4.541974
1	-2.906505	-1.198020	-3.689369
6	-1.461643	-2.575282	-2.834539
6	-0.124090	-2.993982	-2.796266
6	-2.438704	-3.324014	-2.170240
6	0.227673	-4.150547	-2.102764
1	0.635850	-2.421427	-3.321556
6	-2.086718	-4.482132	-1.474381
1	-3.475350	-3.003734	-2.202136
6	-0.753354	-4.895459	-1.439706
1	1.261892	-4.478843	-2.091685
1	-2.852566	-5.061010	-0.967964
1	-0.481799	-5.806561	-0.914659
6	-3.629302	2.757323	1.756604
6	-2.507306	1.967302	1.428706
6	-1.679552	1.527891	2.471006
6	-2.004821	1.865470	3.782054
6	-3.146912	2.629945	4.080036

6	-3.980922	3.089583	3.065584
6	-3.607969	2.618374	-0.492089
6	-2.520644	1.798868	-0.030485
1	-0.792248	0.937998	2.267508
1	-1.363434	1.532951	4.592069
1	-3.377019	2.871775	5.112277
1	-4.858488	3.687031	3.287011
1	-3.209252	0.629416	-0.525066
7	-4.273143	3.122835	0.565448
6	-5.515022	3.894082	0.546960
1	-6.296828	3.347751	1.081139
1	-5.353307	4.857342	1.037023
1	-5.838098	4.066163	-0.477548
6	-4.039314	2.863446	-1.901311
1	-4.989403	2.365017	-2.123768
1	-4.168415	3.933923	-2.085867
1	-3.288557	2.505178	-2.604508
7	-1.397614	-1.199196	0.547005
6	-2.243361	-1.906801	0.906003
6	-3.312992	-2.756715	1.295980
6	-4.536672	-2.662491	0.603813
6	-3.135621	-3.685326	2.338069
6	-5.579463	-3.510251	0.960370
1	-4.646002	-1.941803	-0.199217
6	-4.191160	-4.525005	2.679920
1	-2.188351	-3.741197	2.864055
6	-5.406838	-4.439247	1.993143
1	-6.526986	-3.450722	0.435244
1	-4.068293	-5.245566	3.481479
1	-6.224940	-5.098737	2.264920

$TS(D\text{-}E_a)_{1wat}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2540.3189058
Zero-point correction= 0.834815 (Hartree/Particle)
Thermal correction to Energy= 0.886268
Thermal correction to Enthalpy= 0.887212
Thermal correction to Gibbs Free Energy= 0.748001
Sum of electronic and zero-point Energies= -2539.484047
Sum of electronic and thermal Energies= -2539.432594
Sum of electronic and thermal Enthalpies= -2539.431650
Sum of electronic and thermal Free Energies= -2539.570861

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Cartesian Coordinates

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46	-0.054621	-0.138988	-0.042072
7	1.431525	-1.572566	0.608311
7	1.685388	1.084731	0.035492
8	4.968919	-1.289200	0.172595
8	4.602782	0.487052	2.016620
6	1.264424	-2.899538	0.694358
1	0.247312	-3.265838	0.677783
6	2.350700	-3.764163	0.794823
1	2.184808	-4.831031	0.894530
6	3.639095	-3.250132	0.689071
1	4.494057	-3.915977	0.659861
6	3.813518	-1.869467	0.548203
6	2.670757	-1.036257	0.633366
6	2.736300	0.428446	0.601707

6	3.821872	1.146807	1.146518
6	3.960473	2.501743	0.825714
1	4.813146	3.064600	1.189287
6	2.962287	3.107497	0.073700
1	3.025939	4.153090	-0.204851
6	1.814955	2.385889	-0.254001
1	0.984368	2.859274	-0.749458
6	7.266000	-1.370667	-0.402733
1	7.007601	-1.928450	-1.306199
1	8.273743	-1.659401	-0.093105
1	7.273141	-0.304707	-0.648836
6	6.271533	-1.669903	0.709500
1	6.279446	-2.744051	0.923917
6	6.529325	-0.889834	2.008748
1	7.600377	-0.931236	2.233130
1	6.009098	-1.366191	2.846899
6	6.062168	0.567297	1.959518
1	6.341030	1.038002	1.009518
6	6.558960	1.390368	3.138756
1	6.154338	2.405505	3.110806
1	7.650590	1.456031	3.122579
1	6.252273	0.927555	4.081051
6	-1.565918	1.369188	-0.626376
6	-1.215820	2.731028	-0.058321
6	-1.242487	3.896483	-0.846014
6	-0.958793	2.867398	1.317085
6	-0.985664	5.147437	-0.280995
1	-1.435822	3.829807	-1.909940
6	-0.699113	4.115380	1.879044
1	-0.941751	1.986599	1.948285
6	-0.706678	5.262561	1.081529
1	-1.002948	6.031785	-0.910799
1	-0.488588	4.191454	2.941365
1	-0.502577	6.234994	1.518206
6	-1.256685	1.109507	-2.061869
8	-1.833707	0.276406	-2.796694
8	-0.234542	1.814953	-2.536997
6	0.430694	1.344862	-3.769278
1	0.910977	2.245409	-4.151489
1	-0.332636	1.005074	-4.469065
6	1.424609	0.271826	-3.421836
6	2.740755	0.614519	-3.086735
6	1.029970	-1.072870	-3.370879
6	3.652097	-0.369635	-2.705690
1	3.051273	1.655225	-3.125250
6	1.942669	-2.059233	-2.992729
1	0.011328	-1.338629	-3.633942
6	3.252785	-1.707969	-2.661015
1	4.669021	-0.099644	-2.441955
1	1.636871	-3.100945	-2.972442
1	3.965809	-2.473484	-2.372945
6	-4.705827	1.118380	1.408440
6	-3.386231	0.663192	1.204205
6	-2.756147	-0.018244	2.256885
6	-3.462766	-0.255665	3.433689
6	-4.796900	0.164335	3.584838
6	-5.439879	0.864283	2.568631
6	-4.097618	1.861117	-0.628396
6	-3.004083	1.047235	-0.168677
1	-1.728275	-0.348740	2.170825

1	-2.972501	-0.771287	4.253448
1	-5.324817	-0.042722	4.509713
1	-6.461869	1.207737	2.684931
1	-3.559218	-0.061198	-0.968119
7	-5.098790	1.843695	0.275779
6	-6.421781	2.456127	0.156584
1	-6.463228	3.103457	-0.716543
1	-7.192609	1.684433	0.076579
1	-6.613000	3.061720	1.045147
6	-4.206760	2.590290	-1.926697
1	-5.192972	2.478954	-2.385603
1	-4.026772	3.660276	-1.771385
1	-3.464442	2.227786	-2.636316
8	-3.745856	-0.903366	-1.808364
1	-2.938809	-0.528544	-2.367530
7	-1.494374	-1.582391	-0.073138
6	-2.269606	-2.438902	0.034730
6	-3.254131	-3.450541	0.194073
6	-3.223606	-4.598437	-0.620716
6	-4.254278	-3.274522	1.171557
6	-4.200667	-5.573294	-0.449124
1	-2.448859	-4.713885	-1.371557
6	-5.221509	-4.262069	1.326281
1	-4.257032	-2.383877	1.791157
6	-5.195094	-5.405973	0.520975
1	-4.188906	-6.463293	-1.069317
1	-5.995580	-4.143417	2.077244
1	-5.952852	-6.172324	0.650409
1	-4.572349	-0.742800	-2.289797

E_a

Number of imaginary frequencies : 0 Electronic energy : HF=-2463.8793351
Zero-point correction= 0.813464 (Hartree/Particle)
Thermal correction to Energy= 0.864063
Thermal correction to Enthalpy= 0.865007
Thermal correction to Gibbs Free Energy= 0.725656
Sum of electronic and zero-point Energies= -2463.065871
Sum of electronic and thermal Energies= -2463.015272
Sum of electronic and thermal Enthalpies= -2463.014328
Sum of electronic and thermal Free Energies= -2463.153680

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Cartesian Coordinates

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46	0.586266	-0.572540	-1.107004
7	1.903398	-1.970752	-0.223456
7	2.404905	0.435027	-1.370020
8	5.471814	-2.048227	-0.417576
8	5.173616	0.171378	0.867520
6	1.602573	-3.221512	0.142468
1	0.556153	-3.497689	0.121861
6	2.602601	-4.121541	0.510622
1	2.334689	-5.125302	0.821044
6	3.935787	-3.744699	0.397474
1	4.725269	-4.463719	0.584104
6	4.248891	-2.447694	-0.034555
6	3.185436	-1.534767	-0.231244
6	3.379281	-0.129607	-0.605037
6	4.487807	0.637329	-0.183927

6	4.729151	1.864699	-0.810100
1	5.609929	2.442309	-0.552056
6	3.797214	2.345239	-1.724789
1	3.950472	3.288610	-2.236640
6	2.616738	1.635766	-1.932219
1	1.834963	2.031223	-2.566454
6	7.779643	-2.492033	-0.760554
1	7.513886	-3.250758	-1.500022
1	8.730053	-2.772679	-0.299056
1	7.915908	-1.540455	-1.282585
6	6.697658	-2.384193	0.303181
1	6.574796	-3.351943	0.800921
6	6.962971	-1.298900	1.360801
1	8.013190	-1.358859	1.664882
1	6.360339	-1.485300	2.256587
6	6.638173	0.121221	0.890083
1	7.000215	0.292906	-0.129836
6	7.151469	1.193694	1.839194
1	6.843984	2.191188	1.513642
1	8.243941	1.171276	1.882523
1	6.761508	1.027493	2.847641
6	-1.922588	1.808777	-0.077333
6	-1.903323	1.132305	-1.338752
6	-3.026122	0.544876	-1.986307
6	-0.627595	1.037975	-2.044378
6	-2.904541	-0.034932	-3.235601
1	-3.994404	0.568826	-1.509806
6	-0.568619	0.489080	-3.372613
1	0.079900	1.814188	-1.779648
6	-1.679041	-0.083696	-3.944637
1	-3.793468	-0.451214	-3.702879
1	0.369399	0.538384	-3.918687
1	-1.635201	-0.528562	-4.932346
6	-3.030416	1.880467	0.775878
8	-2.980638	2.553324	1.918154
8	-4.171890	1.280263	0.530394
6	-5.325282	1.508810	1.419822
1	-5.526974	2.584476	1.413426
1	-5.045633	1.213382	2.433265
6	-6.477698	0.704609	0.891251
6	-6.840862	0.779172	-0.460676
6	-7.234323	-0.083144	1.763827
6	-7.941443	0.065297	-0.933166
1	-6.269343	1.407381	-1.138555
6	-8.351340	-0.779745	1.295643
1	-6.959921	-0.145666	2.813538
6	-8.703269	-0.711187	-0.053351
1	-8.220883	0.131925	-1.980231
1	-8.945799	-1.371913	1.984675
1	-9.573451	-1.248831	-0.417221
6	1.423125	2.571034	1.397444
6	0.296278	1.716425	1.287711
6	0.317019	0.465877	1.928135
6	1.456730	0.093464	2.633558
6	2.569723	0.953234	2.723344
6	2.566287	2.206108	2.115273
6	-0.107066	3.628958	0.115747
6	-0.671875	2.406169	0.463953
1	-0.546230	-0.190328	1.871198
1	1.489013	-0.869655	3.133482

1	3.446605	0.635631	3.276696
1	3.420876	2.869328	2.197981
1	-2.086666	2.946927	1.988790
7	1.152825	3.726267	0.678690
6	2.057320	4.864793	0.619723
1	2.200655	5.297470	1.614575
1	3.029140	4.547143	0.229346
1	1.651849	5.631154	-0.039296
6	-0.686164	4.700058	-0.749663
1	-0.803611	5.646021	-0.209512
1	-0.060443	4.900278	-1.627140
1	-1.671281	4.389492	-1.103197
7	-1.094594	-1.625877	-0.605591
6	-2.114207	-2.009531	-0.203742
6	-3.373529	-2.443112	0.287914
6	-3.480882	-2.906169	1.614359
6	-4.503884	-2.372276	-0.550858
6	-4.726349	-3.297687	2.092998
1	-2.601377	-2.955693	2.248004
6	-5.739757	-2.762272	-0.052235
1	-4.400701	-2.008968	-1.566281
6	-5.850424	-3.222570	1.263689
1	-4.822520	-3.659805	3.111115
1	-6.622161	-2.685093	-0.676333
1	-6.821551	-3.519272	1.645230

E_b

Number of imaginary frequencies : 0 Electronic energy : HF=-2463.8688521
Zero-point correction= 0.813430 (Hartree/Particle)
Thermal correction to Energy= 0.863888
Thermal correction to Enthalpy= 0.864832
Thermal correction to Gibbs Free Energy= 0.725386
Sum of electronic and zero-point Energies= -2463.055422
Sum of electronic and thermal Energies= -2463.004964
Sum of electronic and thermal Enthalpies= -2463.004020
Sum of electronic and thermal Free Energies= -2463.143466

Cartesian Coordinates

46	-0.632243	-0.291030	0.286205
7	-2.293830	-1.154614	1.166655
7	-2.086939	0.915544	-0.511199
8	-5.551932	0.257535	1.543612
8	-5.505560	0.058112	-1.031688
6	-2.271380	-2.112493	2.102428
1	-1.320232	-2.594186	2.286888
6	-3.430251	-2.447538	2.802646
1	-3.397536	-3.242498	3.539199
6	-4.591989	-1.709482	2.604717
1	-5.468517	-1.896254	3.214576
6	-4.596014	-0.673222	1.658577
6	-3.442845	-0.496513	0.858739
6	-3.340015	0.459053	-0.243620
6	-4.419910	0.841478	-1.066438
6	-4.238509	1.918874	-1.943604
1	-5.070879	2.280200	-2.537211
6	-2.964051	2.454627	-2.099591
1	-2.782620	3.266734	-2.794392

6	-1.890227	1.876577	-1.422886
1	-0.865189	2.160481	-1.622226
6	-7.610532	1.188496	2.280376
1	-7.173095	1.349806	3.268220
1	-8.686925	1.037174	2.396481
1	-7.450533	2.091403	1.683937
6	-6.986018	-0.026659	1.612105
1	-7.150924	-0.914434	2.231645
6	-7.502874	-0.294507	0.187885
1	-8.589484	-0.160136	0.182888
1	-7.309906	-1.334009	-0.098850
6	-6.866158	0.591424	-0.886622
1	-6.785289	1.631037	-0.549928
6	-7.581913	0.502259	-2.225943
1	-7.070218	1.090138	-2.992342
1	-8.603444	0.881638	-2.133435
1	-7.627298	-0.536534	-2.565216
6	3.374283	0.713392	-0.705310
6	4.657757	0.037342	-1.019361
6	4.889454	-0.642813	-2.228748
6	5.684400	0.069791	-0.057488
6	6.102679	-1.289501	-2.457609
1	4.130633	-0.643200	-3.002588
6	6.894393	-0.581749	-0.286607
1	5.519672	0.598747	0.875701
6	7.107833	-1.266320	-1.485711
1	6.271009	-1.798290	-3.401793
1	7.672073	-0.553147	0.470313
1	8.054868	-1.764020	-1.669892
6	2.188660	0.157188	-1.076235
8	0.964912	0.795926	-0.835827
8	2.026866	-1.066011	-1.594281
6	1.403659	-1.178125	-2.918655
1	1.920281	-2.028177	-3.371709
1	1.634946	-0.279350	-3.498542
6	-0.080660	-1.421449	-2.836223
6	-0.981542	-0.594250	-3.514342
6	-0.573386	-2.501140	-2.086886
6	-2.355735	-0.837183	-3.443116
1	-0.609256	0.237403	-4.106959
6	-1.946311	-2.735207	-2.003554
1	0.123102	-3.152898	-1.567762
6	-2.841513	-1.900212	-2.679986
1	-3.044826	-0.194844	-3.981809
1	-2.316773	-3.574583	-1.423001
1	-3.910398	-2.080406	-2.617910
6	2.836821	3.763211	1.376989
6	2.563447	2.390328	1.132869
6	1.679203	1.713206	1.997675
6	1.042245	2.428315	3.009415
6	1.294950	3.799397	3.198722
6	2.209170	4.480978	2.396281
6	4.141523	3.117445	-0.347036
6	3.390841	1.993862	0.014395
1	1.542678	0.642191	1.911972
1	0.363582	1.913406	3.682602
1	0.792031	4.330776	3.999950
1	2.428590	5.529276	2.568792
1	1.166259	1.624034	-0.343046
7	3.806753	4.169497	0.475152

6	4.353079	5.520982	0.439385
1	3.596016	6.234565	0.099788
1	4.690270	5.808430	1.438758
1	5.205586	5.561688	-0.235993
6	5.135104	3.273589	-1.451998
1	4.874078	4.109351	-2.109846
1	6.141440	3.460217	-1.059626
1	5.182207	2.366651	-2.053033
7	0.771893	-1.580184	1.078973
6	1.743944	-2.176776	1.303186
6	2.959064	-2.872875	1.531601
6	3.254995	-3.392032	2.808195
6	3.868160	-2.997187	0.460508
6	4.469145	-4.039553	3.003725
1	2.545544	-3.283573	3.621802
6	5.080002	-3.641419	0.682311
1	3.625316	-2.578734	-0.508330
6	5.378140	-4.161688	1.945683
1	4.711041	-4.446861	3.979572
1	5.793418	-3.724523	-0.129957
1	6.325755	-4.665023	2.110221

E_c

Number of imaginary frequencies : 0 Electronic energy : HF=-2463.875655
Zero-point correction= 0.813685 (Hartree/Particle)
Thermal correction to Energy= 0.864052
Thermal correction to Enthalpy= 0.864997
Thermal correction to Gibbs Free Energy= 0.725108
Sum of electronic and zero-point Energies= -2463.061970
Sum of electronic and thermal Energies= -2463.011603
Sum of electronic and thermal Enthalpies= -2463.010658
Sum of electronic and thermal Free Energies= -2463.150547

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Cartesian Coordinates

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46	0.046296	-0.002479	0.057388
7	1.502638	1.500093	-0.443302
7	1.818592	-1.177744	-0.030708
8	4.964451	1.306303	0.439338
8	4.863035	-0.232522	-1.672320
6	1.279124	2.821211	-0.463810
1	0.250469	3.143334	-0.549914
6	2.328965	3.730110	-0.343277
1	2.126001	4.794180	-0.393541
6	3.616157	3.265032	-0.090354
1	4.424719	3.963327	0.093257
6	3.840334	1.883642	-0.016985
6	2.760476	1.019790	-0.310757
6	2.891479	-0.435942	-0.420710
6	4.016162	-1.042658	-1.016922
6	4.114851	-2.439054	-0.999433
1	4.989264	-2.927555	-1.414639
6	3.042472	-3.174423	-0.510783
1	3.062849	-4.258270	-0.507349
6	1.890114	-2.514361	-0.085801
1	1.013112	-3.064671	0.220046
6	7.189221	1.345457	1.255828
1	6.823472	1.772191	2.192533

1	8.213343	1.690762	1.092088
1	7.203196	0.256680	1.359170
6	6.304787	1.775033	0.094953
1	6.301557	2.868508	0.026539
6	6.717931	1.181757	-1.261763
1	7.803260	1.283612	-1.365859
1	6.265408	1.752665	-2.080086
6	6.311696	-0.281736	-1.459474
1	6.501656	-0.872662	-0.556131
6	6.972681	-0.916802	-2.674063
1	6.618161	-1.938627	-2.831624
1	8.057687	-0.949781	-2.540164
1	6.750786	-0.336675	-3.574283
6	-1.339056	-1.494724	1.009926
6	-0.511919	-2.413521	1.883487
6	0.413481	-1.926013	2.828638
6	-0.635338	-3.808265	1.740119
6	1.174472	-2.798763	3.599795
1	0.557639	-0.858948	2.943801
6	0.129809	-4.681581	2.515670
1	-1.321796	-4.214449	1.007277
6	1.036555	-4.182436	3.449658
1	1.883069	-2.398363	4.318219
1	0.012942	-5.752919	2.385529
1	1.631675	-4.860227	4.053235
6	-2.107593	-0.488498	1.760718
8	-3.259281	-0.061938	1.314796
8	-1.687308	-0.008274	2.879362
6	-2.382541	1.137471	3.536618
1	-1.991214	1.077620	4.551807
1	-3.453667	0.933263	3.537375
6	-2.025459	2.417990	2.841985
6	-0.698012	2.869601	2.856537
6	-3.002598	3.162711	2.173973
6	-0.356094	4.054751	2.208046
1	0.060924	2.299429	3.385668
6	-2.660550	4.351846	1.526870
1	-4.032880	2.819088	2.169543
6	-1.337115	4.796869	1.541550
1	0.669852	4.407498	2.235675
1	-3.425809	4.928756	1.017736
1	-1.074252	5.729998	1.052208
6	-3.057335	-3.109697	-1.943786
6	-1.977439	-2.331529	-1.451694
6	-0.978170	-1.935243	-2.360401
6	-1.088578	-2.299828	-3.696137
6	-2.181510	-3.059410	-4.159283
6	-3.181188	-3.474527	-3.288835
6	-3.394470	-2.850984	0.267100
6	-2.217307	-2.145762	-0.034702
1	-0.120899	-1.357444	-2.030826
1	-0.316607	-1.998764	-4.397447
1	-2.239567	-3.329583	-5.208535
1	-4.020081	-4.066436	-3.638895
1	-3.438704	-0.614122	0.505354
7	-3.899609	-3.407144	-0.883846
6	-5.119159	-4.193744	-1.025426
1	-5.783939	-3.725895	-1.757266
1	-4.879576	-5.206516	-1.362194
1	-5.640728	-4.254848	-0.071833

6	-4.030603	-3.094766	1.602568
1	-5.009727	-2.611762	1.698122
1	-4.173504	-4.166084	1.775577
1	-3.389992	-2.732201	2.408128
7	-1.500265	1.218135	-0.452221
6	-2.319734	1.885640	-0.931664
6	-3.344861	2.692108	-1.495401
6	-4.639186	2.642651	-0.940960
6	-3.054313	3.530423	-2.588194
6	-5.638295	3.441645	-1.484693
1	-4.840735	1.992148	-0.096941
6	-4.067251	4.323655	-3.118041
1	-2.054485	3.551171	-3.008944
6	-5.352702	4.280739	-2.568295
1	-6.639343	3.413283	-1.067438
1	-3.856791	4.973666	-3.960625
1	-6.137383	4.902549	-2.987412

E_d

Number of imaginary frequencies : 0 Electronic energy : HF=-2464.4346092
Zero-point correction= 0.809612 (Hartree/Particle)
Thermal correction to Energy= 0.860163
Thermal correction to Enthalpy= 0.861107
Thermal correction to Gibbs Free Energy= 0.721053
Sum of electronic and zero-point Energies= -2463.624997
Sum of electronic and thermal Energies= -2463.574446
Sum of electronic and thermal Enthalpies= -2463.573502
Sum of electronic and thermal Free Energies= -2463.713556

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Cartesian Coordinates

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46	-1.980541	-0.528920	0.123751
7	-3.388757	0.583145	-1.060509
7	-3.758574	-0.996087	1.129434
8	-6.813892	-0.359918	-1.440950
8	-6.865387	0.758446	0.905599
6	-3.133161	1.216101	-2.209581
1	-2.102969	1.481357	-2.401410
6	-4.150304	1.506726	-3.114036
1	-3.921165	2.044925	-4.024857
6	-5.434406	1.038187	-2.871933
1	-6.213209	1.173575	-3.611105
6	-5.694309	0.337009	-1.689511
6	-4.653521	0.225072	-0.743278
6	-4.830853	-0.354780	0.592998
6	-6.010258	-0.173274	1.344202
6	-6.155125	-0.872780	2.544165
1	-7.070674	-0.788451	3.115536
6	-5.082247	-1.613571	3.019056
1	-5.146355	-2.149047	3.957454
6	-3.882752	-1.606618	2.317037
1	-3.008634	-2.095935	2.720929
6	-8.994145	-1.120912	-1.991937
1	-9.044433	-1.734079	-1.089400
1	-8.566681	-1.726639	-2.792143
1	-10.010251	-0.839018	-2.275292
6	-8.157337	0.125996	-1.763481
1	-8.115753	0.710556	-2.686154

6	-8.660351	1.018836	-0.619063
1	-9.745302	1.116723	-0.713046
1	-8.242530	2.025897	-0.708852
6	-8.308780	0.509097	0.779091
1	-8.466646	-0.570304	0.859289
6	-9.045207	1.251752	1.881021
1	-10.120423	1.078521	1.795301
1	-8.859679	2.325559	1.806772
1	-8.725778	0.917748	2.869739
6	3.435033	-1.059659	1.087169
6	2.036938	-1.322339	1.164279
6	1.150035	-0.751817	2.137358
6	1.471827	-2.277948	0.247877
6	-0.166628	-1.117480	2.196447
1	1.538438	-0.065464	2.872621
6	0.151108	-2.604100	0.273031
1	2.126092	-2.734533	-0.482719
6	-0.752914	-1.996475	1.218393
1	-0.786194	-0.734880	3.000599
1	-0.242713	-3.326935	-0.432165
1	-1.591762	-2.616138	1.517294
6	4.074055	0.027944	1.712085
8	5.387488	0.161112	1.680028
8	3.428442	0.977884	2.337477
6	4.163407	2.026704	3.105539
1	5.037071	1.562468	3.557924
1	3.443090	2.283759	3.879357
6	4.516222	3.214475	2.260369
6	5.792632	3.341778	1.701920
6	3.580499	4.239100	2.074266
6	6.131391	4.483021	0.977539
1	6.522974	2.554961	1.846992
6	3.915970	5.376701	1.344200
1	2.596382	4.159142	2.525335
6	5.195120	5.501874	0.799940
1	7.128460	4.583551	0.565302
1	3.191447	6.172375	1.217495
1	5.464212	6.395797	0.249494
6	5.784372	-2.827232	-1.215902
6	5.082859	-1.650744	-0.856482
6	5.210408	-0.501806	-1.650150
6	6.040352	-0.549281	-2.760852
6	6.740806	-1.723279	-3.096089
6	6.622150	-2.878074	-2.331510
6	4.602345	-3.294787	0.647646
6	4.333405	-1.964288	0.338078
1	4.673602	0.402922	-1.395808
1	6.155931	0.330880	-3.382363
1	7.385849	-1.728175	-3.966301
1	7.164259	-3.777434	-2.596151
1	5.764740	-0.596320	1.189751
7	5.463929	-3.812475	-0.292917
6	6.050545	-5.147333	-0.299920
1	5.501972	-5.799197	0.375895
1	5.991598	-5.567337	-1.305167
1	7.097887	-5.112747	0.010786
6	4.085254	-4.105492	1.788127
1	4.897971	-4.533540	2.381463
1	3.481526	-3.479949	2.445097
1	3.456635	-4.932536	1.442062

7	-0.326366	0.214393	-0.817066
6	0.613121	0.725622	-1.247618
6	1.763324	1.383326	-1.755788
6	2.500139	2.222417	-0.901827
6	2.132952	1.214769	-3.100737
6	3.598854	2.903110	-1.407687
1	2.215718	2.334418	0.136680
6	3.234913	1.904685	-3.589008
1	1.564006	0.555556	-3.744585
6	3.959988	2.750251	-2.748028
1	4.170727	3.550747	-0.757666
1	3.528123	1.782481	-4.624254
1	4.816139	3.289155	-3.136633

E_e

Number of imaginary frequencies : 0 Electronic energy : HF=-2463.866873
Zero-point correction= 0.812983 (Hartree/Particle)
Thermal correction to Energy= 0.863848
Thermal correction to Enthalpy= 0.864792
Thermal correction to Gibbs Free Energy= 0.725088
Sum of electronic and zero-point Energies= -2463.053890
Sum of electronic anthermal Energies= -2463.003025
Sum of electronic and thermal Enthalpies= -2463.002081
Sum of electronic and thermal Free Energies= -2463.141786

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Cartesian Coordinates

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46	0.448547	0.621592	-1.328535
7	1.437576	-1.222337	-1.101468
7	2.323502	1.306146	-0.771275
8	4.969377	-1.758294	-1.054378
8	4.693422	-0.512073	1.194542
6	0.960718	-2.421958	-1.455632
1	-0.094262	-2.484402	-1.682997
6	1.803782	-3.530688	-1.535139
1	1.391042	-4.496324	-1.805142
6	3.171653	-3.369511	-1.346267
1	3.848075	-4.201679	-1.504355
6	3.673805	-2.100381	-1.022285
6	2.746153	-1.057342	-0.790264
6	3.121031	0.286109	-0.345485
6	4.202291	0.539147	0.525851
6	4.611798	1.865118	0.715286
1	5.475101	2.083399	1.333974
6	3.861455	2.885894	0.141979
1	4.144863	3.924711	0.268881
6	2.689931	2.575548	-0.547220
1	2.041958	3.345921	-0.935076
6	7.251639	-2.304910	-1.418161
1	7.022380	-2.520541	-2.464133
1	8.098178	-2.925012	-1.111850
1	7.547076	-1.254395	-1.342986
6	6.047497	-2.600235	-0.537133
1	5.767228	-3.654009	-0.639380
6	6.260943	-2.271019	0.950140
1	7.250224	-2.634455	1.247060
1	5.528326	-2.802410	1.567438
6	6.133457	-0.782390	1.285348

1	6.640566	-0.162096	0.537672
6	6.614517	-0.449614	2.689632
1	6.451461	0.604712	2.927860
1	7.684459	-0.657029	2.780615
1	6.079683	-1.053217	3.428376
6	-1.991299	1.429857	1.170997
6	-3.419405	1.228311	0.830787
6	-4.193445	0.189987	1.386553
6	-4.055505	2.107178	-0.068637
6	-5.532494	0.030632	1.041858
1	-3.741593	-0.497855	2.089072
6	-5.397459	1.945126	-0.412672
1	-3.500835	2.937613	-0.494143
6	-6.143876	0.902463	0.137518
1	-6.103262	-0.779613	1.485112
1	-5.860792	2.641287	-1.105708
1	-7.189225	0.776452	-0.125412
6	-1.139298	0.429121	1.527765
8	0.167947	0.621691	1.868812
8	-1.473326	-0.864725	1.471506
6	-0.839891	-1.804984	2.394791
1	-1.028588	-1.466754	3.419217
1	0.238060	-1.811398	2.217675
6	-1.463215	-3.141129	2.115888
6	-2.727391	-3.450592	2.633381
6	-0.826298	-4.057817	1.270643
6	-3.348106	-4.656517	2.306469
1	-3.224318	-2.746418	3.295446
6	-1.446349	-5.264033	0.938300
1	0.161122	-3.826945	0.879828
6	-2.710107	-5.562964	1.454031
1	-4.322472	-4.894076	2.722227
1	-0.943768	-5.975062	0.289380
1	-3.189265	-6.504807	1.205078
6	-0.265956	4.496764	-0.079938
6	-0.778883	3.177713	-0.281125
6	-0.686555	2.572066	-1.582666
6	-0.053090	3.333780	-2.619613
6	0.475999	4.591722	-2.375379
6	0.340694	5.205155	-1.103337
6	-1.229967	3.830288	1.833531
6	-1.367556	2.757061	0.932564
1	-1.530646	1.956110	-1.883986
1	-0.029890	2.925305	-3.624855
1	0.947541	5.148228	-3.177876
1	0.697993	6.219947	-0.954852
1	0.321679	1.577169	1.923606
7	-0.555547	4.862939	1.227706
6	-0.283177	6.180106	1.798263
1	0.719553	6.504299	1.511683
1	-1.014527	6.913982	1.447079
1	-0.328235	6.126630	2.885150
6	-1.734864	3.901164	3.233053
1	-0.928743	4.086010	3.952165
1	-2.470423	4.704995	3.348147
1	-2.218350	2.956515	3.486959
7	-1.344890	-0.299213	-1.686211
6	-2.386754	-0.810571	-1.617905
6	-3.630959	-1.489625	-1.574627
6	-3.753027	-2.636429	-0.764452

6	-4.713726	-1.014607	-2.338763
6	-4.968023	-3.309202	-0.737222
1	-2.916603	-2.975589	-0.166223
6	-5.919735	-1.705392	-2.296901
1	-4.605558	-0.119974	-2.941234
6	-6.045797	-2.848826	-1.502000
1	-5.070241	-4.191371	-0.115169
1	-6.762215	-1.351403	-2.881275
1	-6.990696	-3.382663	-1.476401

E_f

Number of imaginary frequencies : 0 Electronic energy : HF=-2463.8607307
Zero-point correction= 0.813138 (Hartree/Particle)
Thermal correction to Energy= 0.863945
Thermal correction to Enthalpy= 0.864889
Thermal correction to Gibbs Free Energy= 0.723408
Sum of electronic and zero-point Energies= -2463.047593
Sum of electronic and thermal Energies= -2462.996786
Sum of electronic and thermal Enthalpies= -2462.995841
Sum of electronic and thermal Free Energies= -2463.137323

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Cartesian Coordinates

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46	-0.718038	1.085398	0.695031
7	-2.346183	2.057113	-0.162582
7	-2.075271	-0.474164	0.664863
8	-5.136376	0.564633	-1.817258
8	-5.635153	-0.245300	0.585208
6	-2.328263	3.297625	-0.668504
1	-1.468207	3.909679	-0.429613
6	-3.372614	3.754142	-1.471262
1	-3.353394	4.770627	-1.847863
6	-4.387583	2.878047	-1.841006
1	-5.150569	3.191708	-2.544339
6	-4.375781	1.563723	-1.350694
6	-3.387481	1.215220	-0.399948
6	-3.320529	-0.076453	0.285779
6	-4.444422	-0.856405	0.626031
6	-4.229362	-2.161236	1.095050
1	-5.076126	-2.804141	1.307926
6	-2.928568	-2.586214	1.340246
1	-2.723313	-3.584789	1.707528
6	-1.868716	-1.693393	1.175215
1	-0.850504	-1.951784	1.430074
6	-6.790082	-0.219431	-3.332395
1	-6.145686	0.065070	-4.167369
1	-7.831650	-0.150929	-3.657073
1	-6.576428	-1.260728	-3.074146
6	-6.557444	0.697502	-2.141297
1	-6.769244	1.733520	-2.426115
6	-7.384355	0.330188	-0.897048
1	-8.402442	0.086307	-1.217761
1	-7.460578	1.189661	-0.222356
6	-6.805488	-0.828532	-0.079687
1	-6.455275	-1.639154	-0.728954
6	-7.773861	-1.348216	0.972439
1	-7.316875	-2.129150	1.585539
1	-8.661400	-1.769669	0.491970

1	-8.088890	-0.536209	1.633758
6	2.072537	-1.068702	-0.421849
6	1.125599	-2.214605	-0.521423
6	0.247816	-2.303691	-1.611478
6	1.128867	-3.234738	0.443038
6	-0.634406	-3.379257	-1.720271
6	0.253758	-4.315801	0.326218
6	-0.634399	-4.386840	-0.751451
6	1.995526	-0.212221	0.629575
8	2.914202	0.735480	0.967358
8	0.890860	-0.172632	1.442674
6	1.137460	-0.115478	2.943146
1	0.151802	0.125892	3.339771
1	1.826006	0.710927	3.112457
6	1.644260	-1.438138	3.400292
6	0.746599	-2.422504	3.837158
6	3.012204	-1.735590	3.315777
6	1.208841	-3.692589	4.177948
1	-0.312574	-2.189815	3.915665
6	3.473858	-3.008305	3.649656
1	3.707089	-0.970024	2.983166
6	2.571825	-3.987717	4.076817
1	0.513491	-4.448720	4.528495
1	4.532923	-3.236106	3.584548
1	2.932846	-4.976349	4.342400
6	4.753472	-1.355884	-2.972298
6	3.895899	-1.970541	-2.029983
6	3.974818	-3.359284	-1.839216
6	4.888703	-4.085893	-2.595447
6	5.728971	-3.453696	-3.531290
6	5.676115	-2.076831	-3.733541
6	3.498986	0.285588	-2.059429
6	3.108004	-0.911048	-1.433731
1	3.328563	-3.857846	-1.125897
1	4.955475	-5.161254	-2.465289
1	6.429932	-4.048894	-4.107365
1	6.323737	-1.593008	-4.456817
7	4.493717	0.013382	-2.964706
6	5.146078	0.957601	-3.860141
1	4.773978	0.847928	-4.884142
1	4.970829	1.978592	-3.522869
1	6.223863	0.776910	-3.856628
6	2.904981	1.652789	-1.921316
1	3.554054	2.346437	-1.371250
1	2.705981	2.097388	-2.901324
1	1.958195	1.590177	-1.383298
1	3.727268	0.525163	0.476971
7	0.550839	2.726594	0.823146
6	1.427397	3.481474	0.926414
6	2.508940	4.393885	1.057042
6	2.336294	5.745576	0.699875
6	3.741834	3.922858	1.553332
6	3.406691	6.622235	0.840738
1	1.379923	6.094371	0.324867
6	4.798471	4.816602	1.687596
1	3.845953	2.879432	1.827173
6	4.632210	6.160050	1.332538
1	3.286508	7.666141	0.571466
1	5.751593	4.470237	2.073194
1	5.461444	6.851632	1.442946

1	0.268478	-1.531141	-2.374678
1	-1.309804	-3.439966	-2.568213
1	-1.307458	-5.233438	-0.847735
1	0.277434	-5.106580	1.070092
1	1.830867	-3.189591	1.267494

E_{free}

Number of imaginary frequencies : 0 Electronic energy : HF=-1171.7706495
Zero-point correction= 0.419068 (Hartree/Particle)
Thermal correction to Energy= 0.443771
Thermal correction to Enthalpy= 0.444715
Thermal correction to Gibbs Free Energy= 0.361656
Sum of electronic and zero-point Energies= -1171.351582
Sum of electronic and thermal Energies= -1171.326878
Sum of electronic and thermal Enthalpies= -1171.325934
Sum of electronic and thermal Free Energies= -1171.408994

Cartesian Coordinates

6	-0.413093	0.302427	0.347212
6	0.105320	1.599917	-0.146645
6	-0.616383	2.297373	-1.136488
6	1.281291	2.200964	0.346869
6	-0.173604	3.523732	-1.627125
1	-1.530610	1.859758	-1.525373
6	1.724326	3.426800	-0.150311
1	1.847126	1.705241	1.125339
6	1.003455	4.097223	-1.140273
1	-0.748835	4.031205	-2.397213
1	2.634712	3.864665	0.250948
1	1.349449	5.053545	-1.521959
6	0.389839	-0.707487	0.780111
8	-0.048688	-1.920863	1.204547
8	1.730448	-0.599375	0.851897
6	2.505599	-1.748436	0.451535
1	2.069901	-2.165665	-0.466951
1	2.454073	-2.522021	1.224357
6	3.925657	-1.300296	0.214356
6	4.992087	-2.130286	0.574571
6	4.192158	-0.074168	-0.409284
6	6.308817	-1.749295	0.307700
1	4.793100	-3.077914	1.069638
6	5.507679	0.310446	-0.666283
1	3.366975	0.579879	-0.672261
6	6.569510	-0.526611	-0.312634
1	7.128541	-2.402370	0.593558
1	5.704164	1.266119	-1.144280
1	7.593368	-0.224942	-0.514744
6	-3.965611	-0.804766	-0.111478
6	-2.580049	-0.982217	-0.374437
6	-2.173199	-2.036893	-1.210835
6	-3.138350	-2.887065	-1.739858
6	-4.505909	-2.702901	-1.453040
6	-4.938642	-1.659974	-0.637643
6	-2.837830	0.821923	0.975921
6	-1.875052	0.061819	0.335672
1	-1.119954	-2.173728	-1.437887
1	-2.836582	-3.705329	-2.387095

1	-5.236750	-3.385551	-1.876442
1	-5.993218	-1.520771	-0.420188
1	-1.012344	-1.954443	1.094667
7	-4.100362	0.310033	0.695184
6	-5.367306	0.792712	1.206671
1	-5.246965	1.799750	1.606259
1	-6.104519	0.831967	0.398772
1	-5.755331	0.143609	2.001298
6	-2.645816	2.031175	1.830337
1	-3.115386	1.917213	2.814536
1	-1.578830	2.202907	1.976980
1	-3.062992	2.931840	1.362479

TS(E_{free}-P)

Number of imaginary frequencies : 1 Electronic energy : HF=-1171.6931417
Zero-point correction= 0.413391 (Hartree/Particle)
Thermal correction to Energy= 0.437852
Thermal correction to Enthalpy= 0.438796
Thermal correction to Gibbs Free Energy= 0.355413
Sum of electronic and zero-point Energies= -1171.279757
Sum of electronic and thermal Energies= -1171.255296
Sum of electronic and thermal Enthalpies= -1171.254352
Sum of electronic and thermal Free Energies= -1171.337736

Cartesian Coordinates

6	-0.639119	0.779655	0.883246
6	-0.203593	1.912533	0.026924
6	-1.010056	2.414755	-1.009230
6	1.031212	2.553566	0.259659
6	-0.594236	3.496266	-1.786150
1	-1.965093	1.939541	-1.208294
6	1.453666	3.622878	-0.525927
1	1.662372	2.215578	1.078667
6	0.641437	4.104087	-1.557111
1	-1.238012	3.859603	-2.583120
1	2.412789	4.092445	-0.322695
1	0.964922	4.943228	-2.166080
6	0.379411	-0.140586	1.354004
8	0.174678	-0.479126	2.581306
8	1.424861	-0.546416	0.679202
6	2.490520	-1.243094	1.383682
1	2.198190	-2.291415	1.494138
1	2.570287	-0.809387	2.386725
6	3.764662	-1.095728	0.593004
6	4.739838	-2.095878	0.673743
6	4.008751	0.044200	-0.182784
6	5.953256	-1.954774	-0.000680
1	4.550426	-2.989235	1.264381
6	5.218486	0.177248	-0.865330
1	3.246781	0.812213	-0.268015
6	6.194770	-0.817069	-0.773098
1	6.703265	-2.737312	0.068716
1	5.396347	1.060317	-1.472236
1	7.135456	-0.709364	-1.305237
6	-3.482882	-1.268200	-0.471050
6	-2.100429	-0.948756	-0.446360
6	-1.224942	-1.622397	-1.312041

6	-1.740203	-2.595209	-2.162584
6	-3.114855	-2.907463	-2.163650
6	-4.005910	-2.249689	-1.318707
6	-3.172257	0.358171	1.065997
6	-1.921291	0.083700	0.546084
1	-0.166432	-1.379289	-1.312312
1	-1.075594	-3.124075	-2.839831
1	-3.487415	-3.674912	-2.836065
1	-5.064333	-2.492577	-1.321428
1	-0.639465	0.434276	2.421475
7	-4.120430	-0.450829	0.446997
6	-5.540350	-0.504817	0.725151
1	-5.828203	0.335738	1.356729
1	-6.110899	-0.444163	-0.207780
1	-5.812408	-1.435909	1.237542
6	-3.544681	1.369053	2.098760
1	-4.043402	0.915545	2.964166
1	-2.635957	1.864595	2.446955
1	-4.214160	2.139984	1.697244

TS(E_a-P)

Number of imaginary frequencies : 1 Electronic energy : HF=-2463.8084202
Zero-point correction= 0.808425 (Hartree/Particle)
Thermal correction to Energy= 0.858505
Thermal correction to Enthalpy= 0.859450
Thermal correction to Gibbs Free Energy= 0.722798
Sum of electronic and zero-point Energies= -2462.999812
Sum of electronic and thermal Energies= -2462.949732
Sum of electronic and thermal Enthalpies= -2462.948787
Sum of electronic and thermal Free Energies= -2463.085439

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Cartesian Coordinates

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46	0.332837	-0.614225	-1.130605
7	1.668904	-1.976462	-0.191115
7	2.144277	0.320650	-1.546297
8	5.236501	-2.066886	-0.412300
8	4.963148	0.275556	0.641876
6	1.375611	-3.195883	0.277493
1	0.329280	-3.474007	0.289327
6	2.380215	-4.062665	0.705456
1	2.118757	-5.039494	1.096798
6	3.711623	-3.692384	0.549546
1	4.505077	-4.393064	0.783546
6	4.018062	-2.434196	0.011525
6	2.950226	-1.540359	-0.249658
6	3.138223	-0.175360	-0.754665
6	4.258245	0.621207	-0.449903
6	4.494320	1.772238	-1.209617
1	5.378172	2.372424	-1.027585
6	3.549174	2.157153	-2.151677
1	3.686678	3.048818	-2.751054
6	2.354358	1.447299	-2.243781
1	1.556685	1.789990	-2.888007
6	7.535464	-2.571581	-0.739744
1	7.251766	-3.402348	-1.389704
1	8.490256	-2.811030	-0.264267
1	7.672151	-1.682895	-1.362715

6	6.470785	-2.338509	0.321343
1	6.345852	-3.245144	0.922848
6	6.761458	-1.146881	1.250421
1	7.818217	-1.177298	1.535595
1	6.180322	-1.234067	2.175260
6	6.428477	0.215566	0.636760
1	6.764163	0.272826	-0.404489
6	6.968218	1.383109	1.448921
1	6.647090	2.339552	1.027645
1	8.061558	1.365085	1.460459
1	6.611776	1.326310	2.481835
6	-1.757434	1.792846	0.246225
6	-1.996353	1.202647	-1.043284
6	-3.281902	0.791975	-1.481876
6	-0.882151	1.033858	-1.967975
6	-3.456245	0.247310	-2.739179
1	-4.143762	0.893101	-0.830932
6	-1.132952	0.534254	-3.295541
1	-0.089575	1.763057	-1.842077
6	-2.383986	0.099136	-3.658250
1	-4.453986	-0.065827	-3.035075
1	-0.313440	0.511676	-4.008391
1	-2.567766	-0.309749	-4.645625
6	-2.917645	1.852644	1.184691
8	-3.314535	3.056712	1.254863
8	-3.472990	0.849957	1.777804
6	-4.833899	1.062509	2.401330
1	-4.795111	1.995294	2.964275
1	-4.911923	0.210056	3.074565
6	-5.852068	1.057585	1.305027
6	-6.335012	2.261929	0.774115
6	-6.252425	-0.161730	0.738816
6	-7.210591	2.244635	-0.312450
1	-6.020522	3.206108	1.207341
6	-7.121275	-0.175580	-0.350655
1	-5.884852	-1.094714	1.153684
6	-7.599883	1.028052	-0.878234
1	-7.590837	3.178319	-0.714228
1	-7.435472	-1.122458	-0.778373
1	-8.284865	1.017292	-1.720481
6	1.762409	2.495382	1.285773
6	0.609479	2.826762	0.528132
6	0.638323	3.953564	-0.309543
6	1.794267	4.727877	-0.352178
6	2.918682	4.397526	0.430648
6	2.921022	3.277379	1.258664
6	0.174399	0.959630	1.757146
6	-0.394992	1.842823	0.842694
1	-0.238179	4.230680	-0.889811
1	1.824870	5.613312	-0.979187
1	3.796440	5.035263	0.395255
1	3.785998	3.026977	1.864014
1	-2.372519	3.168686	0.394989
7	1.479245	1.348908	2.011080
6	2.406252	0.748496	2.960034
1	3.374232	0.587860	2.478218
1	2.541870	1.394827	3.833544
1	2.022998	-0.214421	3.295593
6	-0.422829	-0.239757	2.421105
1	0.169700	-1.140418	2.224175

1	-0.486469	-0.113054	3.507969
1	-1.429846	-0.411464	2.043030
7	-1.349455	-1.636359	-0.590839
6	-2.343151	-2.130054	-0.253133
6	-3.562132	-2.731572	0.163715
6	-4.551676	-3.026036	-0.793242
6	-3.758232	-3.027260	1.527210
6	-5.735652	-3.627457	-0.377314
1	-4.383769	-2.787239	-1.837747
6	-4.949805	-3.625749	1.924236
1	-2.985186	-2.792313	2.251445
6	-5.933942	-3.927377	0.974818
1	-6.501890	-3.868727	-1.106497
1	-5.112021	-3.863685	2.970226
1	-6.858609	-4.399598	1.291041

$TS(E_a\text{-}P)_{1wat}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2540.2955012
Zero-point correction= 0.835301 (Hartree/Particle)
Thermal correction to Energy= 0.887043
Thermal correction to Enthalpy= 0.887987
Thermal correction to Gibbs Free Energy= 0.747818
Sum of electronic and zero-point Energies= -2539.460200
Sum of electronic and thermal Energies= -2539.408459
Sum of electronic and thermal Enthalpies= -2539.407514
Sum of electronic and thermal Free Energies= -2539.547684

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Cartesian Coordinates

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46	-0.385425	-0.683153	-1.129565
7	-1.702206	-2.047016	-0.124939
7	-2.210889	0.275208	-1.456219
8	-4.756668	-1.017376	1.440154
8	-5.483429	-1.103855	-1.049598
6	-1.326475	-3.088447	0.628837
1	-0.342449	-3.496599	0.433970
6	-2.164370	-3.604280	1.616373
1	-1.851102	-4.466438	2.194544
6	-3.368463	-2.962031	1.892247
1	-3.989076	-3.293726	2.716988
6	-3.744877	-1.851063	1.126278
6	-2.920055	-1.478131	0.039964
6	-3.253816	-0.411177	-0.912351
6	-4.576760	-0.158734	-1.332777
6	-4.831624	0.982308	-2.103337
1	-5.847006	1.228076	-2.393336
6	-3.754878	1.741572	-2.543407
1	-3.904282	2.621805	-3.157565
6	-2.456892	1.324822	-2.254371
1	-1.608268	1.852115	-2.665142
6	-6.602967	-0.356907	2.773260
1	-5.921849	-0.168062	3.606779
1	-7.578647	-0.633258	3.180986
1	-6.718153	0.570851	2.204820
6	-6.069972	-1.476650	1.891694
1	-5.949397	-2.385387	2.491023
6	-6.951272	-1.785623	0.670705
1	-7.995742	-1.817459	0.998002

1	-6.712807	-2.777546	0.271983
6	-6.796557	-0.791088	-0.483320
1	-6.770928	0.242418	-0.118033
6	-7.860102	-0.963060	-1.557594
1	-7.687490	-0.288790	-2.400288
1	-8.850703	-0.748548	-1.146602
1	-7.855133	-1.988960	-1.936267
6	1.690298	1.628343	0.346031
6	1.943707	1.123595	-0.978894
6	0.836662	0.963573	-1.921813
6	3.246046	0.806312	-1.453264
6	1.103008	0.533498	-3.272738
1	0.033679	1.677958	-1.791418
6	3.437290	0.330453	-2.733033
1	4.104283	0.928685	-0.804671
6	2.366622	0.168793	-3.656449
1	0.281201	0.517859	-3.982946
1	4.448700	0.090877	-3.050360
1	2.566514	-0.180919	-4.663494
6	2.685040	1.372376	1.437667
8	2.926234	2.207395	2.321259
8	3.288707	0.186518	1.396514
6	4.518315	0.016016	2.210123
1	4.574912	-1.063025	2.350231
1	4.372959	0.515250	3.167828
6	5.684449	0.553191	1.433557
6	6.294802	-0.243689	0.454337
6	6.113737	1.874952	1.614068
6	7.319615	0.274718	-0.336385
1	5.970003	-1.270117	0.319189
6	7.142723	2.391286	0.824810
1	5.640773	2.491969	2.371979
6	7.743439	1.594215	-0.152665
1	7.796043	-0.350810	-1.085486
1	7.479991	3.411941	0.975998
1	8.546534	1.996585	-0.762305
6	-1.863871	2.602210	1.039694
6	-0.646086	2.806308	0.338552
6	-0.581418	3.830848	-0.626147
6	-1.710809	4.613834	-0.859116
6	-2.905381	4.392829	-0.147087
6	-2.997466	3.386044	0.812340
6	-0.388308	1.063522	1.779571
6	0.288816	1.815800	0.820650
1	0.327695	4.005685	-1.197721
1	-1.668917	5.409659	-1.596021
1	-3.766129	5.024488	-0.341277
1	-3.915926	3.226429	1.367592
1	2.022341	3.122646	0.315518
7	-1.680893	1.540696	1.909183
6	-2.684223	1.116499	2.875364
1	-2.362133	0.200107	3.367666
1	-2.836657	1.887731	3.637323
1	-3.629485	0.914594	2.367416
6	0.088822	-0.109550	2.574227
1	0.214879	0.136968	3.634907
1	-0.615784	-0.945443	2.506638
1	1.046487	-0.460308	2.190740
8	2.273245	4.128974	0.834511
1	2.556304	3.655240	1.693023

7	1.306446	-1.766733	-0.783157
6	2.335323	-2.269329	-0.599693
6	3.598905	-2.889294	-0.399198
6	4.491306	-2.994320	-1.482946
6	3.940679	-3.387989	0.872693
6	5.727498	-3.602254	-1.284808
1	4.209859	-2.604603	-2.454903
6	5.181644	-3.990865	1.052424
1	3.240297	-3.300302	1.696646
6	6.071530	-4.098662	-0.022799
1	6.421714	-3.693035	-2.113489
1	5.456238	-4.380434	2.026971
1	7.036716	-4.572676	0.124187
1	1.425759	4.584556	0.983913

$TS(E_a\text{-}P)_{2wat}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2616.7568484
Zero-point correction= 0.860469 (Hartree/Particle)
Thermal correction to Energy= 0.914737
Thermal correction to Enthalpy= 0.915681
Thermal correction to Gibbs Free Energy= 0.770276
Sum of electronic and zero-point Energies= -2615.896416
Sum of electronic and thermal Energies= -2615.842149
Sum of electronic and thermal Enthalpies= -2615.841205
Sum of electronic and thermal Free Energies= -2615.986610

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Cartesian Coordinates

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46	0.583389	-0.908907	1.216316
7	2.005317	-2.153204	0.231807
7	2.278276	0.284154	1.410338
8	4.850269	-0.877725	-1.525758
8	5.681823	-0.689216	0.918945
6	1.734318	-3.283632	-0.432773
1	0.812602	-3.789390	-0.174230
6	2.599451	-3.767436	-1.413213
1	2.375245	-4.700879	-1.917226
6	3.705145	-3.007368	-1.782307
1	4.333388	-3.320503	-2.608468
6	3.966645	-1.805089	-1.111212
6	3.142936	-1.459121	-0.014686
6	3.377546	-0.299946	0.854226
6	4.673278	0.149915	1.186414
6	4.809359	1.370464	1.860393
1	5.795407	1.766046	2.076647
6	3.662795	2.018574	2.300354
1	3.719468	2.958668	2.836069
6	2.418446	1.418268	2.113460
1	1.528928	1.869741	2.528092
6	6.533893	-0.082678	-2.994097
1	5.794321	-0.039441	-3.797331
1	7.516308	-0.263455	-3.437694
1	6.556258	0.889860	-2.493410
6	6.192458	-1.195525	-2.014593
1	6.166259	-2.153160	-2.545226
6	7.157226	-1.299608	-0.822169
1	8.182006	-1.218673	-1.199389
1	7.069978	-2.283004	-0.347731

6	6.920460	-0.253031	0.270145
1	6.745489	0.739899	-0.160658
6	8.038414	-0.211093	1.301091
1	7.812901	0.494572	2.104697
1	8.975665	0.097507	0.829396
1	8.181921	-1.199475	1.746470
6	-1.861848	1.105874	-0.170900
6	-1.966960	0.577581	1.189054
6	-0.795720	0.608903	2.051804
6	-3.172416	0.120013	1.772484
6	-0.884229	0.173467	3.418800
1	-0.101272	1.408837	1.833728
6	-3.201725	-0.339814	3.078345
1	-4.086010	0.130652	1.194542
6	-2.054566	-0.351811	3.909804
1	-0.015920	0.291009	4.060797
1	-4.148523	-0.681909	3.488508
1	-2.125380	-0.706107	4.932306
6	-2.700773	0.586424	-1.284041
8	-2.717484	1.111541	-2.395479
8	-3.487689	-0.460554	-0.978764
6	-4.733996	-0.580748	-1.755046
1	-5.060560	-1.603183	-1.566917
1	-4.508793	-0.446194	-2.813361
6	-5.699961	0.443568	-1.222610
6	-6.480403	0.150774	-0.096306
6	-5.738844	1.737331	-1.766870
6	-7.275245	1.136006	0.492733
1	-6.461695	-0.854736	0.318306
6	-6.535013	2.725065	-1.177142
1	-5.146570	1.964487	-2.647550
6	-7.297114	2.426680	-0.041472
1	-7.882009	0.897795	1.360816
1	-6.579610	3.717364	-1.616905
1	-7.919062	3.192413	0.411328
6	1.412582	2.814359	-0.833887
6	0.162262	2.771585	-0.160063
6	-0.140482	3.772772	0.783243
6	0.801568	4.766500	1.033914
6	2.037384	4.786281	0.355468
6	2.358621	3.814288	-0.589522
6	0.313332	0.978296	-1.550859
6	-0.530628	1.597880	-0.630993
1	-1.098552	3.777515	1.294511
1	0.577766	5.547893	1.753120
1	2.746897	5.580562	0.564532
1	3.309297	3.836161	-1.112179
1	-2.655288	2.257904	-0.023123
7	1.471607	1.725387	-1.687864
6	2.604665	1.442635	-2.556220
1	3.455427	1.052469	-1.989385
1	2.321935	0.710526	-3.311825
1	2.907929	2.357770	-3.071800
6	0.106246	-0.285084	-2.324685
1	-0.165997	-0.084863	-3.367279
1	1.004573	-0.910538	-2.317602
1	-0.700895	-0.869197	-1.880911
8	-3.305200	3.317178	-0.062036
7	-0.988211	-2.176762	0.891374
6	-1.978646	-2.708755	0.603399

6	-3.202743	-3.338627	0.248879
6	-3.353087	-3.889250	-1.037897
6	-4.262062	-3.360135	1.175472
6	-4.570996	-4.461818	-1.391150
1	-2.529717	-3.857833	-1.743462
6	-5.474213	-3.933749	0.803593
1	-4.125683	-2.931674	2.161604
6	-5.628614	-4.482503	-0.474571
1	-4.697763	-4.892583	-2.378719
1	-6.296094	-3.962940	1.511325
1	-6.575397	-4.932421	-0.756126
8	-2.227805	3.829402	-2.288500
1	-2.206631	2.886453	-2.560755
1	-2.935081	3.695886	-0.948133
1	-1.306516	4.092152	-2.155042
1	-4.249548	3.115562	-0.204482

$TS(E_a\text{-}P)_{enol}$

Number of imaginary frequencies : 1 Electronic energy : HF=-3635.6657733
Zero-point correction= 1.228506 (Hartree/Particle)
Thermal correction to Energy= 1.303966
Thermal correction to Enthalpy= 1.304910
Thermal correction to Gibbs Free Energy= 1.112555
Sum of electronic and zero-point Energies= -3634.437267
Sum of electronic and thermal Energies= -3634.361807
Sum of electronic and thermal Enthalpies= -3634.360863
Sum of electronic and thermal Free Energies= -3634.553218

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Cartesian Coordinates

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46	2.561830	-0.289703	1.484217
7	3.777256	-0.726301	-0.297738
7	2.300885	-2.392328	1.309514
8	5.137642	-3.934131	-1.119718
8	2.616837	-4.339450	-1.673828
6	4.626075	0.111590	-0.904218
1	4.497761	1.165813	-0.686392
6	5.617592	-0.357859	-1.763350
1	6.277922	0.340660	-2.265667
6	5.792482	-1.731425	-1.910839
1	6.620996	-2.117619	-2.493583
6	4.929841	-2.609168	-1.241708
6	3.846911	-2.057890	-0.515055
6	2.824381	-2.880052	0.154473
6	2.370016	-4.108129	-0.366950
6	1.601740	-4.945735	0.444897
1	1.280680	-5.914421	0.078608
6	1.209241	-4.485672	1.697011
1	0.598322	-5.094575	2.352048
6	1.522280	-3.180671	2.066659
1	1.138035	-2.759478	2.986131
6	6.371615	-5.906937	-1.576826
1	7.208588	-5.504175	-1.002049
1	6.765828	-6.575732	-2.346540
1	5.743769	-6.491173	-0.897903
6	5.580359	-4.778209	-2.221347
1	6.239064	-4.204958	-2.882924
6	4.350834	-5.249985	-3.015990

1	4.641821	-6.107856	-3.631439
1	4.017831	-4.463284	-3.702391
6	3.150179	-5.619050	-2.140345
1	3.464936	-6.195393	-1.263406
6	2.059131	-6.352878	-2.906454
1	1.188533	-6.538283	-2.271453
1	2.429255	-7.315895	-3.269304
1	1.735136	-5.760533	-3.767508
6	-0.530699	1.248193	1.285167
6	0.192393	1.193330	2.577004
6	0.261760	2.306587	3.436203
6	0.838520	-0.013674	3.013135
6	0.973814	2.256735	4.627786
1	-0.253037	3.223005	3.166875
6	1.517474	-0.055176	4.265135
1	0.464621	-0.941664	2.603551
6	1.629264	1.079769	5.042506
1	1.007473	3.136590	5.264090
1	1.935536	-0.998382	4.604472
1	2.166829	1.057752	5.984365
6	-0.408038	2.499404	0.527424
8	-1.276170	2.824917	-0.364995
8	0.564659	3.337703	0.751568
6	0.592638	4.625783	-0.003051
1	1.262666	5.228731	0.608697
1	-0.414609	5.043687	0.007563
6	1.113205	4.409451	-1.393425
6	2.476481	4.151453	-1.594888
6	0.242819	4.431185	-2.489391
6	2.962312	3.898555	-2.877057
1	3.155465	4.163948	-0.747041
6	0.735144	4.197750	-3.774331
1	-0.813931	4.627446	-2.338726
6	2.090353	3.920899	-3.969807
1	4.020439	3.707953	-3.030068
1	0.061843	4.245728	-4.624552
1	2.470437	3.742432	-4.971136
6	-0.937168	-2.130544	-0.311263
6	-1.153695	-1.248240	0.780178
6	-1.818617	-1.732628	1.920715
6	-2.247341	-3.057208	1.945395
6	-2.026191	-3.910644	0.846396
6	-1.373295	-3.458553	-0.298307
6	0.008477	-0.148353	-0.843840
6	-0.551158	0.017788	0.420928
1	-2.034334	-1.076630	2.756043
1	-2.793859	-3.422445	2.808685
1	-2.383778	-4.934945	0.887374
1	-1.204230	-4.116914	-1.143923
1	-2.165029	2.332210	-0.131505
7	-0.249800	-1.433438	-1.292313
6	0.156267	-2.019297	-2.560356
1	1.019855	-2.681582	-2.441941
1	-0.675600	-2.594630	-2.975120
1	0.403979	-1.232643	-3.271874
6	0.794314	0.814737	-1.673787
1	1.609867	0.312316	-2.199671
1	0.173960	1.337106	-2.411705
1	1.259179	1.573632	-1.045375
7	3.114563	1.699335	1.648531

6	3.409920	2.804234	1.841131
6	3.742758	4.172893	2.053401
6	2.877992	4.982576	2.814733
6	4.914403	4.705786	1.483332
6	3.189805	6.326841	2.993722
1	1.986655	4.547480	3.250849
6	5.210135	6.052619	1.672702
1	5.577631	4.068177	0.908016
6	4.350685	6.860915	2.423479
1	2.532555	6.958857	3.581922
1	6.111751	6.471995	1.239007
1	4.588627	7.909808	2.569011
1	-1.932969	1.378768	1.395663
6	-4.181400	0.461040	-0.758703
6	-4.893999	-0.757921	-1.188326
6	-5.850293	-0.686455	-2.223310
6	-4.588711	-2.020833	-0.645370
6	-6.476082	-1.836833	-2.696103
1	-6.103202	0.282172	-2.643092
6	-5.205889	-3.170188	-1.130359
1	-3.865879	-2.093951	0.154217
6	-6.152328	-3.086002	-2.156117
1	-7.221392	-1.760845	-3.481976
1	-4.945326	-4.133376	-0.701708
1	-6.637607	-3.982898	-2.528703
6	-3.850316	0.711158	0.567752
8	-3.047185	1.708472	0.914389
8	-4.194473	-0.042664	1.624409
6	-5.572892	-0.411397	1.934640
1	-6.138698	-0.597533	1.021291
1	-6.012954	0.442491	2.461834
6	-5.497325	-1.634655	2.806483
6	-6.009259	-2.861789	2.375364
6	-4.853608	-1.557349	4.049106
6	-5.876453	-4.001010	3.173071
1	-6.504705	-2.928464	1.411867
6	-4.713320	-2.694156	4.843635
1	-4.459687	-0.602561	4.387260
6	-5.224242	-3.920753	4.404666
1	-6.285181	-4.948193	2.834041
1	-4.219895	-2.624528	5.808590
1	-5.125789	-4.804856	5.027496
6	-3.375133	3.308434	-3.036661
6	-3.888676	2.855044	-1.795659
6	-4.369133	3.797044	-0.872317
6	-4.303599	5.149398	-1.193991
6	-3.777218	5.579140	-2.426732
6	-3.310772	4.663394	-3.369681
6	-3.213688	1.055158	-3.026332
6	-3.780949	1.409279	-1.793252
1	-4.769296	3.472230	0.081593
1	-4.672954	5.886750	-0.488237
1	-3.744640	6.639738	-2.654916
1	-2.919836	5.001291	-4.324006
7	-2.986055	2.190516	-3.769013
6	-2.375827	2.235820	-5.086964
1	-2.747580	3.107584	-5.627739
1	-1.283242	2.298369	-5.020420
1	-2.647838	1.347249	-5.658005
6	-2.823329	-0.293467	-3.538059

1	-3.542029	-0.672153	-4.274767
1	-1.838008	-0.265864	-4.014626
1	-2.791138	-1.009609	-2.717419

D_{free}

Number of imaginary frequencies : 0 Electronic energy : HF=-1171.7643281
Zero-point correction= 0.419653 (Hartree/Particle)
Thermal correction to Energy= 0.443385
Thermal correction to Enthalpy= 0.444329
Thermal correction to Gibbs Free Energy= 0.364270
Sum of electronic and zero-point Energies= -1171.344675
Sum of electronic and thermal Energies= -1171.320943
Sum of electronic and thermal Enthalpies= -1171.319999
Sum of electronic and thermal Free Energies= -1171.400058

Cartesian Coordinates

6	0.331528	0.094550	0.624591
6	1.030702	1.274777	0.012400
6	1.565646	2.270837	0.838066
6	1.126282	1.422063	-1.374918
6	2.204539	3.382559	0.290233
1	1.468925	2.172310	1.914998
6	1.764767	2.533409	-1.927494
1	0.714382	0.654640	-2.021183
6	2.309487	3.513783	-1.096856
1	2.614506	4.147822	0.943438
1	1.838672	2.630444	-3.006905
1	2.809941	4.377016	-1.526568
6	-1.060479	0.414423	1.071197
8	-1.465718	1.544050	1.269693
8	-1.836077	-0.690650	1.239162
6	-3.216121	-0.463769	1.640838
1	-3.252031	0.413271	2.290425
1	-3.480765	-1.356469	2.211799
6	-4.111525	-0.299685	0.439242
6	-4.248318	0.951351	-0.179195
6	-4.793096	-1.401897	-0.090022
6	-5.056425	1.091864	-1.307333
1	-3.704878	1.799784	0.223432
6	-5.603616	-1.261195	-1.217513
1	-4.689318	-2.374680	0.384931
6	-5.735973	-0.012528	-1.828086
1	-5.157208	2.064727	-1.780035
1	-6.130706	-2.122876	-1.617237
1	-6.366964	0.100011	-2.705256
6	2.932998	-1.181466	-0.012263
6	1.780419	-1.577584	-0.722953
6	1.881081	-2.044497	-2.024802
6	3.141211	-2.078341	-2.639497
6	4.270950	-1.635329	-1.945283
6	4.187119	-1.174651	-0.625980
6	1.169197	-0.908695	1.484912
6	0.607902	-1.360058	0.157955
1	0.991808	-2.357582	-2.565476
1	3.236924	-2.433359	-3.660831
1	5.239803	-1.648751	-2.436923

1	5.071601	-0.830772	-0.100403
1	-0.259437	-2.007074	0.105805
7	2.600172	-0.841258	1.291027
6	3.511218	-0.132221	2.164080
1	4.446044	-0.695138	2.266249
1	3.745100	0.873746	1.790964
1	3.070051	-0.039252	3.157775
6	0.712342	-1.382349	2.844413
1	1.243009	-2.302000	3.109405
1	0.910966	-0.633650	3.619276
1	-0.358275	-1.582661	2.839898

D_2

Number of imaginary frequencies : 0 Electronic energy : HF=-2463.873558
Zero-point correction= 0.812676 (Hartree/Particle)
Thermal correction to Energy= 0.863230
Thermal correction to Enthalpy= 0.864174
Thermal correction to Gibbs Free Energy= 0.721687
Sum of electronic and zero-point Energies= -2463.060882
Sum of electronic and thermal Energies= -2463.010328
Sum of electronic and thermal Enthalpies= -2463.009384
Sum of electronic and thermal Free Energies= -2463.151871

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Cartesian Coordinates

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46	0.502743	0.974430	-0.323843
7	2.503378	1.023788	-0.951531
7	0.940545	-1.056810	-0.266526
8	4.977514	-1.339615	0.064431
8	3.729798	-2.768779	-1.700912
6	3.226477	2.134723	-1.146310
1	2.675770	3.053186	-1.299273
6	4.619555	2.097588	-1.135581
1	5.181927	3.004083	-1.329325
6	5.270494	0.916242	-0.795259
1	6.347853	0.899360	-0.676408
6	4.509913	-0.229837	-0.533466
6	3.114519	-0.168730	-0.748765
6	2.218560	-1.322265	-0.644548
6	2.601383	-2.636925	-0.988918
6	1.737187	-3.690802	-0.667668
1	2.032956	-4.714747	-0.867004
6	0.479722	-3.391714	-0.153579
1	-0.223463	-4.177794	0.098928
6	0.090114	-2.059312	-0.023892
1	-0.916715	-1.791070	0.279781
6	6.729486	-2.602665	1.038858
1	6.810889	-1.856738	1.833159
1	7.709511	-3.064767	0.894529
1	6.027889	-3.375511	1.366461
6	6.262543	-1.953158	-0.255480
1	6.975274	-1.176042	-0.551871
6	6.072561	-2.940428	-1.419071
1	6.928151	-3.623545	-1.438401
1	6.070521	-2.405212	-2.374832
6	4.768598	-3.740863	-1.352619
1	4.571863	-4.096561	-0.334568
6	4.732099	-4.890673	-2.348620

1	3.768035	-5.405419	-2.328138
1	5.512525	-5.619791	-2.112907
1	4.898347	-4.519172	-3.363711
6	-2.934088	-0.758575	0.838724
6	-3.607911	-1.741599	1.704931
6	-2.899325	-2.517945	2.646721
6	-4.993631	-1.972808	1.584122
6	-3.552067	-3.464602	3.432261
1	-1.831961	-2.377783	2.758479
6	-5.645572	-2.918314	2.370908
1	-5.583121	-1.398853	0.876151
6	-4.927315	-3.670599	3.302348
1	-2.981821	-4.048847	4.148259
1	-6.715404	-3.066244	2.259660
1	-5.432578	-4.408625	3.916981
6	-1.872158	0.047567	1.213573
8	-1.420445	0.997297	0.441235
8	-1.291639	-0.159397	2.421501
6	-0.563468	0.925630	3.041601
1	-0.820391	0.847262	4.102266
1	-0.926833	1.883308	2.660724
6	0.929941	0.800990	2.843046
6	1.552530	-0.453633	2.880106
6	1.713820	1.946120	2.657352
6	2.932676	-0.560866	2.715845
1	0.947160	-1.343296	3.021866
6	3.099070	1.842122	2.507659
1	1.238332	2.923264	2.627989
6	3.709048	0.587474	2.532747
1	3.407971	-1.536674	2.730311
1	3.697685	2.737783	2.371960
1	4.783676	0.499272	2.410402
6	-5.169544	-1.358105	-1.946126
6	-3.924777	-1.680287	-1.402153
6	-3.347104	-2.905813	-1.702439
6	-4.043274	-3.778650	-2.546683
6	-5.289779	-3.430711	-3.083641
6	-5.883058	-2.199003	-2.790190
6	-4.630036	0.432472	-0.664731
6	-3.458021	-0.514265	-0.570384
1	-2.385003	-3.183020	-1.285363
1	-3.614508	-4.745770	-2.788043
1	-5.807437	-4.127265	-3.734331
1	-6.849011	-1.929975	-3.202731
1	-2.653802	0.023398	-1.103164
7	-5.549958	-0.062939	-1.459089
6	-6.843054	0.528682	-1.816995
1	-6.892154	0.646264	-2.901614
1	-7.637561	-0.145729	-1.489348
1	-6.966256	1.494851	-1.334118
6	-4.684193	1.726011	0.056806
1	-3.662010	2.084280	0.200964
1	-5.280402	2.483710	-0.453997
1	-5.112135	1.559010	1.053852
7	0.205498	3.024286	-0.516851
6	0.009134	4.167745	-0.552700
6	-0.215114	5.573439	-0.590975
6	-0.290493	6.233391	-1.833306
6	-0.348514	6.285039	0.617712
6	-0.499639	7.608357	-1.856204

1	-0.185153	5.672198	-2.755944
6	-0.557403	7.659336	0.573709
1	-0.286764	5.762885	1.566822
6	-0.632261	8.318339	-0.658125
1	-0.558017	8.127946	-2.806735
1	-0.660137	8.218195	1.497842
1	-0.793724	9.391362	-0.684426

$TS(D_2\text{-}P)^t$

Number of imaginary frequencies : 1 Electronic energy : HF=-2463.8140723
Zero-point correction= 0.808911 (Hartree/Particle)
Thermal correction to Energy= 0.859271
Thermal correction to Enthalpy= 0.860215
Thermal correction to Gibbs Free Energy= 0.718932
Sum of electronic and zero-point Energies= -2463.005088
Sum of electronic and thermal Energies= -2462.954729
Sum of electronic and thermal Enthalpies= -2462.953784
Sum of electronic and thermal Free Energies= -2463.095067

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Cartesian Coordinates

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46	0.814322	0.904289	-0.325599
7	2.717106	1.686059	-0.484994
7	1.893986	-0.731455	0.339508
8	5.669315	0.561336	1.180750
8	5.314881	-1.443618	-0.400571
6	3.012321	2.959020	-0.784039
1	2.206120	3.572318	-1.163368
6	4.300277	3.456603	-0.590241
1	4.522491	4.482523	-0.861306
6	5.260600	2.658801	0.021225
1	6.233367	3.067403	0.269874
6	4.934477	1.341564	0.376963
6	3.668831	0.840894	-0.009458
6	3.235575	-0.543016	0.184464
6	4.109776	-1.650082	0.144591
6	3.625711	-2.896574	0.563449
1	4.290940	-3.751962	0.600488
6	2.274966	-3.025792	0.864778
1	1.861234	-3.977327	1.178301
6	1.421100	-1.938369	0.683358
1	0.352925	-2.039920	0.807621
6	7.588783	0.227101	2.539464
1	7.265137	1.049608	3.181320
1	8.679777	0.167249	2.573211
1	7.178714	-0.703272	2.942979
6	7.126609	0.453592	1.108170
1	7.542364	1.393983	0.731290
6	7.489382	-0.688288	0.143374
1	8.520520	-0.997223	0.343801
1	7.458315	-0.335881	-0.893325
6	6.557793	-1.900408	0.231676
1	6.332397	-2.154415	1.273703
6	7.088873	-3.108937	-0.524538
1	6.377244	-3.938287	-0.502834
1	8.024974	-3.452592	-0.075363
1	7.279352	-2.850124	-1.569887
6	-2.490051	-1.656990	0.425123

6	-3.182956	-2.374188	1.534556
6	-3.080667	-3.770728	1.615993
6	-3.939381	-1.684294	2.492689
6	-3.710110	-4.464492	2.649166
1	-2.509904	-4.310329	0.864325
6	-4.570934	-2.380391	3.522316
1	-4.035356	-0.606197	2.426864
6	-4.457501	-3.770543	3.604715
1	-3.619491	-5.544812	2.708470
1	-5.157023	-1.836541	4.256768
1	-4.953581	-4.311452	4.404411
6	-1.554717	-0.637098	0.704394
8	-1.110353	0.171067	-0.193404
8	-1.165187	-0.531976	1.987042
6	-0.991902	0.804993	2.567945
1	-0.316267	1.389332	1.936151
1	-0.497256	0.603105	3.517760
6	-2.316584	1.490085	2.753486
6	-2.951467	2.106529	1.663871
6	-2.962931	1.461222	3.994905
6	-4.214235	2.680421	1.815569
1	-2.460148	2.113073	0.696159
6	-4.223668	2.041065	4.148712
1	-2.481887	0.978447	4.841117
6	-4.852230	2.648390	3.059101
1	-4.698637	3.154024	0.966387
1	-4.714453	2.018506	5.116638
1	-5.833560	3.096819	3.179222
6	-2.473809	-3.010961	-3.121467
6	-1.783018	-2.309655	-2.108847
6	-0.439045	-1.980560	-2.316933
6	0.165592	-2.337881	-3.519856
6	-0.546845	-3.021744	-4.519030
6	-1.882269	-3.371858	-4.331607
6	-3.953309	-2.746350	-1.436892
6	-2.729701	-2.144392	-1.012410
1	0.120452	-1.449791	-1.564428
1	1.206888	-2.081665	-3.689777
1	-0.052404	-3.284970	-5.448198
1	-2.432951	-3.904930	-5.098743
1	-3.151887	-1.024939	-0.531491
7	-3.774429	-3.267199	-2.675537
6	-4.763865	-3.974695	-3.483778
1	-5.101875	-3.345796	-4.312602
1	-4.312858	-4.884865	-3.885322
1	-5.617855	-4.257137	-2.871660
6	-5.264065	-2.815582	-0.725281
1	-6.097606	-2.639334	-1.409635
1	-5.399770	-3.796864	-0.254771
1	-5.313682	-2.077109	0.073428
7	-0.143314	2.600625	-1.005126
6	-0.904618	3.437584	-1.267501
6	-1.835738	4.471081	-1.558415
6	-2.566798	5.048049	-0.499247
6	-2.017819	4.898436	-2.888612
6	-3.481576	6.055597	-0.785022
1	-2.421315	4.700366	0.517740
6	-2.936523	5.908941	-3.151017
1	-1.447757	4.442737	-3.691311
6	-3.664563	6.485156	-2.104175

1	-4.049733	6.509358	0.020160
1	-3.085719	6.248964	-4.170259
1	-4.378390	7.274432	-2.317973

TS(D_2-P)[b]

Number of imaginary frequencies : 1 Electronic energy : HF=-2463.8483333
Zero-point correction= 0.808215 (Hartree/Particle)
Thermal correction to Energy= 0.858657
Thermal correction to Enthalpy= 0.859601
Thermal correction to Gibbs Free Energy= 0.717006
Sum of electronic and zero-point Energies= -2463.040228
Sum of electronic and thermal Energies= -2462.989786
Sum of electronic and thermal Enthalpies= -2462.988842
Sum of electronic and thermal Free Energies= -2463.131437

Cartesian Coordinates

46	0.038301	0.779694	0.102422
7	1.742393	1.747983	-0.654720
7	1.328875	-0.857937	-0.121733
8	5.082968	0.677841	0.001086
8	4.442821	-1.002640	-1.870063
6	1.875873	3.077133	-0.766401
1	0.963913	3.657918	-0.804193
6	3.136809	3.668283	-0.815935
1	3.220538	4.742104	-0.940229
6	4.270293	2.883870	-0.624665
1	5.248824	3.345024	-0.553767
6	4.123625	1.501612	-0.453275
6	2.833257	0.944254	-0.600423
6	2.553027	-0.491892	-0.584493
6	3.439006	-1.458019	-1.107195
6	3.150574	-2.812451	-0.898008
1	3.840990	-3.574049	-1.242788
6	1.936302	-3.155604	-0.314011
1	1.660503	-4.192913	-0.161964
6	1.022325	-2.153252	0.009855
1	0.025952	-2.395068	0.353772
6	7.289079	0.243134	0.749432
1	7.104288	0.873144	1.622839
1	8.355796	0.280943	0.514012
1	7.029490	-0.787427	1.009134
6	6.475242	0.729364	-0.440440
1	6.746204	1.765572	-0.669789
6	6.635865	-0.131557	-1.704248
1	7.699616	-0.353995	-1.838234
1	6.314245	0.428371	-2.589123
6	5.830940	-1.434259	-1.682698
1	5.901897	-1.930330	-0.707793
6	6.216884	-2.383445	-2.807436
1	5.585610	-3.275694	-2.811090
1	7.256444	-2.702971	-2.691626
1	6.111495	-1.887343	-3.776351
6	-2.412714	-2.206051	0.795808
6	-2.629420	-3.641902	0.945887
6	-2.028676	-4.407361	1.973032
6	-3.462000	-4.310103	0.019975
6	-2.264384	-5.775115	2.065132

1	-1.387869	-3.925801	2.699671
6	-3.687534	-5.679260	0.116028
1	-3.922005	-3.752363	-0.789069
6	-3.092764	-6.419597	1.140949
1	-1.801721	-6.343582	2.866124
1	-4.328386	-6.170597	-0.609416
1	-3.272767	-7.486996	1.219552
6	-1.619593	-1.373625	1.554163
8	-1.627287	-0.070996	1.182198
8	-0.824362	-1.743367	2.558512
6	-0.480049	-0.761856	3.589982
1	-0.391452	-1.371868	4.491571
1	-1.309685	-0.062382	3.714165
6	0.810049	-0.045787	3.284089
6	1.984480	-0.779167	3.065976
6	0.854829	1.352165	3.225219
6	3.180268	-0.124274	2.777364
1	1.953843	-1.864022	3.113085
6	2.058234	2.011782	2.956781
1	-0.051745	1.925928	3.397720
6	3.219348	1.273159	2.727791
1	4.085120	-0.695856	2.597449
1	2.086799	3.096909	2.931314
1	4.156021	1.778158	2.515941
6	-3.910465	-0.819876	-2.349582
6	-2.763687	-1.294687	-1.682688
6	-1.587799	-1.503169	-2.410539
6	-1.590472	-1.222065	-3.775629
6	-2.741846	-0.731343	-4.417728
6	-3.925337	-0.521299	-3.712353
6	-4.507271	-1.084965	-0.189412
6	-3.115305	-1.394373	-0.259933
1	-0.700949	-1.897393	-1.929149
1	-0.691784	-1.394426	-4.359466
1	-2.712738	-0.523191	-5.482133
1	-4.816316	-0.151799	-4.208589
1	-2.505313	-0.274299	0.335720
7	-4.950408	-0.718426	-1.409762
6	-6.290143	-0.253967	-1.759333
1	-6.254611	0.791046	-2.079910
1	-6.683560	-0.864437	-2.575743
1	-6.953739	-0.344244	-0.901401
6	-5.371723	-1.134866	1.023279
1	-4.770377	-1.413716	1.889482
1	-5.852944	-0.172028	1.224128
1	-6.161048	-1.886033	0.907806
7	-1.173221	2.471531	0.105030
6	-1.889514	3.385592	0.121330
6	-2.756623	4.513348	0.139549
6	-3.164968	5.093713	-1.078237
6	-3.186870	5.037430	1.375048
6	-4.005418	6.201321	-1.049177
1	-2.823767	4.679258	-2.021258
6	-4.027615	6.145170	1.382080
1	-2.861912	4.580549	2.303908
6	-4.434626	6.724836	0.175426
1	-4.324973	6.659214	-1.979287
1	-4.364414	6.559332	2.326463
1	-5.088927	7.590775	0.189547

TS(D_2-E_a)

Number of imaginary frequencies : 1 Electronic energy : HF=-2463.8264921
Zero-point correction= 0.809084 (Hartree/Particle)
Thermal correction to Energy= 0.859235
Thermal correction to Enthalpy= 0.860179
Thermal correction to Gibbs Free Energy= 0.721218
Sum of electronic and zero-point Energies= -2463.017408
Sum of electronic and thermal Energies= -2462.967257
Sum of electronic and thermal Enthalpies= -2462.966313
Sum of electronic and thermal Free Energies= -2463.105274

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Cartesian Coordinates

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46	-0.585616	0.029508	0.333833
7	-2.166744	-0.819964	1.355770
7	-2.103296	1.197648	-0.391260
8	-5.533858	0.344113	1.629960
8	-5.428790	0.050711	-0.945505
6	-2.087622	-1.732727	2.331904
1	-1.106503	-2.134691	2.546827
6	-3.224869	-2.123085	3.038602
1	-3.140000	-2.876441	3.813676
6	-4.437972	-1.488859	2.795015
1	-5.306037	-1.715459	3.403497
6	-4.508001	-0.500935	1.801518
6	-3.359761	-0.268783	1.010313
6	-3.319716	0.653857	-0.125739
6	-4.406378	0.918942	-0.982417
6	-4.284415	1.968853	-1.903307
1	-5.124133	2.230444	-2.537675
6	-3.059564	2.618649	-2.035689
1	-2.933566	3.427597	-2.746355
6	-1.959744	2.160877	-1.309072
1	-0.953907	2.533824	-1.456144
6	-7.674145	1.130045	2.299925
1	-7.269219	1.364300	3.287033
1	-8.736584	0.895274	2.405503
1	-7.577318	2.019863	1.671124
6	-6.939711	-0.053735	1.689342
1	-7.043130	-0.928032	2.340735
6	-7.407687	-0.416836	0.269366
1	-8.501532	-0.375415	0.243606
1	-7.122772	-1.446119	0.025324
6	-6.828421	0.479279	-0.829189
1	-6.832771	1.532711	-0.527936
6	-7.519404	0.290158	-2.171092
1	-7.045692	0.890462	-2.952064
1	-8.568456	0.591249	-2.100995
1	-7.479572	-0.759660	-2.475524
6	3.110586	0.684314	-0.809844
6	4.315735	-0.026131	-1.308504
6	4.327982	-1.421835	-1.460281
6	5.480141	0.698667	-1.611793
6	5.475981	-2.077674	-1.898780
1	3.433402	-1.990126	-1.235654
6	6.624287	0.043471	-2.062704
1	5.481590	1.779200	-1.498298
6	6.628031	-1.347549	-2.201835

1	5.471859	-3.158412	-2.003564
1	7.512848	0.616825	-2.307909
1	7.522180	-1.857279	-2.546465
6	1.817983	0.472584	-1.337857
8	0.765173	1.049300	-0.865195
8	1.732369	-0.365226	-2.383122
6	0.481426	-0.463869	-3.107738
1	0.795122	-0.767791	-4.109609
1	0.014752	0.522473	-3.169210
6	-0.468650	-1.471983	-2.503078
6	0.013868	-2.660502	-1.940414
6	-1.849176	-1.240086	-2.526863
6	-0.869139	-3.583446	-1.379616
1	1.083214	-2.850330	-1.946229
6	-2.735398	-2.165134	-1.970863
1	-2.232488	-0.323573	-2.967973
6	-2.245001	-3.334879	-1.386705
1	-0.490829	-4.507192	-0.950342
1	-3.802603	-1.963714	-1.982601
1	-2.930450	-4.057846	-0.955248
6	3.381326	3.934557	1.109571
6	2.725192	3.183930	0.112284
6	1.814794	3.825016	-0.735589
6	1.554688	5.178192	-0.532029
6	2.187747	5.897394	0.497315
6	3.121739	5.286878	1.331287
6	4.273836	1.862667	1.211622
6	3.288203	1.840482	0.179645
1	1.338682	3.281282	-1.540573
1	0.857598	5.693455	-1.185231
1	1.960062	6.949343	0.633999
1	3.630517	5.847629	2.107667
7	4.315476	3.105876	1.746495
6	5.181425	3.574091	2.824285
1	4.591302	3.787253	3.720265
1	5.933407	2.822739	3.057253
1	5.690626	4.487189	2.506617
6	5.143729	0.746217	1.685846
1	5.170812	0.693564	2.778255
1	4.791357	-0.208745	1.295422
1	6.170433	0.871498	1.321777
7	0.862688	-1.263040	1.028361
6	1.705912	-2.040647	1.210022
6	2.750387	-2.990445	1.374098
6	2.766863	-4.132548	0.548617
6	3.774213	-2.757356	2.312418
6	3.821812	-5.031421	0.660648
1	1.966232	-4.297879	-0.163950
6	4.820838	-3.668212	2.409429
1	3.740143	-1.879330	2.948398
6	4.846603	-4.798074	1.584677
1	3.846217	-5.914611	0.031122
1	5.615585	-3.501574	3.128709
1	5.667357	-5.503592	1.665981
1	2.711243	0.733203	0.465277

TS(D-P)

Number of imaginary frequencies : 1 Electronic energy : HF=-2463.8133936

Zero-point correction= 0.808320 (Hartree/Particle)
Thermal correction to Energy= 0.858745
Thermal correction to Enthalpy= 0.859689
Thermal correction to Gibbs Free Energy= 0.720162
Sum of electronic and zero-point Energies= -2463.005073
Sum of electronic and thermal Energies= -2462.954648
Sum of electronic and thermal Enthalpies= -2462.953704
Sum of electronic and thermal Free Energies= -2463.093232

Cartesian Coordinates

46	0.666278	0.884753	0.049670
7	2.502690	1.953506	-0.150184
7	1.986261	-0.711808	-0.358336
8	5.691750	0.555540	0.671360
8	5.285711	-0.421197	-1.717832
6	2.671382	3.255466	0.115833
1	1.786818	3.878999	0.078590
6	3.930446	3.763518	0.435789
1	4.049535	4.825651	0.618753
6	5.005949	2.893036	0.583853
1	5.967365	3.264854	0.919279
6	4.815914	1.523110	0.352410
6	3.554459	1.100089	-0.122038
6	3.259976	-0.269993	-0.552539
6	4.190604	-1.051164	-1.270066
6	3.859259	-2.376623	-1.577686
1	4.575252	-3.009332	-2.090105
6	2.574195	-2.826894	-1.298308
1	2.263135	-3.829699	-1.568378
6	1.642167	-1.951200	-0.744322
1	0.602446	-2.233208	-0.646210
6	7.776788	-0.226670	1.485851
1	7.489440	0.094856	2.489517
1	8.865283	-0.172848	1.401415
1	7.471229	-1.269408	1.359767
6	7.130547	0.665116	0.436501
1	7.446759	1.701708	0.595843
6	7.441311	0.255679	-1.012565
1	8.513169	0.044825	-1.088262
1	7.232287	1.086222	-1.695706
6	6.638847	-0.948330	-1.514651
1	6.583738	-1.736137	-0.754570
6	7.164583	-1.497095	-2.832784
1	6.539221	-2.313109	-3.203809
1	8.181048	-1.879634	-2.703527
1	7.183048	-0.709938	-3.591742
6	-1.312272	-0.233526	0.685603
6	-2.070425	0.533511	1.754159
6	-1.539955	1.523015	2.586176
6	-3.411783	0.145698	1.931395
6	-2.337424	2.139019	3.555890
1	-0.503754	1.824656	2.484458
6	-4.208474	0.768778	2.888333
1	-3.831259	-0.635659	1.305063
6	-3.673852	1.771712	3.704634
1	-1.908011	2.906458	4.192151
1	-5.244869	0.466382	3.002712
1	-4.292814	2.253364	4.454780
6	-1.789283	-0.175931	-0.755947

8	-1.257427	-0.806954	-1.652515
8	-2.823747	0.647913	-0.903855
6	-3.475679	0.650013	-2.224716
1	-2.711158	0.773414	-2.994192
1	-4.104969	1.540133	-2.176827
6	-4.266750	-0.616182	-2.404945
6	-3.946240	-1.524555	-3.418841
6	-5.301408	-0.917798	-1.507590
6	-4.659439	-2.719893	-3.541651
1	-3.133629	-1.301980	-4.103942
6	-6.003185	-2.116532	-1.620539
1	-5.551106	-0.210906	-0.720146
6	-5.683787	-3.018576	-2.640746
1	-4.414050	-3.415286	-4.338422
1	-6.804972	-2.344304	-0.925027
1	-6.239201	-3.946493	-2.737184
6	-1.402187	-3.936889	1.570563
6	-1.677646	-2.946368	0.600146
6	-2.436308	-3.303420	-0.525392
6	-2.864551	-4.623328	-0.649291
6	-2.558493	-5.593582	0.318060
6	-1.821726	-5.260807	1.452448
6	-0.514411	-2.033554	2.397712
6	-1.107533	-1.709456	1.140060
1	-2.690929	-2.592126	-1.295705
1	-3.454940	-4.896556	-1.517192
1	-2.907376	-6.612727	0.188748
1	-1.597521	-6.000535	2.212903
7	-0.697306	-3.348628	2.632176
6	-0.274011	-4.114235	3.802920
1	0.467520	-4.863109	3.512074
1	0.151072	-3.455049	4.556142
1	-1.142648	-4.618699	4.232781
6	0.229101	-1.132048	3.324852
1	1.033663	-1.657349	3.843112
1	0.674089	-0.300193	2.775396
1	-0.445643	-0.697310	4.070793
7	-0.520011	2.562996	-0.020097
6	-1.440908	3.234393	-0.245344
6	-2.615207	4.001524	-0.453968
6	-3.788376	3.604307	0.222693
6	-2.609311	5.108834	-1.323810
6	-4.955658	4.330615	0.015899
1	-3.768846	2.744574	0.882257
6	-3.788640	5.821259	-1.512782
1	-1.697456	5.397145	-1.836024
6	-4.956309	5.433544	-0.846108
1	-5.866678	4.040453	0.528754
1	-3.800092	6.677507	-2.178616
1	-5.872507	5.995130	-0.999353
1	-0.177963	-0.893728	0.681743

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Number of imaginary frequencies : 0 Electronic energy : HF=-2463.8519089
Zero-point correction= 0.812367 (Hartree/Particle)
Thermal correction to Energy= 0.862709
Thermal correction to Enthalpy= 0.863653
Thermal correction to Gibbs Free Energy= 0.724763

Sum of electronic and zero-point Energies= -2463.039542
Sum of electronic and thermal Energies= -2462.989200
Sum of electronic and thermal Enthalpies= -2462.988256
Sum of electronic and thermal Free Energies= -2463.127146

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Cartesian Coordinates

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46	-0.745107	-0.326623	0.525897
7	-2.072537	-0.999683	-0.893714
7	-2.430445	0.596285	1.213796
8	-5.628660	-1.143735	-0.609065
8	-5.353139	1.424516	-0.657771
6	-1.814478	-1.902863	-1.848889
1	-0.777481	-2.161642	-2.011002
6	-2.850909	-2.488170	-2.575715
1	-2.616334	-3.200193	-3.358897
6	-4.171120	-2.217165	-2.234811
1	-4.982141	-2.744704	-2.723707
6	-4.438706	-1.307076	-1.201152
6	-3.349394	-0.612670	-0.626135
6	-3.483999	0.452865	0.366204
6	-4.562278	1.361302	0.421087
6	-4.655680	2.214058	1.529907
1	-5.503964	2.882259	1.627197
6	-3.616570	2.240551	2.455298
1	-3.648920	2.906634	3.310017
6	-2.480380	1.462476	2.235051
1	-1.590407	1.539748	2.846436
6	-7.917199	-1.747121	-0.399884
1	-7.616030	-2.769984	-0.162600
1	-8.897699	-1.775634	-0.882401
1	-8.009319	-1.191502	0.537849
6	-6.903232	-1.092977	-1.325845
1	-6.822101	-1.671301	-2.252257
6	-7.218645	0.374193	-1.664709
1	-8.290954	0.459544	-1.868834
1	-6.695750	0.675742	-2.578800
6	-6.817952	1.369709	-0.572055
1	-7.082694	0.997228	0.423962
6	-7.387071	2.760967	-0.806490
1	-7.036530	3.469488	-0.051750
1	-8.479522	2.732823	-0.762931
1	-7.088090	3.133741	-1.790232
6	2.080271	1.666329	1.026778
6	1.243696	1.975347	-0.134985
6	1.720710	1.789842	-1.453762
6	-0.047036	2.531123	0.006651
6	0.932354	2.098920	-2.560444
1	2.714116	1.375034	-1.603138
6	-0.844258	2.822525	-1.102784
1	-0.401325	2.764970	1.004701
6	-0.363573	2.601266	-2.394738
1	1.326261	1.944375	-3.561604
1	-1.832098	3.250874	-0.954938
1	-0.973248	2.844084	-3.259125
6	1.730998	1.000873	2.194771
8	2.387713	0.804272	3.213344
8	0.354918	0.356826	2.209822
6	0.186230	-0.617093	3.318830
1	-0.888070	-0.622542	3.515853

1	0.717862	-0.201916	4.172852
6	0.683432	-1.987243	2.946080
6	-0.223365	-2.981090	2.551351
6	2.055585	-2.280321	2.968239
6	0.227928	-4.245686	2.168229
1	-1.290505	-2.769891	2.561832
6	2.505735	-3.546429	2.593038
1	2.751893	-1.514234	3.291968
6	1.595223	-4.529585	2.187827
1	-0.484469	-5.012869	1.880596
1	3.566644	-3.775866	2.640136
1	1.947612	-5.520596	1.916282
6	5.332460	1.966079	-0.519636
6	4.563148	1.175410	0.334912
6	4.839028	-0.178858	0.456098
6	5.893905	-0.705574	-0.298369
6	6.653943	0.105779	-1.151194
6	6.386360	1.473495	-1.278963
6	3.833030	3.398521	0.399555
6	3.547079	2.061562	1.014111
1	4.246431	-0.803291	1.116979
1	6.122722	-1.763522	-0.230467
1	7.468532	-0.329461	-1.720398
1	6.981839	2.103749	-1.930386
1	3.835173	2.154706	2.077615
7	4.832392	3.309343	-0.450164
6	5.413426	4.384112	-1.257486
1	5.372174	4.094105	-2.309780
1	4.856329	5.307183	-1.114935
1	6.455317	4.531406	-0.963508
6	3.060215	4.629226	0.692983
1	3.699111	5.506387	0.824041
1	2.361893	4.825422	-0.130974
1	2.464402	4.467923	1.592540
7	0.874970	-1.256777	-0.282562
6	1.805005	-1.733273	-0.782206
6	2.931113	-2.290732	-1.447688
6	3.544582	-3.452725	-0.944177
6	3.408849	-1.658378	-2.611783
6	4.643227	-3.978129	-1.617903
1	3.157323	-3.917324	-0.044740
6	4.507983	-2.198698	-3.269636
1	2.921444	-0.760818	-2.977269
6	5.122154	-3.354911	-2.775544
1	5.124018	-4.876345	-1.244658
1	4.886208	-1.722704	-4.168104
1	5.977003	-3.774237	-3.296914

TS(G-P)

Number of imaginary frequencies : 1 Electronic energy : HF=-2463.8112655
Zero-point correction= 0.808824 (Hartree/Particle)
Thermal correction to Energy= 0.858832
Thermal correction to Enthalpy= 0.859776
Thermal correction to Gibbs Free Energy= 0.722884
Sum of electronic and zero-point Energies= -2463.002441
Sum of electronic and thermal Energies= -2462.952434
Sum of electronic and thermal Enthalpies= -2462.951489
Sum of electronic and thermal Free Energies= -2463.088382

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Cartesian Coordinates

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46	-0.640424	-0.460798	0.492846
7	-1.915381	-1.004980	-1.011552
7	-2.377262	0.233416	1.297225
8	-5.470036	-1.298540	-0.869228
8	-5.292234	1.246319	-0.487037
6	-1.596796	-1.752223	-2.077312
1	-0.546968	-1.952101	-2.240216
6	-2.591601	-2.256916	-2.914268
1	-2.309949	-2.841155	-3.783020
6	-3.929654	-2.076747	-2.582845
1	-4.707598	-2.551255	-3.170047
6	-4.259093	-1.336878	-1.436970
6	-3.211803	-0.701432	-0.729750
6	-3.408084	0.189206	0.411301
6	-4.527851	1.028502	0.589362
6	-4.691377	1.660693	1.830054
1	-5.577152	2.256125	2.021275
6	-3.672424	1.573846	2.773322
1	-3.755263	2.075501	3.730788
6	-2.489253	0.911458	2.446911
1	-1.613301	0.945107	3.079595
6	-7.738337	-2.010618	-0.844234
1	-7.403100	-3.047574	-0.769582
1	-8.702390	-1.992596	-1.359278
1	-7.880375	-1.623153	0.168795
6	-6.725836	-1.175415	-1.612417
1	-6.593012	-1.586847	-2.618509
6	-7.089653	0.316221	-1.713265
1	-8.158936	0.397615	-1.934067
1	-6.556014	0.783696	-2.547873
6	-6.756594	1.128784	-0.458641
1	-7.032179	0.586668	0.452900
6	-7.370806	2.520276	-0.476707
1	-7.064841	3.104053	0.395223
1	-8.462156	2.449875	-0.470978
1	-7.062731	3.061234	-1.375920
6	1.796877	1.802957	1.035167
6	0.600761	2.295562	0.313518
6	0.509333	2.171806	-1.087878
6	-0.461830	2.914515	0.995248
6	-0.626687	2.599286	-1.772382
1	1.340146	1.729811	-1.630788
6	-1.599038	3.344578	0.309710
1	-0.383709	3.056613	2.068945
6	-1.691988	3.179351	-1.073795
1	-0.681076	2.488914	-2.851492
1	-2.407163	3.821880	0.855424
1	-2.572790	3.522544	-1.607346
6	1.774758	0.843145	2.082553
8	2.654966	0.525935	2.860545
8	0.485627	0.130486	2.210314
6	0.479182	-0.926277	3.266119
1	-0.562970	-0.966473	3.587532
1	1.105185	-0.553528	4.074595
6	0.942829	-2.252947	2.737231
6	0.004327	-3.187028	2.273614
6	2.308858	-2.565033	2.680343

6	0.421544	-4.405647	1.735384
1	-1.058478	-2.969808	2.355855
6	2.725183	-3.786517	2.150550
1	3.031049	-1.851930	3.061487
6	1.784556	-4.705083	1.670969
1	-0.312682	-5.129236	1.394842
1	3.783130	-4.030850	2.129571
1	2.111025	-5.663014	1.276520
6	5.266171	2.030059	-0.488018
6	4.348679	1.293170	0.291765
6	4.679163	-0.010463	0.682223
6	5.912882	-0.529310	0.297533
6	6.815456	0.224122	-0.471658
6	6.504735	1.519743	-0.879306
6	3.492551	3.392077	-0.170393
6	3.195185	2.169025	0.499962
1	3.998627	-0.597523	1.281816
1	6.182838	-1.536876	0.596541
1	7.773346	-0.204588	-0.747610
1	7.206470	2.105967	-1.462479
1	2.796239	2.594760	1.595871
7	4.707725	3.283899	-0.766070
6	5.414408	4.323525	-1.507762
1	5.860445	3.885311	-2.403231
1	4.719648	5.102182	-1.817724
1	6.205498	4.765295	-0.894443
6	2.665308	4.631628	-0.234661
1	3.276549	5.531230	-0.128118
1	2.119436	4.694294	-1.184618
1	1.918375	4.631649	0.559836
7	1.051086	-1.144792	-0.431333
6	2.031373	-1.502341	-0.938464
6	3.224514	-1.916520	-1.586476
6	3.770229	-3.182172	-1.300280
6	3.855615	-1.034285	-2.485083
6	4.955615	-3.558021	-1.923370
1	3.270928	-3.836962	-0.595451
6	5.038928	-1.428721	-3.095854
1	3.431612	-0.054310	-2.673979
6	5.586571	-2.685821	-2.816559
1	5.389304	-4.530142	-1.713870
1	5.540830	-0.756251	-3.782795
1	6.512575	-2.986563	-3.296479

X

Number of imaginary frequencies : 0 Electronic energy : HF=-2059.0837653
Zero-point correction= 0.680672 (Hartree/Particle)
Thermal correction to Energy= 0.724570
Thermal correction to Enthalpy= 0.725514
Thermal correction to Gibbs Free Energy= 0.597577
Sum of electronic and zero-point Energies= -2058.403093
Sum of electronic and thermal Energies= -2058.359196
Sum of electronic and thermal Enthalpies= -2058.358251
Sum of electronic and thermal Free Energies= -2058.486188

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Cartesian Coordinates

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46	1.328437	0.675054	-0.673322

7	-0.123689	2.143719	-0.290452
7	-0.401588	-0.272893	-1.499534
8	-3.496562	2.234724	-1.504535
8	-3.647460	0.083030	-0.030579
6	0.070696	3.424864	0.058059
1	1.074542	3.716945	0.311915
6	-0.969058	4.352227	0.061797
1	-0.765628	5.372372	0.366774
6	-2.223988	3.982556	-0.401195
1	-3.015459	4.716849	-0.497556
6	-2.424544	2.660194	-0.817632
6	-1.373328	1.729097	-0.647584
6	-1.518336	0.315088	-1.009226
6	-2.703387	-0.427778	-0.845189
6	-2.779214	-1.697473	-1.430717
1	-3.693669	-2.274617	-1.351617
6	-1.655029	-2.219393	-2.062188
1	-1.680105	-3.199237	-2.525331
6	-0.459264	-1.503270	-2.022544
1	0.465517	-1.916205	-2.401761
6	-5.596854	2.671878	-2.524874
1	-5.110513	3.373685	-3.206080
1	-6.631296	2.991895	-2.374655
1	-5.604526	1.686606	-2.999871
6	-4.866482	2.633028	-1.191064
1	-4.864201	3.633542	-0.745786
6	-5.449445	1.628833	-0.183844
1	-6.540488	1.722366	-0.191870
1	-5.116386	1.870000	0.831697
6	-5.050044	0.175695	-0.454059
1	-5.094089	-0.054552	-1.524145
6	-5.873939	-0.821162	0.346593
1	-5.512867	-1.841872	0.198862
1	-6.922560	-0.778914	0.039173
1	-5.818628	-0.587430	1.414426
6	3.003600	3.314239	1.672035
6	3.252158	2.933115	0.341515
6	3.505758	3.915237	-0.617398
6	3.493208	5.253422	-0.214074
6	3.229660	5.609652	1.118452
6	2.979847	4.638875	2.094237
6	2.939369	1.052888	1.662543
6	3.137946	1.471128	0.279953
1	3.698348	3.646744	-1.651183
1	3.694333	6.032922	-0.941459
1	3.230900	6.657012	1.401514
1	2.788681	4.915717	3.125210
1	3.861251	0.910736	-0.305936
7	2.798695	2.132942	2.432504
6	2.496845	2.171185	3.862909
1	1.614181	2.794574	4.025586
1	2.296476	1.167687	4.232008
1	3.344052	2.599686	4.404474
6	2.935949	-0.339939	2.190994
1	3.530953	-0.415372	3.105437
1	1.918858	-0.688798	2.397973
1	3.350206	-1.014169	1.442831
7	2.502095	-0.924577	-1.139080
7	0.332793	-2.140441	1.058255
6	3.616363	-3.243824	-1.327673

6	4.664741	-3.501141	-2.232337
6	3.121774	-4.249313	-0.470326
6	5.217435	-4.776667	-2.272644
1	5.030451	-2.715045	-2.884446
6	3.690842	-5.516501	-0.527544
1	2.311820	-4.020131	0.215252
6	4.733318	-5.778562	-1.424123
1	6.025355	-4.991525	-2.963818
1	3.325751	-6.302098	0.125594
1	5.171969	-6.770712	-1.461874
6	-0.636170	-2.687923	1.403532
6	-1.816403	-3.379396	1.824510
6	-1.747572	-4.758224	2.096014
6	-3.029803	-2.681197	1.970072
6	-2.892028	-5.433090	2.511960
1	-0.806031	-5.285548	1.984119
6	-4.163467	-3.370951	2.391810
1	-3.079011	-1.619371	1.753810
6	-4.097326	-4.741453	2.661869
1	-2.843452	-6.496044	2.723930
1	-5.100599	-2.838972	2.517139
1	-4.985392	-5.270412	2.993047
6	3.025702	-1.954961	-1.249540

TS(X-Y)

Number of imaginary frequencies : 1 Electronic energy : HF=-2058.9313583
Zero-point correction= 0.675360 (Hartree/Particle)
Thermal correction to Energy= 0.719065
Thermal correction to Enthalpy= 0.720009
Thermal correction to Gibbs Free Energy= 0.592460
Sum of electronic and zero-point Energies= -2058.316277
Sum of electronic and thermal Energies= -2058.272572
Sum of electronic and thermal Enthalpies= -2058.271628
Sum of electronic and thermal Free Energies= -2058.399177

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Cartesian Coordinates

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46	0.864776	0.237912	-0.351207
7	-0.686390	1.508138	0.090555
7	-0.729260	-0.637483	-1.642095
8	-3.811306	1.938819	-1.582770
8	-4.149378	-0.455704	-0.624010
6	-0.620583	2.588429	0.885998
1	0.309541	2.766541	1.402144
6	-1.705548	3.454482	1.000344
1	-1.626478	4.310096	1.661215
6	-2.832512	3.262082	0.211715
1	-3.637805	3.987410	0.220586
6	-2.890254	2.143451	-0.630909
6	-1.838004	1.198167	-0.573005
6	-1.907073	-0.105943	-1.247379
6	-3.101300	-0.843737	-1.376142
6	-3.081468	-2.010246	-2.151322
1	-3.996458	-2.572506	-2.303432
6	-1.869351	-2.464733	-2.662492
1	-1.819961	-3.370572	-3.256341
6	-0.697248	-1.782247	-2.330210
1	0.283184	-2.154385	-2.604441

6	-5.733072	2.534833	-2.836962
1	-5.166181	3.347691	-3.296079
1	-6.787766	2.820380	-2.805969
1	-5.631764	1.648776	-3.469984
6	-5.228479	2.265948	-1.427479
1	-5.328807	3.175769	-0.826307
6	-5.936841	1.103545	-0.714019
1	-7.016368	1.217702	-0.857950
1	-5.753741	1.152718	0.365405
6	-5.495321	-0.285556	-1.182500
1	-5.415268	-0.331592	-2.273952
6	-6.388293	-1.398839	-0.655596
1	-6.001944	-2.382552	-0.934512
1	-7.398545	-1.300219	-1.062402
1	-6.451392	-1.350849	0.436015
6	3.647720	2.971414	1.455008
6	2.603507	2.742792	0.520952
6	2.129466	3.819836	-0.249322
6	2.676839	5.080732	-0.053316
6	3.705257	5.288331	0.888420
6	4.208931	4.238134	1.647606
6	3.171371	0.759781	1.542098
6	2.324361	1.330411	0.595313
1	1.346130	3.667516	-0.988169
1	2.316486	5.919328	-0.640154
1	4.118434	6.283293	1.016005
1	5.012196	4.398407	2.358830
1	1.692969	1.282845	-1.088143
7	3.974010	1.760311	2.048835
6	4.997533	1.627296	3.079175
1	4.660561	2.072090	4.020768
1	5.231123	0.577094	3.245197
1	5.909719	2.133375	2.753298
6	3.272422	-0.642592	2.051320
1	4.207087	-1.119792	1.731339
1	3.247672	-0.667767	3.145331
1	2.440231	-1.244933	1.691166
7	2.312738	-1.090286	-0.989167
7	-0.127849	-1.283832	1.190911
6	4.449204	-2.394011	-1.612026
6	5.257690	-1.942966	-2.676153
6	4.788483	-3.547394	-0.873833
6	6.407909	-2.655879	-2.994300
1	4.982301	-1.053507	-3.232918
6	5.942926	-4.244515	-1.209597
1	4.153430	-3.880785	-0.059755
6	6.748419	-3.800830	-2.265082
1	7.039743	-2.321280	-3.810040
1	6.216647	-5.133973	-0.652258
1	7.647773	-4.351882	-2.521325
6	-0.946780	-1.837522	1.802979
6	-1.974084	-2.509180	2.528711
6	-1.636616	-3.424522	3.543183
6	-3.320301	-2.244547	2.207802
6	-2.654130	-4.074596	4.234649
1	-0.595400	-3.616998	3.779112
6	-4.322002	-2.905859	2.910710
1	-3.568873	-1.534686	1.425912
6	-3.992140	-3.817039	3.919562
1	-2.405526	-4.781415	5.019141

1	-5.363279	-2.712034	2.673921
1	-4.780381	-4.327953	4.463424
6	3.278321	-1.669940	-1.271933

Y

Number of imaginary frequencies : 0 Electronic energy : HF=-2058.9976983
Zero-point correction= 0.677243 (Hartree/Particle)
Thermal correction to Energy= 0.721053
Thermal correction to Enthalpy= 0.721997
Thermal correction to Gibbs Free Energy= 0.594132
Sum of electronic and zero-point Energies= -2058.320455
Sum of electronic and thermal Energies= -2058.276646
Sum of electronic and thermal Enthalpies= -2058.275701
Sum of electronic and thermal Free Energies= -2058.403566

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Cartesian Coordinates

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46	0.800560	0.257045	-0.392825
7	-0.732690	1.505144	0.212091
7	-0.847553	-0.394548	-1.795101
8	-3.906473	2.139350	-1.300464
8	-4.213180	-0.358370	-0.590277
6	-0.600177	2.521520	1.078756
1	0.354673	2.622674	1.572879
6	-1.655098	3.405169	1.296822
1	-1.529073	4.209603	2.012469
6	-2.818558	3.294072	0.545734
1	-3.605163	4.033543	0.642405
6	-2.938460	2.246695	-0.378766
6	-1.902390	1.286040	-0.447674
6	-2.002294	0.070088	-1.272369
6	-3.203028	-0.648861	-1.434167
6	-3.223393	-1.709697	-2.348441
1	-4.145468	-2.253478	-2.523777
6	-2.039133	-2.089102	-2.974610
1	-2.021307	-2.912532	-3.679860
6	-0.851754	-1.443505	-2.623303
1	0.112672	-1.767804	-2.998604
6	-5.887279	2.871682	-2.380452
1	-5.340937	3.731491	-2.774320
1	-6.937720	3.150592	-2.263540
1	-5.822583	2.062295	-3.113159
6	-5.311967	2.447075	-1.038023
1	-5.376530	3.283303	-0.333770
6	-5.989058	1.211847	-0.423022
1	-7.073909	1.341297	-0.497533
1	-5.750796	1.140287	0.644303
6	-5.580664	-0.116667	-1.065296
1	-5.548321	-0.037940	-2.157332
6	-6.460341	-1.279297	-0.630824
1	-6.095339	-2.225793	-1.038086
1	-7.486340	-1.130489	-0.978659
1	-6.475986	-1.356740	0.460870
6	3.708147	2.536780	1.691700
6	2.686978	2.420057	0.706969
6	2.369768	3.537593	-0.085657
6	3.053566	4.728053	0.121548
6	4.044376	4.831058	1.119398

6	4.379301	3.743630	1.918297
6	2.956753	0.401529	1.779476
6	2.202105	1.077668	0.838269
1	1.596796	3.473380	-0.849019
1	2.821468	5.594501	-0.489084
1	4.554276	5.777135	1.267831
1	5.135086	3.832051	2.691568
1	1.258361	1.356711	-1.300415
7	3.859780	1.308285	2.314570
6	4.750901	1.086174	3.446007
1	4.363539	1.562703	4.352503
1	4.866467	0.018979	3.629807
1	5.735976	1.501836	3.219757
6	2.945909	-1.026946	2.217783
1	3.925326	-1.493717	2.060079
1	2.703835	-1.123205	3.282114
1	2.205852	-1.593568	1.656076
7	2.310344	-0.875595	-1.146381
7	-0.112917	-1.353637	0.937551
6	4.555066	-1.968542	-1.786985
6	5.426783	-1.295365	-2.668828
6	4.888539	-3.229193	-1.248084
6	6.634080	-1.895624	-3.006394
1	5.154732	-0.325691	-3.072082
6	6.100584	-3.810289	-1.600199
1	4.204921	-3.732258	-0.572326
6	6.968706	-3.146636	-2.475466
1	7.315042	-1.390797	-3.683145
1	6.371084	-4.779902	-1.196063
1	7.913036	-3.608412	-2.745991
6	-0.895666	-1.999654	1.503382
6	-1.878668	-2.781462	2.174340
6	-1.482879	-3.808842	3.051850
6	-3.241469	-2.510382	1.937295
6	-2.459832	-4.565109	3.691210
1	-0.429661	-4.004008	3.223645
6	-4.201263	-3.279471	2.586525
1	-3.534231	-1.713484	1.261616
6	-3.813923	-4.302121	3.459164
1	-2.167591	-5.358937	4.370309
1	-5.254529	-3.083077	2.413995
1	-4.570257	-4.896618	3.961836
6	3.326618	-1.360527	-1.429385

A_{H2O}

Number of imaginary frequencies : 0 Electronic energy : HF=-1504.5615823
Zero-point correction= 0.318042 (Hartree/Particle)
Thermal correction to Energy= 0.339287
Thermal correction to Enthalpy= 0.340231
Thermal correction to Gibbs Free Energy= 0.268912
Sum of electronic and zero-point Energies= -1504.243540
Sum of electronic and thermal Energies= -1504.222296
Sum of electronic and thermal Enthalpies= -1504.221352
Sum of electronic and thermal Free Energies= -1504.292670

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Cartesian Coordinates

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46	2.450775	0.196092	0.042287

7	1.006427	-1.204335	-0.266758
7	0.799575	1.379649	0.353261
8	-2.403775	-1.088711	0.792345
8	-2.490566	0.852215	-0.930235
6	1.217466	-2.514789	-0.449146
1	2.238722	-2.827158	-0.619853
6	0.157168	-3.418618	-0.392485
1	0.351046	-4.471078	-0.565559
6	-1.110302	-2.978090	-0.033652
1	-1.915294	-3.689334	0.113534
6	-1.315503	-1.611033	0.202638
6	-0.249543	-0.719916	-0.047278
6	-0.355623	0.736904	0.039268
6	-1.514722	1.481489	-0.254302
6	-1.523210	2.847662	0.057493
1	-2.422351	3.431639	-0.103007
6	-0.353016	3.449337	0.508802
1	-0.323763	4.508359	0.738667
6	0.818997	2.696830	0.587917
1	1.780100	3.136090	0.826827
6	-4.520498	-1.429770	1.809510
1	-4.040861	-2.066069	2.558483
1	-5.550250	-1.770885	1.668515
1	-4.544762	-0.403093	2.188610
6	-3.770335	-1.506227	0.489147
1	-3.765498	-2.538190	0.127902
6	-4.341089	-0.582818	-0.599035
1	-5.434162	-0.633315	-0.558192
1	-4.038596	-0.935414	-1.591080
6	-3.885843	0.873588	-0.481887
1	-3.902106	1.217902	0.557288
6	-4.685406	1.809188	-1.375955
1	-4.305294	2.832798	-1.321335
1	-5.734464	1.815374	-1.063997
1	-4.634524	1.475554	-2.417383
17	4.314375	-1.167264	-0.425178
8	3.809086	1.773596	0.502832
1	4.331638	1.977275	-0.295425
1	4.459187	1.436399	1.147568

A_{OH}

Number of imaginary frequencies : 0 Electronic energy : HF=-1504.4928404
Zero-point correction= 0.313255 (Hartree/Particle)
Thermal correction to Energy= 0.335037
Thermal correction to Enthalpy= 0.335981
Thermal correction to Gibbs Free Energy= 0.263233
Sum of electronic and zero-point Energies= -1504.179585
Sum of electronic and thermal Energies= -1504.157804
Sum of electronic and thermal Enthalpies= -1504.156859
Sum of electronic and thermal Free Energies= -1504.229608

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Cartesian Coordinates

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46	2.444691	0.234889	0.100833
7	0.982398	-1.245600	-0.226907
7	0.777062	1.356369	0.417421
8	-2.438661	-1.078027	0.808901
8	-2.462662	0.822389	-0.971745

6	1.175406	-2.562913	-0.364590
1	2.193934	-2.900475	-0.516057
6	0.113057	-3.462631	-0.287109
1	0.297617	-4.522166	-0.424366
6	-1.154980	-2.998435	0.043592
1	-1.969526	-3.696373	0.201561
6	-1.348097	-1.624016	0.240985
6	-0.267192	-0.752885	-0.019399
6	-0.363594	0.708881	0.063076
6	-1.513390	1.453753	-0.259954
6	-1.539972	2.816460	0.065038
1	-2.438146	3.395447	-0.120447
6	-0.388029	3.417201	0.563318
1	-0.371463	4.473419	0.807250
6	0.786209	2.670970	0.669703
1	1.747890	3.092741	0.937052
6	-4.587897	-1.311928	1.782112
1	-4.146851	-1.922491	2.574874
1	-5.623675	-1.629431	1.630614
1	-4.589987	-0.267413	2.109437
6	-3.805621	-1.477534	0.488502
1	-3.818711	-2.527970	0.183828
6	-4.326552	-0.602248	-0.662496
1	-5.420496	-0.652097	-0.667082
1	-3.981235	-0.997471	-1.624024
6	-3.874506	0.858127	-0.586620
1	-3.939757	1.244871	0.435508
6	-4.626763	1.760065	-1.552858
1	-4.238053	2.781863	-1.520733
1	-5.689102	1.786432	-1.290911
1	-4.530414	1.384997	-2.576928
17	4.590759	-0.929020	-0.553510
8	3.647052	1.705051	0.618738
1	3.830385	2.187743	-0.204535
1	4.238393	-1.971084	-1.244263

A'

Number of imaginary frequencies : 0 Electronic energy : HF=-1752.5648029
Zero-point correction= 0.393367 (Hartree/Particle)
Thermal correction to Energy= 0.419889
Thermal correction to Enthalpy= 0.420833
Thermal correction to Gibbs Free Energy= 0.333316
Sum of electronic and zero-point Energies= -1752.171435
Sum of electronic and thermal Energies= -1752.144914
Sum of electronic and thermal Enthalpies= -1752.143970
Sum of electronic and thermal Free Energies= -1752.231487

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Cartesian Coordinates

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46	-1.024338	0.669550	-0.131356
7	0.182172	-1.004517	0.157345
7	0.813661	1.571979	-0.249730
8	3.592142	-1.346969	-0.860179
8	3.909604	0.360668	1.070453
6	-0.237620	-2.275223	0.209842
1	-1.300237	-2.429348	0.347473
6	0.658762	-3.332888	0.069062
1	0.299737	-4.353638	0.135876

6	1.989243	-3.065423	-0.236849
1	2.675100	-3.876608	-0.453077
6	2.416999	-1.734588	-0.333447
6	1.497214	-0.711997	-0.008588
6	1.832151	0.714957	0.039407
6	3.086956	1.215361	0.436324
6	3.346252	2.580818	0.262279
1	4.321059	2.982357	0.515318
6	2.320647	3.411704	-0.173469
1	2.481794	4.475793	-0.303162
6	1.041421	2.887566	-0.365507
1	0.181776	3.504363	-0.596029
6	5.675376	-1.886419	-1.855088
1	5.144125	-2.351070	-2.688955
1	6.640327	-2.385567	-1.732209
1	5.857154	-0.838090	-2.109318
6	4.860809	-2.002496	-0.574619
1	4.685092	-3.059758	-0.347228
6	5.513099	-1.321419	0.641050
1	6.582923	-1.555548	0.639684
1	5.098489	-1.724921	1.571249
6	5.308754	0.196344	0.686115
1	5.446628	0.644815	-0.304609
6	6.197453	0.875462	1.719255
1	5.991443	1.947061	1.779528
1	7.251480	0.745039	1.457141
1	6.027769	0.440990	2.708599
7	-2.819925	-0.247530	0.070695
6	-3.959232	-0.453274	0.139836
6	-5.367997	-0.637077	0.197672
6	-5.919571	-1.860501	0.620283
6	-6.189320	0.444475	-0.177866
6	-7.302910	-1.996068	0.663498
1	-5.271083	-2.681287	0.907715
6	-7.570526	0.287600	-0.126684
1	-5.738802	1.378526	-0.497243
6	-8.124477	-0.926570	0.291369
1	-7.742180	-2.933641	0.987456
1	-8.215162	1.112087	-0.412327
1	-9.203366	-1.040575	0.328328
17	-2.222399	2.611089	-0.597968

B'

Number of imaginary frequencies : 0 Electronic energy : HF=-2266.8220857
Zero-point correction= 0.533002 (Hartree/Particle)
Thermal correction to Energy= 0.569358
Thermal correction to Enthalpy= 0.570302
Thermal correction to Gibbs Free Energy= 0.462588
Sum of electronic and zero-point Energies= -2266.289083
Sum of electronic and thermal Energies= -2266.252727
Sum of electronic and thermal Enthalpies= -2266.251783
Sum of electronic and thermal Free Energies= -2266.359498

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Cartesian Coordinates

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46	-1.269944	-0.869074	0.757385
7	0.301916	-2.193219	0.273468
7	0.414783	0.430116	1.012411

8	3.337404	-1.105663	-1.285066
8	3.828643	-0.658761	1.277393
6	0.136372	-3.428316	-0.220892
1	-0.808469	-3.910239	-0.002324
6	1.132656	-4.026380	-0.992515
1	0.986072	-5.035099	-1.361878
6	2.263881	-3.296718	-1.346502
1	2.995391	-3.715073	-2.028667
6	2.415688	-1.996062	-0.852086
6	1.452742	-1.512221	0.055334
6	1.572448	-0.237702	0.769611
6	2.798245	0.211198	1.295384
6	2.848526	1.467511	1.904797
1	3.788696	1.849777	2.285679
6	1.665491	2.177338	2.061122
1	1.654684	3.149232	2.540056
6	0.460876	1.608548	1.651255
1	-0.476401	2.112837	1.835127
6	5.226919	-0.441675	-2.540931
1	4.615139	-0.475514	-3.445520
1	6.263769	-0.657404	-2.812010
1	5.180263	0.573520	-2.135191
6	4.727608	-1.459611	-1.524831
1	4.780057	-2.462128	-1.964546
6	5.504101	-1.445283	-0.198363
1	6.575188	-1.413591	-0.425249
1	5.323106	-2.371916	0.357256
6	5.129776	-0.288114	0.733507
1	5.013193	0.648563	0.175366
6	6.120065	-0.115412	1.877353
1	5.801371	0.673945	2.562850
1	7.108669	0.146990	1.489216
1	6.204764	-1.045244	2.447108
17	-2.817959	-2.595529	1.017910
6	-2.982894	0.480555	0.591649
6	-4.015172	-0.034693	-0.397877
6	-5.373142	-0.092585	-0.070576
6	-3.591145	-0.412743	-1.678716
6	-6.300070	-0.538808	-1.013480
1	-5.726226	0.200983	0.913547
6	-4.521949	-0.847369	-2.617093
1	-2.539003	-0.366433	-1.934108
6	-5.878154	-0.917425	-2.286972
1	-7.350990	-0.586880	-0.747209
1	-4.185680	-1.140789	-3.606600
1	-6.599873	-1.265523	-3.018949
6	-2.480076	1.899130	0.341800
8	-2.374301	2.735863	1.216205
8	-2.170441	2.046323	-0.939226
6	-1.594827	3.325005	-1.356967
1	-2.013812	4.123393	-0.742150
1	-1.947480	3.431976	-2.385166
6	-0.089865	3.284654	-1.278327
6	0.619941	4.375141	-0.766323
6	0.611289	2.165195	-1.746077
6	2.016204	4.353052	-0.733457
1	0.082436	5.243260	-0.394290
6	2.003707	2.132395	-1.694505
1	0.060607	1.312441	-2.132269
6	2.707907	3.230870	-1.192435

1	2.559826	5.207915	-0.342718
1	2.534913	1.248735	-2.033863
1	3.793769	3.212610	-1.159833
7	-3.456379	0.445314	1.909620
7	-3.809543	0.396664	2.965985

TS(B'-C')

Number of imaginary frequencies : 1 Electronic energy : HF=-2266.8138848
Zero-point correction= 0.531110 (Hartree/Particle)
Thermal correction to Energy= 0.567512
Thermal correction to Enthalpy= 0.568456
Thermal correction to Gibbs Free Energy= 0.461254
Sum of electronic and zero-point Energies= -2266.282775
Sum of electronic and thermal Energies= -2266.246373
Sum of electronic and thermal Enthalpies= -2266.245428
Sum of electronic and thermal Free Energies= -2266.352631

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Cartesian Coordinates

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46	-1.315775	-1.016043	0.745690
7	0.338524	-2.329843	0.372889
7	0.335417	0.305039	1.069060
8	3.253190	-1.118727	-1.327730
8	3.812954	-0.592360	1.204749
6	0.230218	-3.585461	-0.081464
1	-0.679174	-4.112411	0.181359
6	1.230847	-4.150624	-0.872548
1	1.132094	-5.177136	-1.207352
6	2.303837	-3.367675	-1.289129
1	3.033694	-3.764435	-1.985814
6	2.397875	-2.045889	-0.837179
6	1.440526	-1.593158	0.091558
6	1.517127	-0.300391	0.782313
6	2.734744	0.215722	1.264365
6	2.738204	1.469069	1.882583
1	3.670433	1.904690	2.222507
6	1.523220	2.098749	2.113310
1	1.475744	3.057826	2.615084
6	0.339953	1.465905	1.740080
1	-0.614988	1.904138	1.989675
6	5.061455	-0.402727	-2.676929
1	4.407810	-0.482282	-3.548790
1	6.090764	-0.591248	-2.993469
1	5.001431	0.621272	-2.296018
6	4.649397	-1.408956	-1.611012
1	4.737786	-2.421368	-2.021129
6	5.474403	-1.310234	-0.317773
1	6.531934	-1.219255	-0.588041
1	5.373026	-2.229668	0.269088
6	5.063813	-0.152280	0.597701
1	4.861622	0.758425	0.021619
6	6.088247	0.115848	1.692294
1	5.750656	0.904151	2.369794
1	7.040908	0.427577	1.253882
1	6.255941	-0.789622	2.282536
17	-2.846423	-2.769796	0.927222
6	-2.883321	0.296503	0.444565
6	-3.922256	0.057002	-0.600027

6	-5.031480	0.927203	-0.661695
6	-3.773942	-0.934626	-1.582033
6	-5.980115	0.790456	-1.666924
1	-5.153105	1.703681	0.089933
6	-4.712194	-1.045353	-2.607459
1	-2.930392	-1.610075	-1.545401
6	-5.818355	-0.196257	-2.646299
1	-6.839753	1.452221	-1.693110
1	-4.584336	-1.809454	-3.367252
1	-6.555645	-0.300640	-3.436275
6	-2.495945	1.760412	0.531902
8	-2.671846	2.485234	1.490110
8	-1.910416	2.082485	-0.620070
6	-1.369256	3.426231	-0.793176
1	-1.682681	4.050061	0.046134
1	-1.841418	3.794456	-1.708631
6	0.133870	3.369230	-0.924758
6	0.909320	4.444029	-0.476110
6	0.763841	2.268076	-1.517670
6	2.297841	4.421046	-0.622531
1	0.429233	5.301257	-0.010735
6	2.152020	2.235283	-1.645225
1	0.166326	1.428387	-1.856938
6	2.921606	3.314336	-1.202191
1	2.889824	5.263284	-0.277272
1	2.626406	1.361461	-2.079797
1	4.002483	3.296231	-1.311943
7	-3.747594	0.150279	1.942708
7	-4.278604	-0.245318	2.828790

C'

Number of imaginary frequencies : 0 Electronic energy : HF=-2157.3328671
Zero-point correction= 0.523848 (Hartree/Particle)
Thermal correction to Energy= 0.558171
Thermal correction to Enthalpy= 0.559115
Thermal correction to Gibbs Free Energy= 0.455883
Sum of electronic and zero-point Energies= -2156.809019
Sum of electronic and thermal Energies= -2156.774696
Sum of electronic and thermal Enthalpies= -2156.773752
Sum of electronic and thermal Free Energies= -2156.876984

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Cartesian Coordinates

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46	1.237327	0.528273	0.478789
7	-0.639296	1.095662	1.345032
7	-0.091722	0.055803	-1.101502
8	-3.691777	1.813839	-0.383621
8	-3.557511	-0.760260	-0.768411
6	-0.803737	1.731841	2.508821
1	0.069218	1.788100	3.148944
6	-2.029985	2.306336	2.846373
1	-2.146722	2.800120	3.804600
6	-3.061733	2.309886	1.914257
1	-3.983436	2.842947	2.118669
6	-2.871711	1.673563	0.680538
6	-1.667225	0.966966	0.474291
6	-1.391552	0.155576	-0.721707
6	-2.388392	-0.566012	-1.411135

6	-2.069074	-1.148660	-2.640131
1	-2.833125	-1.667396	-3.208475
6	-0.749805	-1.105163	-3.082194
1	-0.461382	-1.553574	-4.026159
6	0.223554	-0.548538	-2.257161
1	1.273497	-0.604565	-2.506034
6	-5.648434	2.681018	-1.397167
1	-5.243379	3.689528	-1.286478
1	-6.740047	2.736330	-1.369452
1	-5.345064	2.298938	-2.376365
6	-5.140389	1.781276	-0.279020
1	-5.451496	2.193984	0.687067
6	-5.624173	0.325087	-0.386629
1	-6.690129	0.327234	-0.638333
1	-5.524620	-0.180315	0.580351
6	-4.844933	-0.510271	-1.406590
1	-4.666908	0.055601	-2.328277
6	-5.516457	-1.842776	-1.710198
1	-4.908022	-2.449367	-2.386034
1	-6.490928	-1.680326	-2.179920
1	-5.666792	-2.409954	-0.786764
17	2.518360	1.158044	2.326946
6	2.935242	-0.047326	-0.322118
6	3.955743	0.733944	-0.897524
6	5.136549	0.126101	-1.424438
6	3.823663	2.153201	-0.957330
6	6.125039	0.906494	-1.995704
1	5.260375	-0.949130	-1.353632
6	4.819065	2.922968	-1.531851
1	2.939966	2.609984	-0.525812
6	5.965008	2.300321	-2.050221
1	7.024496	0.447580	-2.391865
1	4.722643	4.002561	-1.571903
1	6.747475	2.908637	-2.494786
6	3.102953	-1.513683	-0.105890
8	3.866796	-1.917671	0.744532
8	2.251980	-2.247323	-0.833319
6	1.785528	-3.507476	-0.211942
1	2.634509	-3.988405	0.275548
1	1.447886	-4.109497	-1.055264
6	0.675513	-3.158217	0.740506
6	0.976215	-2.736698	2.044728
6	-0.652211	-3.124595	0.297269
6	-0.038605	-2.278995	2.885628
1	2.005134	-2.747750	2.389668
6	-1.668585	-2.674891	1.141160
1	-0.888238	-3.439888	-0.715954
6	-1.359946	-2.244945	2.434084
1	0.205838	-1.947398	3.889763
1	-2.692478	-2.639437	0.784065
1	-2.148946	-1.888769	3.090071

TS(C'-D')

Number of imaginary frequencies : 1 Electronic energy : HF=-2599.6996573
Zero-point correction= 0.709823 (Hartree/Particle)
Thermal correction to Energy= 0.754682
Thermal correction to Enthalpy= 0.755626
Thermal correction to Gibbs Free Energy= 0.628546

Sum of electronic and zero-point Energies= -2598.987338
Sum of electronic and thermal Energies= -2598.942478
Sum of electronic and thermal Enthalpies= -2598.941534
Sum of electronic and thermal Free Energies= -2599.068614

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Cartesian Coordinates

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46	-0.185861	0.487731	0.957580
7	1.709191	1.195590	1.744568
7	1.150020	0.102408	-0.695869
8	4.994416	0.358651	0.560576
8	4.168938	1.915418	-1.369804
6	1.941922	1.534429	3.017916
1	1.064724	1.696863	3.632987
6	3.241215	1.642716	3.512060
1	3.400400	1.934450	4.544263
6	4.312711	1.300921	2.695568
1	5.321148	1.283866	3.094078
6	4.066822	0.920250	1.371110
6	2.737803	0.976003	0.894485
6	2.364344	0.680427	-0.498678
6	3.183456	1.022279	-1.596450
6	2.858060	0.520026	-2.859807
1	3.491583	0.735893	-3.713373
6	1.686323	-0.213814	-3.004896
1	1.399933	-0.623941	-3.966904
6	0.830287	-0.356276	-1.915269
1	-0.125030	-0.850358	-2.013534
6	7.221470	-0.351878	0.145165
1	7.112280	-1.110972	0.923529
1	8.273351	-0.057308	0.092416
1	6.941350	-0.804074	-0.811062
6	6.353100	0.860393	0.458876
1	6.660535	1.280956	1.422571
6	6.414617	1.964482	-0.612919
1	7.457411	2.091157	-0.924537
1	6.092453	2.922059	-0.188765
6	5.532196	1.699696	-1.837936
1	5.620899	0.658738	-2.170062
6	5.827692	2.656662	-2.987414
1	5.151186	2.489793	-3.830009
1	6.853353	2.519269	-3.342999
1	5.711297	3.694181	-2.660477
17	-1.292548	1.222047	2.884951
6	-1.801769	-0.375995	0.088198
6	-2.354518	0.170787	-1.124793
6	-3.103111	-0.600051	-2.057706
6	-2.174369	1.552104	-1.404143
6	-3.601198	-0.023064	-3.218072
1	-3.250079	-1.657790	-1.877238
6	-2.687294	2.124085	-2.561043
1	-1.624937	2.157331	-0.691607
6	-3.402705	1.340475	-3.471343
1	-4.146754	-0.632933	-3.932265
1	-2.538009	3.181798	-2.752287
1	-3.800975	1.786816	-4.377656
6	-1.678511	-1.846002	0.373187
8	-1.801857	-2.358350	1.467611
8	-1.295810	-2.529005	-0.736039
6	-0.928104	-3.941878	-0.551023

1	-1.208603	-4.405921	-1.498091
1	-1.539441	-4.344748	0.256833
6	0.542359	-4.103509	-0.274088
6	1.437634	-4.330859	-1.327498
6	1.033288	-4.032523	1.038151
6	2.801881	-4.484207	-1.078309
1	1.062145	-4.403313	-2.345561
6	2.397722	-4.183587	1.287018
1	0.342030	-3.861560	1.857558
6	3.283407	-4.409468	0.230303
1	3.484990	-4.673868	-1.901100
1	2.767297	-4.138458	2.307223
1	4.343525	-4.539306	0.427586
6	-5.421701	0.935655	0.002909
6	-4.396462	1.230416	0.930083
6	-4.052552	2.570347	1.152236
6	-4.747149	3.564057	0.458509
6	-5.759224	3.242592	-0.457894
6	-6.114094	1.912891	-0.704062
6	-4.748122	-1.033086	0.883115
6	-3.912988	-0.033873	1.435275
1	-3.267806	2.819802	1.857261
1	-4.504059	4.607073	0.636644
1	-6.284345	4.037240	-0.978680
1	-6.905384	1.667062	-1.404567
1	-3.278174	-0.183937	2.294469
7	-5.597067	-0.459747	-0.011487
6	-6.640583	-1.118790	-0.782118
1	-7.629026	-0.807649	-0.429066
1	-6.542906	-0.853555	-1.838446
1	-6.552886	-2.199167	-0.680877
6	-4.820982	-2.483474	1.230688
1	-5.803393	-2.728399	1.651455
1	-4.669752	-3.129851	0.357406
1	-4.055163	-2.725323	1.964503

D'

Number of imaginary frequencies : 0 Electronic energy : HF=-2599.8750934
Zero-point correction= 0.714140 (Hartree/Particle)
Thermal correction to Energy= 0.758147
Thermal correction to Enthalpy= 0.759091
Thermal correction to Gibbs Free Energy= 0.637118
Sum of electronic and zero-point Energies= -2599.160953
Sum of electronic and thermal Energies= -2599.116946
Sum of electronic and thermal Enthalpies= -2599.116002
Sum of electronic and thermal Free Energies= -2599.237975

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Cartesian Coordinates

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46	-0.367152	-0.638522	0.602325
7	1.537165	-0.727198	1.643093
7	0.883541	0.627729	-0.642778
8	4.767634	-0.035354	0.260379
8	3.816567	2.389486	0.421779
6	1.834197	-1.558930	2.649956
1	0.994392	-2.053902	3.120979
6	3.152960	-1.790274	3.035194
1	3.361285	-2.449998	3.870169

6	4.186665	-1.237872	2.286932
1	5.218237	-1.495907	2.498911
6	3.873902	-0.404830	1.209411
6	2.518503	-0.071960	0.986679
6	2.084691	0.868858	-0.057663
6	2.855948	1.986808	-0.437525
6	2.523807	2.667065	-1.611877
1	3.127882	3.503503	-1.946234
6	1.389680	2.268184	-2.309917
1	1.099319	2.754433	-3.234354
6	0.567054	1.282755	-1.767239
1	-0.361970	1.006277	-2.237747
6	6.954506	0.032900	-0.632797
1	6.902067	-1.044380	-0.808730
1	7.999153	0.310465	-0.467996
1	6.598225	0.541690	-1.533466
6	6.109875	0.410879	0.576946
1	6.483236	-0.125707	1.456601
6	6.092576	1.919226	0.875771
1	7.114894	2.305227	0.798196
1	5.759250	2.097049	1.904137
6	5.157064	2.714256	-0.039780
1	5.255020	2.383849	-1.080731
6	5.366299	4.219090	0.067162
1	4.643182	4.761564	-0.547686
1	6.372994	4.490449	-0.264400
1	5.241332	4.544753	1.104020
17	-1.280141	-2.266929	2.045844
6	-2.249531	-0.463908	-0.459103
6	-2.434944	0.901417	-1.090659
6	-2.895247	1.046798	-2.412813
6	-2.226528	2.071243	-0.338861
6	-3.123819	2.309340	-2.963671
1	-3.032408	0.167818	-3.032913
6	-2.456625	3.332437	-0.886270
1	-1.858131	1.988374	0.676841
6	-2.906686	3.458989	-2.202335
1	-3.465553	2.391652	-3.991494
1	-2.275666	4.217932	-0.284154
1	-3.079657	4.441318	-2.631381
6	-1.956937	-1.616145	-1.373509
8	-2.362848	-2.756994	-1.215319
8	-1.120764	-1.263945	-2.385504
6	-0.371406	-2.344726	-3.021281
1	-0.151559	-1.969503	-4.022171
1	-1.013439	-3.224622	-3.088439
6	0.884295	-2.614094	-2.234378
6	2.080414	-1.965576	-2.564998
6	0.843518	-3.449957	-1.109456
6	3.226439	-2.157135	-1.793521
1	2.111252	-1.304667	-3.427872
6	1.989999	-3.642383	-0.337077
1	-0.090169	-3.928020	-0.831962
6	3.181746	-3.001718	-0.681172
1	4.147978	-1.643177	-2.047414
1	1.947924	-4.288777	0.534027
1	4.073394	-3.152311	-0.080598
6	-4.948206	0.857111	1.336069
6	-3.740489	0.201942	1.584475
6	-3.014844	0.555043	2.718692

6	-3.518372	1.564871	3.547207
6	-4.723242	2.217768	3.259583
6	-5.472750	1.864824	2.134736
6	-4.773280	-0.664826	-0.332611
6	-3.496414	-0.781786	0.461971
1	-2.088220	0.049512	2.955436
1	-2.962721	1.844118	4.436862
1	-5.087273	2.997821	3.920084
1	-6.414277	2.353284	1.909672
1	-3.373255	-1.814283	0.811271
7	-5.526986	0.292264	0.158801
6	-6.802655	0.775973	-0.367680
1	-6.704676	1.842301	-0.583944
1	-7.062691	0.245800	-1.280383
1	-7.582524	0.628175	0.382967
6	-5.169852	-1.492641	-1.503137
1	-6.204344	-1.835582	-1.405043
1	-5.097383	-0.903283	-2.425035
1	-4.508336	-2.352618	-1.585528

TS(D'-E')

Number of imaginary frequencies : 1 Electronic energy : HF=-2599.8450626
Zero-point correction= 0.708178 (Hartree/Particle)
Thermal correction to Energy= 0.752227
Thermal correction to Enthalpy= 0.753171
Thermal correction to Gibbs Free Energy= 0.630949
Sum of electronic and zero-point Energies= -2599.134156
Sum of electronic and thermal Energies= -2599.090107
Sum of electronic and thermal Enthalpies= -2599.089163
Sum of electronic and thermal Free Energies= -2599.211385

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Cartesian Coordinates

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46	-0.495892	-0.509010	0.137047
7	1.269049	-1.535492	0.991130
7	1.034560	0.996176	-0.074356
8	4.665678	-0.777774	0.145946
8	4.116965	1.220469	1.732181
6	1.341951	-2.831942	1.318096
1	0.401422	-3.344823	1.479472
6	2.566247	-3.485541	1.437175
1	2.597840	-4.529911	1.727100
6	3.731306	-2.800310	1.106634
1	4.684573	-3.316542	1.090163
6	3.650811	-1.456657	0.728359
6	2.391736	-0.815628	0.788549
6	2.204304	0.618992	0.504070
6	3.174456	1.585785	0.838847
6	3.049087	2.876728	0.316487
1	3.806620	3.623923	0.526329
6	1.919272	3.184892	-0.431970
1	1.782251	4.170310	-0.862472
6	0.905956	2.235695	-0.560607
1	-0.023875	2.465860	-1.057757
6	6.897667	-0.588415	-0.610040
1	6.681852	-1.326127	-1.386838
1	7.957536	-0.654187	-0.349921
1	6.703469	0.406212	-1.022368

6	6.036237	-0.847605	0.618629
1	6.246822	-1.853465	0.999350
6	6.240853	0.173955	1.749323
1	7.315483	0.340166	1.881483
1	5.859628	-0.227358	2.694752
6	5.526856	1.507886	1.510927
1	5.653303	1.840470	0.473770
6	5.969420	2.594424	2.481784
1	5.398140	3.514171	2.331146
1	7.030597	2.821649	2.343433
1	5.815164	2.264823	3.513371
6	-2.250985	0.550518	-0.612094
6	-2.215298	2.028336	-0.308803
6	-2.496260	2.985151	-1.302986
6	-1.978104	2.491614	0.998774
6	-2.510560	4.348324	-1.004981
1	-2.687934	2.667805	-2.320759
6	-1.981426	3.852516	1.292841
1	-1.773517	1.782581	1.789599
6	-2.243876	4.790489	0.291242
1	-2.730772	5.064029	-1.791538
1	-1.781123	4.180478	2.308468
1	-2.248429	5.851638	0.520620
6	-1.986707	0.114449	-2.031384
8	-2.452861	-0.890328	-2.541772
8	-1.083079	0.910788	-2.656795
6	-0.412711	0.340694	-3.821856
1	-0.089746	1.209550	-4.397389
1	-1.135803	-0.237521	-4.399233
6	0.754471	-0.496574	-3.366879
6	2.017515	0.084581	-3.200402
6	0.569121	-1.844295	-3.027298
6	3.084350	-0.667220	-2.708922
1	2.162527	1.132081	-3.452674
6	1.636816	-2.598403	-2.537057
1	-0.414315	-2.288906	-3.136747
6	2.894308	-2.011962	-2.380856
1	4.058409	-0.209474	-2.571260
1	1.486612	-3.643432	-2.282661
1	3.725785	-2.597233	-2.001249
6	-5.044762	-0.684733	1.599674
6	-3.676389	-0.364657	1.443236
6	-2.838198	-0.454077	2.566792
6	-3.381043	-0.812595	3.795541
6	-4.750883	-1.107345	3.926848
6	-5.600583	-1.056510	2.826833
6	-4.730185	-0.204900	-0.584195
6	-3.460817	-0.107860	0.022183
1	-1.772435	-0.257244	2.481217
1	-2.737906	-0.869979	4.668246
1	-5.149257	-1.384246	4.897572
1	-6.654974	-1.292245	2.923916
1	-2.902669	-1.781427	-0.172137
7	-5.654788	-0.585914	0.354080
6	-7.061834	-0.892375	0.132722
1	-7.700619	-0.081941	0.498175
1	-7.251741	-1.049378	-0.927600
1	-7.318862	-1.812989	0.662563
6	-5.132132	0.106505	-1.990306
1	-4.488604	0.884151	-2.402034

1	-5.031895	-0.767787	-2.640414
1	-6.159652	0.473351	-2.036993
17	-1.875187	-2.684283	-0.007348

E'

Number of imaginary frequencies : 0 Electronic energy : HF=-2600.3864236
Zero-point correction= 0.709509 (Hartree/Particle)
Thermal correction to Energy= 0.753999
Thermal correction to Enthalpy= 0.754943
Thermal correction to Gibbs Free Energy= 0.631791
Sum of electronic and zero-point Energies= -2599.676914
Sum of electronic and thermal Energies= -2599.632425
Sum of electronic and thermal Enthalpies= -2599.631481
Sum of electronic and thermal Free Energies= -2599.754632

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Cartesian Coordinates

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46	0.454887	-0.623679	0.119569
7	-1.249259	-1.713780	-0.597283
7	-1.032970	0.908267	0.096613
8	-4.684916	-0.832719	-0.138944
8	-4.001016	0.968161	-1.889856
6	-1.314135	-3.038933	-0.762729
1	-0.374697	-3.572580	-0.756623
6	-2.535906	-3.688336	-0.901795
1	-2.557770	-4.759115	-1.058432
6	-3.710833	-2.964774	-0.752976
1	-4.668048	-3.470225	-0.745107
6	-3.640102	-1.585880	-0.548842
6	-2.374069	-0.965429	-0.596051
6	-2.181358	0.485915	-0.490016
6	-3.113566	1.417767	-0.982660
6	-2.997635	2.752589	-0.593084
1	-3.727468	3.481424	-0.922519
6	-1.910562	3.124722	0.183782
1	-1.781366	4.146335	0.516003
6	-0.919645	2.188462	0.460031
1	-0.013626	2.470915	0.969145
6	-6.972461	-0.571759	0.417145
1	-6.826693	-1.225749	1.278458
1	-8.007227	-0.665345	0.081058
1	-6.805213	0.458526	0.739823
6	-6.020974	-0.953080	-0.706003
1	-6.201732	-1.991704	-0.995935
6	-6.134508	-0.054870	-1.947222
1	-7.194436	0.104969	-2.164472
1	-5.701476	-0.554669	-2.818571
6	-5.422120	1.290600	-1.802466
1	-5.609781	1.729730	-0.817886
6	-5.782026	2.271223	-2.907529
1	-5.205833	3.194078	-2.819116
1	-6.844085	2.523597	-2.858669
1	-5.573246	1.832722	-3.886077
6	2.328213	0.635267	0.479374
6	2.107084	2.033409	-0.045957
6	2.411670	3.153344	0.741203
6	1.706784	2.242767	-1.372330
6	2.277915	4.442256	0.228853

1	2.747764	3.025014	1.761365
6	1.570097	3.529233	-1.882098
1	1.494222	1.396015	-2.008704
6	1.846420	4.637152	-1.081652
1	2.518193	5.293661	0.855515
1	1.251219	3.665561	-2.909041
1	1.742243	5.639797	-1.479599
6	2.032185	0.337581	1.846670
8	2.500368	-0.713642	2.493807
8	1.361698	1.195835	2.588100
6	0.683769	0.725368	3.825398
1	0.507709	1.655393	4.361082
1	1.378670	0.103443	4.384463
6	-0.594444	0.015554	3.486973
6	-1.782623	0.740051	3.348987
6	-0.601769	-1.363675	3.250707
6	-2.959602	0.100013	2.972234
1	-1.784086	1.809282	3.532970
6	-1.780846	-2.005770	2.878839
1	0.315713	-1.931124	3.344470
6	-2.958434	-1.274780	2.737055
1	-3.875727	0.668177	2.862417
1	-1.774992	-3.073769	2.695855
1	-3.875045	-1.769687	2.439973
6	5.067864	-0.865837	-1.590403
6	3.693782	-0.558523	-1.439879
6	2.819868	-0.877791	-2.488812
6	3.325522	-1.448604	-3.647659
6	4.697482	-1.725636	-3.780807
6	5.585462	-1.444929	-2.750400
6	4.801750	0.034343	0.457907
6	3.539972	0.001291	-0.119596
1	1.753767	-0.709500	-2.393130
1	2.653350	-1.694346	-4.461553
1	5.066781	-2.171348	-4.696747
1	6.640779	-1.667777	-2.849864
1	2.703762	-1.438854	1.852710
7	5.718336	-0.509713	-0.421197
6	7.152470	-0.637455	-0.221440
1	7.699123	0.124852	-0.784692
1	7.394499	-0.538199	0.834488
1	7.481935	-1.624314	-0.551813
6	5.240154	0.604465	1.767675
1	4.434309	1.164935	2.237325
1	5.553909	-0.174029	2.471041
1	6.078196	1.294102	1.634708
17	1.736158	-2.601135	0.331244

F_{H2O}

Number of imaginary frequencies : 0 Electronic energy : HF=-2215.4752024
Zero-point correction= 0.725785 (Hartree/Particle)
Thermal correction to Energy= 0.770238
Thermal correction to Enthalpy= 0.771182
Thermal correction to Gibbs Free Energy= 0.648365
Sum of electronic and zero-point Energies= -2214.749417
Sum of electronic and thermal Energies= -2214.704964
Sum of electronic and thermal Enthalpies= -2214.704020
Sum of electronic and thermal Free Energies= -2214.826838

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Cartesian Coordinates

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46	-0.528488	-1.105357	-0.192665
7	0.987375	-0.984033	-1.683941
7	1.135866	-1.117254	1.005252
8	3.985366	0.861051	-1.026813
8	4.597468	-1.438702	0.144407
6	0.762576	-0.715040	-2.978126
1	-0.200150	-1.021884	-3.369349
6	1.710043	-0.048522	-3.752920
1	1.518241	0.129703	-4.805226
6	2.861678	0.447852	-3.144670
1	3.558122	1.060977	-3.705761
6	3.071104	0.208267	-1.782007
6	2.153617	-0.612752	-1.096295
6	2.296780	-0.993498	0.316831
6	3.521029	-1.276659	0.942883
6	3.528795	-1.486695	2.328368
1	4.466327	-1.677845	2.838279
6	2.323623	-1.492515	3.022044
1	2.298707	-1.647839	4.094511
6	1.126415	-1.344072	2.320077
1	0.149002	-1.380339	2.786687
6	5.787142	2.376218	-0.798067
1	5.140576	3.191318	-1.133317
1	6.818318	2.616700	-1.070049
1	5.721196	2.315356	0.292329
6	5.364370	1.061966	-1.440655
1	5.410748	1.158272	-2.531539
6	6.212842	-0.142569	-1.000376
1	7.267305	0.153720	-1.009327
1	6.105807	-0.963961	-1.717095
6	5.834331	-0.703010	0.375078
1	5.626106	0.103475	1.088032
6	6.888233	-1.653637	0.927396
1	6.569852	-2.089460	1.877731
1	7.830808	-1.123525	1.093211
1	7.066965	-2.470650	0.222329
6	-2.726447	1.197920	0.687267
6	-3.896323	1.988926	0.253738
6	-3.829273	3.397544	0.301979
6	-5.069929	1.408558	-0.274379
6	-4.885419	4.186694	-0.146580
1	-2.938594	3.866838	0.706790
6	-6.120180	2.200103	-0.729948
1	-5.155255	0.329716	-0.323308
6	-6.037355	3.594055	-0.668004
1	-4.809911	5.268451	-0.084794
1	-7.009017	1.726833	-1.137425
1	-6.860391	4.208382	-1.019788
6	-2.801228	-0.086655	1.235382
8	-1.764988	-0.836182	1.463308
8	-4.029557	-0.611667	1.519653
6	-4.077383	-2.018137	1.833983
1	-5.105506	-2.170988	2.170216
1	-3.395253	-2.246095	2.656780
6	-3.767583	-2.871753	0.624068
6	-4.578621	-2.781953	-0.516938
6	-2.645087	-3.706527	0.592462

6	-4.263876	-3.505094	-1.672960
1	-5.457844	-2.143314	-0.498785
6	-2.330308	-4.436630	-0.556486
1	-2.002005	-3.763224	1.465203
6	-3.134195	-4.332987	-1.694519
1	-4.902753	-3.431946	-2.548028
1	-1.455178	-5.079197	-0.565453
1	-2.891309	-4.898054	-2.589070
6	0.826430	2.337065	0.916219
6	-0.341438	1.834361	1.542134
6	-0.309319	1.527348	2.909178
6	0.877534	1.711941	3.610960
6	2.037071	2.188087	2.965578
6	2.027372	2.512363	1.611099
6	-0.809706	2.256227	-0.642808
6	-1.375637	1.766129	0.532369
1	-1.200514	1.151993	3.401091
1	0.915087	1.487792	4.672930
1	2.950621	2.319257	3.537762
1	2.917622	2.892106	1.120826
7	0.521295	2.575752	-0.417268
6	1.415632	3.225790	-1.357286
1	1.370797	4.317742	-1.269239
1	2.438320	2.894576	-1.167473
1	1.154661	2.942505	-2.377775
6	-1.410817	2.385347	-2.003910
1	-0.914853	1.723667	-2.725845
1	-2.470390	2.131253	-1.974283
1	-1.336422	3.409491	-2.386425
8	-2.188578	-0.915461	-1.624763
1	-2.786705	-1.686522	-1.598398
1	-2.701101	-0.176770	-1.241945

TS(F_{H2O}-P)

Number of imaginary frequencies : 1 Electronic energy : HF=-2215.4609142
Zero-point correction= 0.722101 (Hartree/Particle)
Thermal correction to Energy= 0.765529
Thermal correction to Enthalpy= 0.766473
Thermal correction to Gibbs Free Energy= 0.645530
Sum of electronic and zero-point Energies= -2214.738362
Sum of electronic and thermal Energies= -2214.694935
Sum of electronic and thermal Enthalpies= -2214.693991
Sum of electronic and thermal Free Energies= -2214.814934

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Cartesian Coordinates

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46	0.408028	1.117133	-0.177143
7	-1.054983	0.969550	-1.605117
7	-1.217327	1.213727	1.039636
8	-4.125865	-0.750541	-1.007624
8	-4.691216	1.500274	0.228416
6	-0.814056	0.707725	-2.896590
1	0.181786	0.944108	-3.250965
6	-1.788362	0.108735	-3.693716
1	-1.588452	-0.067286	-4.744647
6	-2.969865	-0.340263	-3.108544
1	-3.685304	-0.912685	-3.688370
6	-3.187722	-0.116333	-1.743211

6	-2.251597	0.662961	-1.034773
6	-2.389114	1.057417	0.372088
6	-3.607469	1.336494	1.013338
6	-3.595733	1.549067	2.398834
1	-4.527134	1.730713	2.922849
6	-2.380415	1.577202	3.073678
1	-2.341502	1.742932	4.144074
6	-1.191581	1.448511	2.353768
1	-0.209998	1.518800	2.805763
6	-5.940386	-2.263473	-0.863395
1	-5.297334	-3.064255	-1.237484
1	-6.971827	-2.481908	-1.152495
1	-5.879737	-2.259490	0.229027
6	-5.506186	-0.920381	-1.434173
1	-5.550954	-0.955235	-2.528579
6	-6.342794	0.266593	-0.926502
1	-7.397916	-0.026955	-0.923118
1	-6.250130	1.117164	-1.610326
6	-5.931517	0.768669	0.461903
1	-5.714120	-0.066501	1.137994
6	-6.965725	1.705940	1.071238
1	-6.628499	2.100628	2.032861
1	-7.909683	1.177006	1.232658
1	-7.149885	2.551802	0.402620
6	2.628973	-1.006721	0.356833
6	3.832289	-1.885884	0.158251
6	3.854098	-3.193118	0.663686
6	4.938327	-1.430753	-0.574477
6	4.961087	-4.016952	0.457726
1	2.996342	-3.560276	1.219845
6	6.047380	-2.251113	-0.778359
1	4.921663	-0.427248	-0.990227
6	6.062904	-3.548576	-0.261349
1	4.963679	-5.025722	0.860583
1	6.894645	-1.882414	-1.349718
1	6.923187	-4.191024	-0.423292
6	2.733903	0.147728	1.198741
8	1.784152	0.996315	1.377897
8	3.931685	0.448442	1.702017
6	4.209310	1.864658	1.937297
1	5.206331	1.851620	2.379742
1	3.494688	2.266497	2.657809
6	4.175989	2.614718	0.629113
6	5.133818	2.329663	-0.354097
6	3.145578	3.516668	0.338434
6	5.054806	2.926105	-1.613576
1	5.932399	1.627453	-0.132448
6	3.068536	4.122762	-0.918450
1	2.390497	3.723123	1.090412
6	4.019265	3.822703	-1.899009
1	5.800191	2.697145	-2.368958
1	2.266971	4.823280	-1.132736
1	3.959016	4.290498	-2.876969
6	-0.874348	-2.314634	0.781776
6	0.304541	-1.771584	1.359490
6	0.313477	-1.468728	2.729963
6	-0.838654	-1.690884	3.477300
6	-2.008284	-2.201828	2.878162
6	-2.040342	-2.526743	1.524256
6	0.682518	-2.153425	-0.848580

6	1.275349	-1.641824	0.296765
1	1.208373	-1.070236	3.196895
1	-0.839176	-1.472273	4.541134
1	-2.893415	-2.362369	3.486347
1	-2.936322	-2.934502	1.067394
7	-0.621728	-2.539656	-0.562459
6	-1.535245	-3.226451	-1.455926
1	-1.532049	-4.308915	-1.282603
1	-2.548760	-2.846624	-1.302034
1	-1.254097	-3.035243	-2.491735
6	1.260325	-2.291001	-2.217435
1	0.706941	-1.695347	-2.953617
1	2.295072	-1.949039	-2.219435
1	1.252198	-3.333508	-2.555624
8	1.963103	0.777873	-1.474984
1	2.561102	1.544715	-1.486129
1	2.486817	-0.092683	-0.730972

F_{HCl}

Number of imaginary frequencies : 0 Electronic energy : HF=-2599.8356331
Zero-point correction= 0.708111 (Hartree/Particle)
Thermal correction to Energy= 0.753886
Thermal correction to Enthalpy= 0.754831
Thermal correction to Gibbs Free Energy= 0.627244
Sum of electronic and zero-point Energies= -2599.127522
Sum of electronic and thermal Energies= -2599.081747
Sum of electronic and thermal Enthalpies= -2599.080803
Sum of electronic and thermal Free Energies= -2599.208389

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Cartesian Coordinates

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46	-1.133024	0.467570	1.474885
7	0.078290	-1.296492	1.380561
7	1.004074	1.320263	1.095434
8	3.173097	-1.604385	-0.408061
8	3.967078	-0.542440	1.914990
6	-0.450487	-2.522717	1.239171
1	-1.464238	-2.649238	1.601363
6	0.261402	-3.564349	0.651679
1	-0.194730	-4.542224	0.548460
6	1.526713	-3.313014	0.127741
1	2.051883	-4.080580	-0.428281
6	2.070526	-2.034426	0.262617
6	1.346812	-1.056176	0.974733
6	1.882110	0.304867	1.202200
6	3.222664	0.532630	1.565729
6	3.674010	1.854864	1.650730
1	4.708512	2.056614	1.907627
6	2.763909	2.891586	1.460209
1	3.076276	3.927982	1.526208
6	1.421821	2.583351	1.226525
1	0.664706	3.352365	1.118670
6	5.091195	-1.913820	-1.751886
1	4.441766	-2.046836	-2.620792
1	6.010736	-2.482516	-1.913442
1	5.350501	-0.853299	-1.676484
6	4.387732	-2.395131	-0.489934
1	4.128980	-3.453826	-0.607816

6	5.217007	-2.218773	0.791922
1	6.230770	-2.587696	0.600848
1	4.799830	-2.833508	1.597058
6	5.269794	-0.778576	1.314143
1	5.405709	-0.066628	0.490795
6	6.345630	-0.578047	2.373403
1	6.318427	0.439695	2.771361
1	7.339017	-0.757260	1.951329
1	6.189925	-1.271313	3.205159
6	-1.985551	0.931310	-1.224610
6	-2.473681	-0.231118	-1.997820
6	-2.430741	-0.206500	-3.403759
6	-2.961632	-1.386789	-1.358869
6	-2.869058	-1.299300	-4.149959
1	-2.063333	0.683732	-3.904023
6	-3.397072	-2.479088	-2.102664
1	-2.982376	-1.423006	-0.275829
6	-3.354805	-2.441393	-3.504265
1	-2.839645	-1.259350	-5.234358
1	-3.765842	-3.365284	-1.594588
1	-3.705059	-3.289873	-4.084387
6	-2.772895	1.409572	-0.117482
8	-2.278491	2.108335	0.828879
8	-4.071994	1.040830	-0.101174
6	-4.735622	1.070618	1.197010
1	-5.786751	0.916781	0.950841
1	-4.604401	2.055792	1.648945
6	-4.202797	-0.027872	2.081960
6	-4.604918	-1.353541	1.878368
6	-3.236050	0.248427	3.070764
6	-4.074589	-2.384799	2.656105
1	-5.345079	-1.574379	1.114029
6	-2.709807	-0.789844	3.858105
1	-2.982630	1.282004	3.292277
6	-3.124515	-2.104924	3.645348
1	-4.414763	-3.404980	2.504117
1	-1.988723	-0.559683	4.635803
1	-2.724205	-2.906759	4.258271
6	0.923425	3.128795	-1.888355
6	-0.413933	2.998264	-1.445741
6	-1.084907	4.139332	-0.983190
6	-0.406529	5.354993	-0.951449
6	0.927949	5.456811	-1.384000
6	1.611248	4.342555	-1.865263
6	0.364424	0.952592	-2.132319
6	-0.780107	1.601216	-1.611208
1	-2.106836	4.075622	-0.632595
1	-0.916741	6.240884	-0.586851
1	1.432210	6.417261	-1.348008
1	2.639191	4.425873	-2.201376
7	1.363833	1.866551	-2.297953
6	2.732747	1.545770	-2.675120
1	3.273660	1.102807	-1.831214
1	2.740158	0.843826	-3.510739
1	3.241595	2.455464	-2.991633
6	0.610606	-0.497071	-2.386949
1	0.437132	-0.763790	-3.435255
1	1.634525	-0.777425	-2.133598
1	-0.061863	-1.109628	-1.788760
1	-1.253346	-3.305203	-3.083442

17	-0.101700	-3.899606	-3.037030

TS(F_{HCl}-P)

Number of imaginary frequencies : 1 Electronic energy : HF=-2599.8000078
Zero-point correction= 0.708076 (Hartree/Particle)
Thermal correction to Energy= 0.752325
Thermal correction to Enthalpy= 0.753269
Thermal correction to Gibbs Free Energy= 0.630664
Sum of electronic and zero-point Energies= -2599.113968
Sum of electronic and thermal Energies= -2599.069719
Sum of electronic and thermal Enthalpies= -2599.068775
Sum of electronic and thermal Free Energies= -2599.191380

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Cartesian Coordinates

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46	-0.479724	-1.131651	-0.209347
7	1.094400	-1.078757	-1.699725
7	1.189430	-1.114136	1.018059
8	4.041762	0.835763	-0.983050
8	4.653192	-1.482595	0.182856
6	0.923518	-0.849959	-3.011221
1	0.000402	-1.210142	-3.448309
6	1.878929	-0.173506	-3.766310
1	1.723776	-0.030951	-4.830075
6	2.992950	0.369438	-3.128730
1	3.695690	0.985399	-3.678684
6	3.158221	0.159243	-1.756162
6	2.231172	-0.663755	-1.085118
6	2.353622	-1.019567	0.336980
6	3.570543	-1.314697	0.972341
6	3.566223	-1.526876	2.357112
1	4.497376	-1.733673	2.872697
6	2.356100	-1.514763	3.042398
1	2.320924	-1.673394	4.114211
6	1.167233	-1.340846	2.332167
1	0.186781	-1.357326	2.793687
6	5.836272	2.344195	-0.680123
1	5.197859	3.167122	-1.012090
1	6.873353	2.591042	-0.922096
1	5.744417	2.258683	0.406674
6	5.429304	1.045214	-1.362910
1	5.498338	1.169860	-2.449812
6	6.272498	-0.167896	-0.937934
1	7.327449	0.126966	-0.938878
1	6.166675	-0.977010	-1.668719
6	5.889165	-0.750299	0.426950
1	5.679655	0.044757	1.152331
6	6.940306	-1.710279	0.968059
1	6.617054	-2.160497	1.910040
1	7.882861	-1.184010	1.145835
1	7.120722	-2.516443	0.251045
6	-2.633688	1.308925	0.711958
6	-3.806122	2.115921	0.324690
6	-3.699673	3.525120	0.331155
6	-5.028036	1.552515	-0.111105
6	-4.760375	4.330409	-0.072513
1	-2.776078	3.979912	0.673192
6	-6.080954	2.362209	-0.523893

1	-5.146411	0.476143	-0.125187
6	-5.957079	3.754875	-0.506297
1	-4.654900	5.410864	-0.042876
1	-7.005564	1.903983	-0.862399
1	-6.784460	4.382271	-0.822968
6	-2.709967	0.016909	1.282014
8	-1.676343	-0.726780	1.476690
8	-3.930440	-0.480355	1.596327
6	-3.993321	-1.875308	1.995200
1	-4.999363	-1.969680	2.408605
1	-3.261604	-2.063722	2.784268
6	-3.791086	-2.805385	0.823284
6	-4.771568	-2.894701	-0.172292
6	-2.616360	-3.555812	0.690489
6	-4.577514	-3.709650	-1.287800
1	-5.690511	-2.322449	-0.070629
6	-2.418951	-4.373867	-0.423943
1	-1.854937	-3.491624	1.461919
6	-3.398112	-4.447637	-1.417762
1	-5.346576	-3.774135	-2.051690
1	-1.506288	-4.956175	-0.512283
1	-3.249380	-5.087580	-2.282510
6	0.944080	2.359400	0.861952
6	-0.219125	1.880005	1.511432
6	-0.164332	1.575010	2.877991
6	1.041413	1.733437	3.553462
6	2.196951	2.180853	2.882241
6	2.164122	2.506274	1.528321
6	-0.732613	2.350847	-0.656376
6	-1.281917	1.853818	0.528109
1	-1.051869	1.221126	3.391635
1	1.096708	1.509115	4.614490
1	3.125908	2.290518	3.433611
1	3.051012	2.866779	1.018821
7	0.609860	2.622771	-0.461351
6	1.509321	3.221448	-1.431159
1	2.525028	2.873441	-1.236763
1	1.234252	2.908894	-2.439492
1	1.488348	4.316225	-1.379373
6	-1.359126	2.535725	-1.999670
1	-1.223729	3.558390	-2.368696
1	-0.926099	1.853235	-2.742085
1	-2.431769	2.352528	-1.949800
1	-2.849266	0.150560	-1.119604
17	-2.454225	-0.843080	-1.886557

HCl

Number of imaginary frequencies : 0 Electronic energy : HF=-460.7758002
Zero-point correction= 0.006760 (Hartree/Particle)
Thermal correction to Energy= 0.009120
Thermal correction to Enthalpy= 0.010064
Thermal correction to Gibbs Free Energy= -0.011134
Sum of electronic and zero-point Energies= -460.769041
Sum of electronic and thermal Energies= -460.766680
Sum of electronic and thermal Enthalpies= -460.765736
Sum of electronic and thermal Free Energies= -460.786934

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Cartesian Coordinates

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17	0.000000	0.000000	0.071667
1	0.000000	0.000000	-1.218333

E_{enol}

Number of imaginary frequencies : 0 Electronic energy : HF=-2599.8574666
Zero-point correction= 0.713867 (Hartree/Particle)
Thermal correction to Energy= 0.758314
Thermal correction to Enthalpy= 0.759259
Thermal correction to Gibbs Free Energy= 0.635846
Sum of electronic and zero-point Energies= -2599.143600
Sum of electronic and thermal Energies= -2599.099152
Sum of electronic and thermal Enthalpies= -2599.098208
Sum of electronic and thermal Free Energies= -2599.221620

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Cartesian Coordinates

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46	-0.242157	-1.840358	0.565742
7	-2.188194	-2.051082	-0.228365
7	-1.189313	-0.151763	1.436662
8	-5.175028	-0.291327	0.682172
8	-3.762035	1.710275	-0.201900
6	-2.665822	-3.119759	-0.878297
1	-1.942291	-3.887367	-1.126321
6	-4.022533	-3.224456	-1.184319
1	-4.383304	-4.092920	-1.724008
6	-4.905279	-2.254722	-0.723016
1	-5.973975	-2.374339	-0.861349
6	-4.404981	-1.156523	-0.012261
6	-3.004682	-1.028384	0.128031
6	-2.358908	0.111370	0.796593
6	-2.869612	1.421860	0.770789
6	-2.335379	2.373613	1.643182
1	-2.739662	3.378675	1.664055
6	-1.241532	2.024384	2.426008
1	-0.786944	2.737604	3.102637
6	-0.656616	0.773882	2.246446
1	0.259410	0.509673	2.758714
6	-7.315159	0.457896	1.370523
1	-7.472891	-0.496006	1.878990
1	-8.285207	0.853433	1.057363
1	-6.871051	1.154810	2.087401
6	-6.409861	0.269358	0.161076
1	-6.874117	-0.439549	-0.533449
6	-6.094908	1.576895	-0.586935
1	-7.017486	2.160216	-0.678042
1	-5.753182	1.358895	-1.604972
6	-5.003640	2.420423	0.078416
1	-5.140096	2.455648	1.165213
6	-4.906633	3.825661	-0.499885
1	-4.068530	4.374290	-0.061882
1	-5.825257	4.385786	-0.302753
1	-4.755349	3.780124	-1.582772
6	2.731068	-0.480259	-0.961764
6	2.727907	-1.417994	0.148423
6	3.577240	-2.532652	0.261334
6	1.793654	-1.187487	1.226184
6	3.509587	-3.368498	1.371457

1	4.271527	-2.758741	-0.535873
6	1.793222	-2.031032	2.379584
1	1.464659	-0.160006	1.324975
6	2.619453	-3.138353	2.434956
1	4.163140	-4.235415	1.409949
1	1.148372	-1.782261	3.218258
1	2.592670	-3.811403	3.284582
6	3.855765	-0.188011	-1.693180
8	3.891510	0.779680	-2.621767
8	5.030745	-0.793478	-1.514516
6	6.173749	0.106996	-1.314504
1	6.386065	0.634320	-2.246969
1	6.992375	-0.579921	-1.093307
6	5.896618	1.058147	-0.178281
6	5.835257	2.437841	-0.397024
6	5.623333	0.552728	1.101158
6	5.532558	3.307626	0.653693
1	6.020759	2.831548	-1.392376
6	5.309591	1.417968	2.147901
1	5.642029	-0.520836	1.266993
6	5.269735	2.799124	1.926812
1	5.496127	4.377991	0.475358
1	5.105122	1.018270	3.136887
1	5.035715	3.474290	2.744753
6	-0.027700	2.040573	-1.223136
6	1.221795	1.634934	-0.681351
6	1.897192	2.480164	0.214180
6	1.327648	3.712025	0.523318
6	0.103261	4.113533	-0.049000
6	-0.592571	3.285351	-0.928017
6	0.469908	0.010867	-2.087136
6	1.525515	0.341984	-1.247071
1	2.855508	2.184344	0.630475
1	1.845989	4.385076	1.199821
1	-0.303079	5.090937	0.194085
1	-1.535211	3.596468	-1.366727
1	3.016883	1.207237	-2.636986
7	-0.476613	1.025303	-2.053443
6	-1.683211	1.105882	-2.860790
1	-2.509277	1.473960	-2.248293
1	-1.544188	1.773236	-3.719024
1	-1.944206	0.113475	-3.227984
6	0.310087	-1.199010	-2.946219
1	-0.619043	-1.733229	-2.724372
1	0.308485	-0.939950	-4.011592
1	1.128184	-1.892461	-2.750420
17	0.542187	-3.761853	-0.492843

$TS(D'-E_{enol})$

Number of imaginary frequencies : 1 Electronic energy : HF=-2599.8369175
Zero-point correction= 0.708731 (Hartree/Particle)
Thermal correction to Energy= 0.753038
Thermal correction to Enthalpy= 0.753982
Thermal correction to Gibbs Free Energy= 0.629089
Sum of electronic and zero-point Energies= -2599.128186
Sum of electronic and thermal Energies= -2599.083880
Sum of electronic and thermal Enthalpies= -2599.082936
Sum of electronic and thermal Free Energies= -2599.207829

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Cartesian Coordinates

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46	-0.341929	0.153888	-0.838901
7	1.690158	0.445993	-1.554814
7	0.722007	-1.405085	0.208439
8	4.519720	-0.135793	0.570633
8	4.064545	-2.541086	-0.464790
6	2.090504	1.484750	-2.299528
1	1.335703	1.928283	-2.938321
6	3.397392	1.966202	-2.223658
1	3.701551	2.794365	-2.854480
6	4.277470	1.420768	-1.292478
1	5.265927	1.844907	-1.156183
6	3.849428	0.349073	-0.500594
6	2.563134	-0.177436	-0.732721
6	2.047775	-1.387870	-0.072018
6	2.847743	-2.531140	0.122415
6	2.296386	-3.632997	0.782655
1	2.902000	-4.513591	0.965578
6	0.947785	-3.602251	1.122281
1	0.474248	-4.450390	1.604103
6	0.182394	-2.491321	0.774927
1	-0.883017	-2.464291	0.947910
6	6.387329	-0.270800	2.012444
1	6.117847	0.703852	2.425967
1	7.470261	-0.399130	2.092006
1	5.900501	-1.041905	2.616676
6	5.952418	-0.363968	0.556091
1	6.447755	0.428424	-0.017242
6	6.256593	-1.723076	-0.095742
1	7.278599	-2.014602	0.170135
1	6.223298	-1.635827	-1.187377
6	5.275140	-2.835114	0.289627
1	5.033214	-2.796838	1.358301
6	5.781834	-4.218457	-0.098276
1	5.043415	-4.990670	0.132425
1	6.703201	-4.453544	0.442965
1	5.988811	-4.256753	-1.171764
17	-1.247194	1.459989	-2.575321
6	-2.134678	0.265086	0.374343
6	-1.600908	0.087295	1.776524
6	-0.636521	0.968513	2.314506
6	-1.998471	-0.999726	2.575846
6	-0.109148	0.765084	3.585885
1	-0.294229	1.812482	1.730181
6	-1.466444	-1.203284	3.850760
1	-2.724287	-1.713001	2.199321
6	-0.517681	-0.322070	4.364287
1	0.629758	1.461950	3.970272
1	-1.797662	-2.054753	4.438178
1	-0.102301	-0.476513	5.355276
6	-2.627679	1.641195	0.016926
8	-3.678960	1.721005	-0.668913
8	-1.970890	2.683857	0.436182
6	-2.216074	3.996133	-0.194661
1	-3.069839	4.455326	0.308832
1	-2.462073	3.803853	-1.240750
6	-0.946418	4.778333	-0.026544
6	-0.899599	5.921381	0.775841

6	0.220901	4.330109	-0.663023
6	0.300397	6.618719	0.937153
1	-1.800376	6.269442	1.274910
6	1.419738	5.016847	-0.488527
1	0.172624	3.445608	-1.289895
6	1.461271	6.164554	0.309939
1	0.328350	7.510252	1.556178
1	2.320949	4.660593	-0.979883
1	2.394620	6.704421	0.439991
6	-4.323964	-2.645616	-0.618956
6	-3.190253	-1.860075	-0.904862
6	-2.296562	-2.307238	-1.885254
6	-2.551272	-3.519011	-2.523016
6	-3.689171	-4.285304	-2.214995
6	-4.604039	-3.853281	-1.258269
6	-4.460274	-0.846726	0.733705
6	-3.282947	-0.649757	-0.071119
1	-1.434113	-1.707928	-2.157835
1	-1.864305	-3.871837	-3.285793
1	-3.864008	-5.220773	-2.736519
1	-5.492427	-4.431297	-1.027260
1	-3.828043	0.425229	-0.718175
7	-5.075127	-1.987340	0.370419
6	-6.374540	-2.475246	0.821139
1	-7.067410	-2.515836	-0.023861
1	-6.263195	-3.478953	1.239422
1	-6.781597	-1.814582	1.583898
6	-5.027326	0.087789	1.750465
1	-5.923831	0.587404	1.366000
1	-5.296760	-0.442037	2.668483
1	-4.296700	0.850744	2.013914

$TS(E_{enol}\text{-}P)_{2wat}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2752.7365402
Zero-point correction= 0.760893 (Hartree/Particle)
Thermal correction to Energy= 0.808696
Thermal correction to Enthalpy= 0.809640
Thermal correction to Gibbs Free Energy= 0.680587
Sum of electronic and zero-point Energies= -2751.974398
Sum of electronic and thermal Energies= -2751.926595
Sum of electronic and thermal Enthalpies= -2751.925651
Sum of electronic and thermal Free Energies= -2752.054704

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Cartesian Coordinates

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46	0.581900	-1.893148	0.351025
7	2.287936	-1.839732	-0.926030
7	1.808823	-0.531546	1.416587
8	4.411620	1.026036	-1.258285
8	5.323909	-0.003186	0.970688
6	2.374782	-2.410187	-2.134809
1	1.678728	-3.217883	-2.327795
6	3.291895	-1.953050	-3.080966
1	3.360408	-2.448045	-4.043263
6	4.050359	-0.817959	-2.807543
1	4.688407	-0.386087	-3.570512
6	3.932357	-0.207715	-1.554636
6	3.110431	-0.818589	-0.585179

6	3.005628	-0.347542	0.803110
6	4.103056	0.179583	1.512028
6	3.882641	0.745548	2.771376
1	4.704332	1.196655	3.316126
6	2.612186	0.658785	3.327280
1	2.398910	1.075404	4.304817
6	1.615982	-0.037032	2.646042
1	0.645177	-0.194107	3.094764
6	5.629688	2.988002	-1.755583
1	4.874703	3.262220	-2.496783
1	6.588182	3.415704	-2.061253
1	5.342752	3.430008	-0.796727
6	5.738965	1.473055	-1.644264
1	5.997500	1.057100	-2.624734
6	6.769859	1.000981	-0.605870
1	7.684207	1.591236	-0.729721
1	7.037440	-0.045619	-0.787618
6	6.278097	1.088694	0.842253
1	5.749116	2.031876	1.024040
6	7.399527	0.895734	1.854366
1	7.014088	0.896925	2.877157
1	8.137098	1.698777	1.764792
1	7.902468	-0.060407	1.683086
6	-2.558079	-0.244853	-0.108662
6	-2.373444	-1.449153	0.712251
6	-1.219097	-1.486366	1.593787
6	-3.232862	-2.565737	0.767955
6	-1.013799	-2.581616	2.493145
1	-0.828688	-0.519528	1.882961
6	-2.959260	-3.643675	1.599680
1	-4.098451	-2.605283	0.125858
6	-1.849813	-3.676472	2.465458
1	-0.195233	-2.528301	3.205837
1	-3.632263	-4.496423	1.575761
1	-1.675029	-4.533366	3.106366
6	-3.563135	-0.103616	-1.171109
8	-3.596143	0.859469	-1.949713
8	-4.575873	-1.001017	-1.161771
6	-5.815547	-0.554826	-1.786048
1	-6.426748	-1.458067	-1.824550
1	-5.614530	-0.201185	-2.797951
6	-6.438132	0.516469	-0.923963
6	-6.921263	0.181910	0.351485
6	-6.436810	1.857554	-1.321803
6	-7.399106	1.175599	1.211595
1	-6.915309	-0.857094	0.670658
6	-6.916922	2.852213	-0.465826
1	-6.030948	2.122527	-2.292404
6	-7.396129	2.515128	0.801274
1	-7.777787	0.906747	2.193166
1	-6.900495	3.889828	-0.783376
1	-7.764600	3.287734	1.468942
6	0.445414	2.043488	-0.204617
6	-0.705749	1.565087	0.487535
6	-0.973795	2.067982	1.777188
6	-0.110941	3.008590	2.333071
6	1.025110	3.458634	1.631998
6	1.314921	2.984702	0.354825
6	-0.571090	0.517900	-1.522196
6	-1.338559	0.590417	-0.368777

1	-1.847435	1.734489	2.328053
1	-0.318454	3.405579	3.322269
1	1.679607	4.194196	2.089349
1	2.190003	3.334585	-0.183424
1	-3.432515	0.633508	0.785710
7	0.505777	1.392089	-1.424046
6	1.394460	1.768638	-2.509863
1	2.351573	2.092716	-2.100797
1	1.582925	0.908323	-3.152514
1	0.967268	2.575588	-3.116515
6	-0.794331	-0.325234	-2.733098
1	-1.322724	0.231834	-3.515030
1	0.147208	-0.699852	-3.144187
1	-1.391915	-1.198617	-2.467532
8	-4.058088	1.471437	1.293770
8	-3.379358	3.107806	-0.471489
1	-3.354941	2.430409	-1.192498
1	-3.870507	2.265327	0.630750
1	-2.449643	3.294763	-0.270676
1	-5.007253	1.239827	1.249810
17	-0.481489	-3.527395	-0.925651

TS_{SEAr}

Number of imaginary frequencies : 1 Electronic energy : HF=-1870.4020185
Zero-point correction= 0.473683 (Hartree/Particle)
Thermal correction to Energy= 0.504285
Thermal correction to Enthalpy= 0.505229
Thermal correction to Gibbs Free Energy= 0.410956
Sum of electronic and zero-point Energies= -1870.010182
Sum of electronic and thermal Energies= -1869.979579
Sum of electronic and thermal Enthalpies= -1869.978635
Sum of electronic and thermal Free Energies= -1870.072908

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Cartesian Coordinates

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46	0.932786	-0.940203	-0.113296
7	-0.192610	0.788749	0.123116
7	-1.092972	-1.743603	-0.472597
8	-3.539062	1.384989	-1.009476
8	-3.999248	-0.241744	0.993177
6	0.310466	2.031301	0.204990
1	1.372336	2.106392	0.396483
6	-0.501643	3.148698	0.028353
1	-0.070988	4.139865	0.115284
6	-1.833568	2.980351	-0.333079
1	-2.451278	3.839208	-0.569472
6	-2.347987	1.683823	-0.452427
6	-1.517054	0.593228	-0.111286
6	-1.994836	-0.802748	-0.107445
6	-3.285723	-1.168100	0.323641
6	-3.698168	-2.493384	0.141113
1	-4.700578	-2.791236	0.428582
6	-2.787970	-3.423350	-0.352285
1	-3.071773	-4.460335	-0.493179
6	-1.474954	-3.020313	-0.598152
1	-0.708607	-3.727594	-0.896401
6	-5.597675	2.002168	-2.002173
1	-5.051935	2.382025	-2.868930

1	-6.526050	2.569763	-1.895774
1	-5.850607	0.955184	-2.192652
6	-4.753568	2.139633	-0.742904
1	-4.505157	3.195590	-0.587716
6	-5.429173	1.587619	0.523523
1	-6.468629	1.932360	0.541552
1	-4.942679	1.990150	1.418852
6	-5.381781	0.060626	0.639164
1	-5.601265	-0.414725	-0.324034
6	-6.301955	-0.475505	1.727192
1	-6.201653	-1.559035	1.830971
1	-7.345466	-0.248673	1.489659
1	-6.056315	-0.018138	2.690007
6	4.727076	0.908967	0.198642
6	3.685336	0.314732	-0.569023
6	3.831628	0.220309	-1.965543
6	4.995550	0.699866	-2.552135
6	6.021273	1.274190	-1.772243
6	5.903270	1.386018	-0.391054
6	3.096054	0.290266	1.639171
6	2.663994	-0.074449	0.375185
1	3.044864	-0.223244	-2.569865
1	5.122456	0.631603	-3.628041
1	6.921606	1.634779	-2.259562
1	6.697780	1.823807	0.204799
1	3.345140	-2.105261	-0.173891
7	4.343309	0.896992	1.528401
6	5.193936	1.354521	2.614780
1	5.558769	2.363871	2.402832
1	4.628269	1.383160	3.545452
1	6.055315	0.690425	2.746814
6	2.411519	0.130653	2.959210
1	2.996063	-0.482358	3.655037
1	2.230614	1.096919	3.445914
1	1.445422	-0.356852	2.814407
17	2.383781	-2.937293	-0.513463

Int_{SEAr}

Number of imaginary frequencies : 0 Electronic energy : HF=-1870.5463638
Zero-point correction= 0.479859 (Hartree/Particle)
Thermal correction to Energy= 0.509806
Thermal correction to Enthalpy= 0.510750
Thermal correction to Gibbs Free Energy= 0.418718
Sum of electronic and zero-point Energies= -1870.066505
Sum of electronic and thermal Energies= -1870.036558
Sum of electronic and thermal Enthalpies= -1870.035613
Sum of electronic and thermal Free Energies= -1870.127646

Cartesian Coordinates

46	-1.134050	1.135582	-0.515770
7	-0.119516	-0.720501	-0.069496
7	0.910670	1.761454	-0.574535
8	3.316025	-1.416965	-0.838762
8	3.618388	0.211876	1.185754
6	-0.639873	-1.956185	-0.025386
1	-1.710742	-2.031564	0.049865
6	0.155299	-3.097224	-0.095343

1	-0.312190	-4.073638	-0.037940
6	1.520277	-2.968790	-0.319606
1	2.139052	-3.844031	-0.480812
6	2.068925	-1.684775	-0.399404
6	1.229720	-0.573035	-0.154557
6	1.744975	0.801401	-0.110994
6	2.999793	1.142017	0.430411
6	3.471778	2.446847	0.250369
1	4.452086	2.723791	0.622656
6	2.643631	3.382992	-0.359378
1	2.972583	4.405129	-0.509619
6	1.342059	3.022353	-0.710863
1	0.620999	3.736099	-1.089499
6	5.446026	-2.087273	-1.624029
1	4.978052	-2.457852	-2.538948
1	6.345488	-2.676587	-1.426301
1	5.741701	-1.047657	-1.791706
6	4.479669	-2.198504	-0.452902
1	4.192878	-3.247889	-0.320635
6	5.041118	-1.656608	0.871965
1	6.064453	-2.027637	0.994191
1	4.458139	-2.041131	1.716212
6	5.020442	-0.128358	0.975226
1	5.350187	0.333803	0.037484
6	5.837811	0.393765	2.148835
1	6.894393	0.140861	2.020606
1	5.484146	-0.050384	3.083893
1	5.753020	1.480097	2.235885
6	-3.873127	-1.308005	0.683629
6	-3.623666	-0.749427	-0.584526
6	-3.686038	-1.565036	-1.716619
6	-3.984611	-2.917843	-1.544621
6	-4.216241	-3.456520	-0.267254
6	-4.165771	-2.655947	0.876993
6	-3.474598	0.890833	1.034561
6	-3.293714	0.660723	-0.377612
1	-3.494121	-1.155265	-2.703023
1	-4.041176	-3.567674	-2.411911
1	-4.447983	-4.511849	-0.166375
1	-4.349625	-3.070632	1.862245
7	-3.755956	-0.276950	1.641000
6	-3.921621	-0.515279	3.070126
1	-4.918929	-0.920288	3.261193
1	-3.172034	-1.234445	3.412751
1	-3.802103	0.414808	3.621837
6	-3.449804	2.192151	1.764356
1	-4.404081	2.357292	2.277004
1	-2.653806	2.215358	2.516307
1	-3.271377	3.002737	1.058936
1	-3.610386	1.425349	-1.079824
17	-1.873457	3.252559	-1.201413

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me-B

Number of imaginary frequencies : 0 Electronic energy : HF=-1939.0829323
Zero-point correction= 0.580552 (Hartree/Particle)
Thermal correction to Energy= 0.619381
Thermal correction to Enthalpy= 0.620325
Thermal correction to Gibbs Free Energy= 0.505985

Sum of electronic and zero-point Energies= -1938.502381
Sum of electronic and thermal Energies= -1938.463551
Sum of electronic and thermal Enthalpies= -1938.462607
Sum of electronic and thermal Free Energies= -1938.576947

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Cartesian Coordinates

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46	0.746572	0.282827	0.799216
7	-1.169866	1.109165	0.975285
7	-0.393135	-1.342383	0.145126
8	-4.110620	-0.081327	-0.676031
8	-3.790573	-2.013612	0.999792
6	-1.497195	2.387658	1.215358
1	-0.710745	3.066642	1.503486
6	-2.797877	2.857655	1.036674
1	-3.021063	3.890317	1.279598
6	-3.757098	2.035012	0.464967
1	-4.741265	2.420077	0.224071
6	-3.399103	0.723737	0.126312
6	-2.127902	0.246872	0.524781
6	-1.718398	-1.142357	0.349691
6	-2.600574	-2.242932	0.438581
6	-2.135455	-3.501146	0.034225
1	-2.805445	-4.353819	0.038966
6	-0.794128	-3.646766	-0.304808
1	-0.397238	-4.610277	-0.604283
6	0.069381	-2.559244	-0.180116
1	1.133765	-2.657024	-0.336311
6	-5.988028	-0.533375	-2.055402
1	-5.656891	0.246806	-2.744902
1	-7.076709	-0.609332	-2.116221
1	-5.556815	-1.484491	-2.380753
6	-5.570897	-0.198716	-0.631626
1	-6.002893	0.764417	-0.340766
6	-5.956423	-1.264410	0.407132
1	-6.991567	-1.568882	0.220801
1	-5.927058	-0.839770	1.416477
6	-5.047376	-2.496004	0.410452
1	-4.832116	-2.834727	-0.609411
6	-5.588471	-3.633510	1.261982
1	-4.886349	-4.470470	1.299513
1	-6.532008	-3.998525	0.846629
1	-5.767964	-3.292071	2.285217
6	1.898916	1.947980	1.721371
6	1.799216	3.000719	0.615116
8	1.020938	3.921096	0.701482
8	2.577048	2.694075	-0.419665
6	2.145487	3.242414	-1.731990
1	1.984271	4.315564	-1.624821
1	3.006634	3.055058	-2.372711
6	0.910299	2.497738	-2.158675
6	1.011927	1.162151	-2.577556
6	-0.354701	3.087677	-2.048448
6	-0.134556	0.422610	-2.867341
1	1.993458	0.706107	-2.679305
6	-1.501549	2.350091	-2.350260
1	-0.438401	4.119170	-1.721014
6	-1.395411	1.015936	-2.748360
1	-0.046491	-0.607217	-3.199805
1	-2.477356	2.818528	-2.273744

1	-2.290868	0.443349	-2.970163
7	2.496445	-0.690002	0.393887
6	3.481426	-1.234903	0.100369
6	4.686527	-1.894308	-0.250561
6	5.265659	-1.651730	-1.514702
6	5.289189	-2.775749	0.672661
6	6.450612	-2.297473	-1.845945
1	4.790128	-0.970537	-2.212607
6	6.474268	-3.410187	0.319784
1	4.831976	-2.951489	1.640858
6	7.051880	-3.172104	-0.932925
1	6.908127	-2.120986	-2.813483
1	6.949851	-4.089621	1.018906
1	7.977914	-3.671554	-1.199655
7	3.232796	1.536222	1.812844
7	4.295479	1.213537	1.910060
6	1.422819	2.344446	3.125291
1	1.609537	1.536103	3.835023
1	1.918993	3.258452	3.464596
1	0.351103	2.525808	3.100623

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me-C

Number of imaginary frequencies : 0 Electronic energy : HF=-1829.5605496
Zero-point correction= 0.568639 (Hartree/Particle)
Thermal correction to Energy= 0.606095
Thermal correction to Enthalpy= 0.607039
Thermal correction to Gibbs Free Energy= 0.494850
Sum of electronic and zero-point Energies= -1828.991911
Sum of electronic and thermal Energies= -1828.954455
Sum of electronic and thermal Enthalpies= -1828.953511
Sum of electronic and thermal Free Energies= -1829.065700

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Cartesian Coordinates

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46	0.788952	-0.043562	-0.997619
7	-0.452035	1.473258	-0.202731
7	-1.054625	-0.959172	-1.215554
8	-3.967167	1.846002	-0.720957
8	-3.974516	-0.293593	0.722991
6	-0.073140	2.706605	0.152151
1	0.991523	2.888937	0.224385
6	-1.018023	3.703173	0.400839
1	-0.689698	4.689610	0.708643
6	-2.364522	3.442144	0.175805
1	-3.097957	4.234614	0.272078
6	-2.756478	2.161110	-0.245054
6	-1.765862	1.153604	-0.311315
6	-2.048519	-0.252917	-0.606439
6	-3.238852	-0.905210	-0.213222
6	-3.500693	-2.184977	-0.715651
1	-4.435782	-2.680060	-0.478249
6	-2.516258	-2.831885	-1.456605
1	-2.675354	-3.831607	-1.844657
6	-1.279641	-2.218402	-1.631560
1	-0.457100	-2.744606	-2.095208
6	-6.189877	2.441500	-1.314903
1	-5.793303	3.119171	-2.074184
1	-7.150082	2.831980	-0.967861

1	-6.361306	1.467458	-1.782177
6	-5.224787	2.328436	-0.145302
1	-5.065351	3.317030	0.297465
6	-5.672170	1.345045	0.949182
1	-6.736345	1.509153	1.147667
1	-5.139937	1.547620	1.885169
6	-5.432373	-0.127067	0.605263
1	-5.710667	-0.344718	-0.431722
6	-6.118291	-1.081056	1.570519
1	-7.203914	-0.968285	1.502807
1	-5.812492	-0.869209	2.599133
1	-5.871341	-2.122187	1.347025
6	1.840028	-1.502797	-1.782922
6	2.315918	-2.415921	-0.722373
8	3.401723	-2.104273	-0.263054
8	1.458325	-3.323520	-0.323561
6	1.475314	-3.662194	1.146364
1	2.511886	-3.822151	1.442583
1	0.919847	-4.597330	1.187265
6	0.806164	-2.522102	1.853004
6	1.566569	-1.442572	2.328374
6	-0.592809	-2.466899	1.929625
6	0.933089	-0.320963	2.866032
1	2.650194	-1.485048	2.276192
6	-1.224993	-1.346734	2.469626
1	-1.184424	-3.302923	1.566305
6	-0.461659	-0.270294	2.931306
1	1.526912	0.503421	3.248682
1	-2.307668	-1.308088	2.530106
1	-0.953453	0.598184	3.358848
7	2.564118	0.892739	-0.585784
6	3.657181	1.163912	-0.297962
6	4.995601	1.445701	0.070322
6	5.486764	2.766862	0.031417
6	5.813543	0.366914	0.472077
6	6.805459	3.001331	0.402023
1	4.844734	3.582003	-0.285259
6	7.128955	0.627265	0.837596
1	5.412149	-0.640900	0.485405
6	7.621623	1.937101	0.803694
1	7.200341	4.011279	0.377275
1	7.772869	-0.188693	1.148027
1	8.650428	2.130392	1.090720
6	2.304521	-1.612539	-3.161336
1	1.819459	-0.925646	-3.854942
1	3.379269	-1.347410	-3.104662
1	2.294962	-2.649887	-3.524719

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me-C1

Number of imaginary frequencies : 0 Electronic energy : HF=-1947.5535025
Zero-point correction= 0.656268 (Hartree/Particle)
Thermal correction to Energy= 0.696371
Thermal correction to Enthalpy= 0.697315
Thermal correction to Gibbs Free Energy= 0.582982
Sum of electronic and zero-point Energies= -1946.897235
Sum of electronic and thermal Energies= -1946.857132
Sum of electronic and thermal Enthalpies= -1946.856187
Sum of electronic and thermal Free Energies= -1946.970520

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Cartesian Coordinates

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46	-1.055859	-0.634347	-0.372613
7	0.519847	-1.889498	0.491046
7	0.707967	0.215238	-1.287262
8	3.882861	-2.148186	-0.707093
8	3.915838	0.252403	0.284262
6	0.410733	-3.015901	1.215553
1	-0.568995	-3.267369	1.601125
6	1.501231	-3.841363	1.480129
1	1.369694	-4.723885	2.096089
6	2.726820	-3.557660	0.887448
1	3.571487	-4.228469	0.998888
6	2.837644	-2.416886	0.084357
6	1.737032	-1.531055	0.009040
6	1.832750	-0.234475	-0.674498
6	3.001961	0.558892	-0.651971
6	3.063002	1.678029	-1.491796
1	3.954406	2.292141	-1.526255
6	1.940885	2.027752	-2.230909
1	1.952260	2.893675	-2.882419
6	0.760286	1.309384	-2.062185
1	-0.157110	1.627248	-2.535231
6	5.967010	-3.399276	-0.807602
1	7.004834	-3.438965	-0.464914
1	5.963049	-3.348586	-1.900011
1	5.473174	-4.327211	-0.507797
6	5.265619	-2.185232	-0.218445
1	5.235771	-2.241959	0.875775
6	5.869892	-0.859294	-0.688670
1	5.649207	-0.766083	-1.757756
1	6.960097	-0.894388	-0.591985
6	5.356500	0.375156	0.069664
1	5.559654	1.273905	-0.522779
6	5.950083	0.546462	1.459751
1	5.521049	1.422991	1.951476
1	7.032278	0.682700	1.390419
1	5.750108	-0.327011	2.086725
6	-2.304549	0.618613	-1.140548
6	-2.389951	1.885370	-0.352944
8	-3.040854	1.932646	0.673668
8	-1.644907	2.830634	-0.897815
6	-1.277133	4.010082	-0.064731
1	-2.003350	4.076176	0.746746
1	-1.393474	4.862013	-0.733932
6	0.135075	3.837898	0.418808
6	1.131219	4.743874	0.042116
6	0.463101	2.764877	1.263132
6	2.437565	4.591762	0.515542
1	0.885936	5.579127	-0.608228
6	1.769201	2.600716	1.717744
1	-0.310267	2.066289	1.573874
6	2.757910	3.519441	1.348210
1	3.199076	5.312794	0.235195
1	2.020389	1.766836	2.365939
1	3.771412	3.402559	1.719768
6	-4.819056	-0.861398	0.458357
6	-3.915988	-1.712912	-0.202610
6	-4.289697	-2.319957	-1.400768

6	-5.543228	-2.008839	-1.934246
6	-6.407852	-1.108074	-1.287167
6	-6.062746	-0.522084	-0.065125
6	-2.997168	-0.949408	1.789622
6	-2.672563	-1.720971	0.594668
1	-3.619648	-3.003086	-1.913620
1	-5.857758	-2.467625	-2.865931
1	-7.371092	-0.880396	-1.731269
1	-6.742234	0.150858	0.445818
1	-2.151438	-2.664044	0.731919
7	-4.224992	-0.453427	1.675837
6	-4.898979	0.460874	2.597624
1	-4.325577	0.558158	3.516603
1	-4.988077	1.438535	2.120301
1	-5.887938	0.061984	2.831428
6	-2.122376	-0.708089	2.971546
1	-1.163041	-1.208161	2.839642
1	-1.936750	0.363932	3.098810
1	-2.588696	-1.078782	3.890773
6	-3.080904	0.519360	-2.377874
1	-2.907958	-0.394813	-2.943065
1	-4.152864	0.571358	-2.111042
1	-2.901293	1.417335	-2.989749

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me-D

Number of imaginary frequencies : 0 Electronic energy : HF=-2272.1409422
Zero-point correction= 0.761319 (Hartree/Particle)
Thermal correction to Energy= 0.808234
Thermal correction to Enthalpy= 0.809179
Thermal correction to Gibbs Free Energy= 0.677571
Sum of electronic and zero-point Energies= -2271.379624
Sum of electronic and thermal Energies= -2271.332708
Sum of electronic and thermal Enthalpies= -2271.331764
Sum of electronic and thermal Free Energies= -2271.463372

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Cartesian Coordinates

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46	-0.060513	0.225380	-0.158156
7	-1.595497	-0.481243	1.224797
7	-1.777491	0.295142	-1.393917
8	-4.887364	0.924434	1.120278
8	-5.042132	-1.005344	-0.643902
6	-1.435420	-0.729638	2.532470
1	-0.447489	-1.043488	2.847544
6	-2.488860	-0.589307	3.435894
1	-2.339459	-0.835037	4.481510
6	-3.703598	-0.073245	2.991272
1	-4.512858	0.126672	3.685227
6	-3.853875	0.239211	1.634247
6	-2.802044	-0.088075	0.754933
6	-2.913380	-0.012135	-0.708491
6	-4.085106	-0.419527	-1.386408
6	-4.113239	-0.339668	-2.784218
1	-5.001219	-0.631491	-3.333422
6	-2.956688	0.033104	-3.455783
1	-2.927679	0.063554	-4.539152
6	-1.792566	0.299366	-2.737338
1	-0.851849	0.478065	-3.242052

6	-6.935991	1.554981	2.262480
1	-7.976376	1.278934	2.456453
1	-6.920826	2.538926	1.785046
1	-6.418214	1.633188	3.222170
6	-6.274561	0.520685	1.364321
1	-6.262013	-0.463591	1.846420
6	-6.908718	0.444925	-0.027613
1	-6.648259	1.372037	-0.549920
1	-8.000023	0.426091	0.062228
6	-6.468878	-0.774979	-0.854275
1	-6.652385	-0.575770	-1.915737
6	-7.154102	-2.073775	-0.456401
1	-6.775259	-2.904483	-1.056150
1	-8.232432	-1.991395	-0.616029
1	-6.977270	-2.306175	0.597757
6	1.283742	1.395846	-1.336608
6	1.696672	0.353938	-2.334541
8	1.196526	0.241436	-3.441680
8	2.666549	-0.465726	-1.861011
6	3.030757	-1.632420	-2.661341
1	4.121384	-1.622582	-2.720374
1	2.615721	-1.501091	-3.663301
6	2.528941	-2.894828	-2.008576
6	1.183595	-3.012579	-1.630145
6	3.388468	-3.982194	-1.820176
6	0.710956	-4.194916	-1.061225
1	0.501518	-2.183543	-1.796072
6	2.910344	-5.177168	-1.273953
1	4.432672	-3.902934	-2.111023
6	1.573009	-5.283590	-0.886643
1	-0.333004	-4.276554	-0.773096
1	3.583061	-6.020273	-1.149900
1	1.201048	-6.209721	-0.459643
6	2.865411	4.066323	0.420975
6	2.138478	2.893362	0.636118
6	1.290257	2.828449	1.736705
6	1.201456	3.940962	2.583128
6	1.944960	5.101981	2.342075
6	2.802927	5.184795	1.241799
6	3.477808	2.712585	-1.291803
6	2.476747	1.915711	-0.468583
1	0.704797	1.940716	1.941548
1	0.542148	3.902370	3.444211
1	1.857133	5.949164	3.013690
1	3.381866	6.081254	1.051247
1	3.025326	1.049480	-0.083062
7	3.657327	3.897845	-0.762000
6	4.526568	4.984049	-1.232860
1	3.908769	5.866214	-1.413536
1	5.262281	5.207169	-0.457278
1	5.033069	4.703707	-2.151839
6	4.147995	2.204174	-2.513904
1	4.476211	1.177633	-2.336839
1	3.422694	2.159726	-3.336957
1	4.996235	2.807339	-2.833903
7	1.465495	-0.415011	1.045748
6	2.230690	-1.091629	1.599460
6	3.157611	-1.955940	2.239872
6	3.910796	-1.512093	3.344789
6	3.296955	-3.264143	1.735071

6	4.807621	-2.390751	3.941886
1	3.787750	-0.501629	3.720765
6	4.201137	-4.124994	2.347490
1	2.705672	-3.586431	0.886801
6	4.952405	-3.691778	3.444860
1	5.393787	-2.065752	4.794907
1	4.317983	-5.134352	1.967371
1	5.654631	-4.370822	3.918251
6	0.540698	2.580207	-1.951939
1	0.170435	3.245765	-1.169252
1	1.205758	3.164585	-2.603894
1	-0.299081	2.279819	-2.569533

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me-P

Number of imaginary frequencies : 0 Electronic energy : HF=-980.0664648
Zero-point correction= 0.367848 (Hartree/Particle)
Thermal correction to Energy= 0.388618
Thermal correction to Enthalpy= 0.389562
Thermal correction to Gibbs Free Energy= 0.317941
Sum of electronic and zero-point Energies= -979.698617
Sum of electronic and thermal Energies= -979.677847
Sum of electronic and thermal Enthalpies= -979.676903
Sum of electronic and thermal Free Energies= -979.748524

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Cartesian Coordinates

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6	-0.258002	-2.484467	0.244298
6	-1.587797	-1.950591	-0.267175
8	-2.605761	-1.841560	0.385440
8	-1.459275	-1.499945	-1.539740
6	-2.412803	-0.482783	-1.933941
1	-3.425872	-0.795892	-1.670337
1	-2.317570	-0.433364	-3.021393
6	-2.046277	0.828011	-1.277674
6	-2.958751	1.517755	-0.474514
6	-0.746461	1.330623	-1.427441
6	-2.588735	2.711847	0.149695
1	-3.955343	1.111378	-0.326230
6	-0.372733	2.517057	-0.800195
1	-0.018911	0.770216	-2.006224
6	-1.296448	3.214831	-0.015336
1	-3.306153	3.243045	0.768794
1	0.642508	2.885228	-0.914079
1	-1.009009	4.145176	0.467399
6	2.163256	0.396483	0.424924
6	1.729251	-0.824369	-0.160526
6	2.419728	-1.328067	-1.274606
6	3.507231	-0.619829	-1.774693
6	3.921642	0.588590	-1.179917
6	3.256343	1.112781	-0.074845
6	0.326613	-0.302438	1.542818
6	0.573816	-1.260225	0.576467
1	2.101517	-2.252583	-1.748312
1	4.044126	-0.998658	-2.639494
1	4.770756	1.124673	-1.593715
1	3.572836	2.050889	0.370728
7	1.311074	0.679059	1.476058
6	1.360442	1.876251	2.290366

1	2.389724	2.236777	2.342140
1	0.723451	2.667660	1.879286
1	1.031878	1.653955	3.307651
6	-0.796114	-0.170186	2.522376
1	-0.457664	-0.302527	3.558102
1	-1.256446	0.821339	2.443848
1	-1.575149	-0.901361	2.313277
1	0.229620	-2.986924	-0.597166
6	-0.431331	-3.481219	1.395780
1	-0.999342	-4.358156	1.069386
1	0.548942	-3.810597	1.750380
1	-0.968360	-3.031970	2.232796

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me-Pel

Number of imaginary frequencies : 0 Electronic energy : HF=-537.539376
Zero-point correction= 0.177005 (Hartree/Particle)
Thermal correction to Energy= 0.187913
Thermal correction to Enthalpy= 0.188858
Thermal correction to Gibbs Free Energy= 0.138027
Sum of electronic and zero-point Energies= -537.362371
Sum of electronic and thermal Energies= -537.351463
Sum of electronic and thermal Enthalpies= -537.350518
Sum of electronic and thermal Free Energies= -537.401349

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Cartesian Coordinates

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6	-3.492801	0.629117	-0.193381
6	-2.524776	-0.451956	0.116510
8	-2.850585	-1.549224	0.526447
8	-1.240612	-0.086958	-0.106429
6	-0.244485	-1.089662	0.191323
1	-0.434423	-1.479164	1.198238
1	-0.356005	-1.928177	-0.504164
6	1.116293	-0.453419	0.086128
6	2.162098	-1.122143	-0.557343
6	1.362384	0.797231	0.668225
6	3.438433	-0.557325	-0.612138
1	1.978183	-2.088713	-1.019952
6	2.633056	1.366761	0.605698
1	0.548337	1.323531	1.157560
6	3.676205	0.689065	-0.031974
1	4.242048	-1.087377	-1.115278
1	2.811596	2.339146	1.056067
1	4.666577	1.132725	-0.078450
6	-3.155438	1.833453	-0.661191
1	-2.118584	2.094433	-0.846656
1	-4.525187	0.350038	-0.006221
1	-3.908781	2.586271	-0.872428

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me-TS(A_1-B_1)

Number of imaginary frequencies : 1 Electronic energy : HF=-2057.0418684
Zero-point correction= 0.666083 (Hartree/Particle)
Thermal correction to Energy= 0.708352
Thermal correction to Enthalpy= 0.709296
Thermal correction to Gibbs Free Energy= 0.589691
Sum of electronic and zero-point Energies= -2056.375786

Sum of electronic and thermal Energies= -2056.333516
Sum of electronic and thermal Enthalpies= -2056.332572
Sum of electronic and thermal Free Energies= -2056.452178

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Cartesian Coordinates

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46	0.614144	-0.156520	-0.172027
7	-0.888311	1.196469	0.448206
7	-1.122589	-1.162127	-0.890256
8	-4.294419	1.296373	-0.630479
8	-4.346642	-0.954141	0.629764
6	-0.708128	2.434618	0.926654
1	0.300676	2.729461	1.166864
6	-1.774017	3.318388	1.073696
1	-1.596356	4.305613	1.485118
6	-3.034533	2.954498	0.615541
1	-3.850701	3.667575	0.630039
6	-3.216110	1.679545	0.063933
6	-2.132148	0.764451	0.105713
6	-2.245933	-0.622954	-0.351688
6	-3.420692	-1.394305	-0.231569
6	-3.492932	-2.607076	-0.933157
1	-4.403010	-3.196255	-0.902914
6	-2.370556	-3.058134	-1.617975
1	-2.390178	-3.991929	-2.168620
6	-1.174831	-2.339982	-1.528361
1	-0.249262	-2.706419	-1.960159
6	-6.431781	1.746201	-1.564476
1	-5.982624	2.517308	-2.194410
1	-7.471441	2.020012	-1.366923
1	-6.421728	0.803410	-2.118668
6	-5.672570	1.620022	-0.252638
1	-5.688148	2.579912	0.274327
6	-6.202415	0.517570	0.679126
1	-7.295416	0.580007	0.701122
1	-5.853576	0.684904	1.704019
6	-5.772044	-0.897476	0.282868
1	-5.862823	-1.051058	-0.798327
6	-6.511507	-1.981323	1.051658
1	-6.390527	-1.835297	2.128754
1	-6.133973	-2.975068	0.797247
1	-7.578700	-1.950820	0.814618
6	2.834184	-0.904192	-2.764144
6	2.686585	-2.120173	-1.974226
8	1.828606	-2.958102	-2.208430
8	3.558988	-2.179435	-0.936761
6	3.533691	-3.380826	-0.109549
1	4.572926	-3.542231	0.178706
1	3.192737	-4.216744	-0.725555
6	2.646065	-3.193452	1.095845
6	3.141229	-3.381718	2.388726
6	1.282756	-2.879370	0.928189
6	2.294463	-3.255809	3.498022
1	4.185583	-3.642744	2.535967
6	0.443023	-2.730643	2.038517
1	0.871734	-2.890251	-0.073248
6	0.950057	-2.916244	3.327488
1	2.689644	-3.423604	4.495174
1	-0.611049	-2.515313	1.890239
1	0.297581	-2.825901	4.190166

7	3.907700	-0.171329	-2.527024
7	4.808024	0.476124	-2.286256
6	2.602667	3.162977	0.694289
6	2.451462	2.194256	-0.312722
6	2.316195	2.613883	-1.637295
6	2.362437	3.982898	-1.914476
6	2.529366	4.925804	-0.890198
6	2.647580	4.528832	0.446908
6	2.589224	1.169323	1.767169
6	2.397498	0.877714	0.348702
1	2.163352	1.893181	-2.432130
1	2.269884	4.324563	-2.940033
1	2.568598	5.981833	-1.135151
1	2.775846	5.258686	1.238817
1	3.009258	0.044071	-0.014043
7	2.672752	2.483197	1.945826
6	2.847949	3.196302	3.212653
1	3.817252	3.701092	3.210881
1	2.056091	3.941439	3.318923
1	2.799418	2.499311	4.046428
6	2.704123	0.169479	2.857569
1	3.588335	0.351982	3.476260
1	1.824767	0.194522	3.511249
1	2.771157	-0.828356	2.430558
6	2.022108	-0.666717	-4.014627
1	0.972777	-0.882721	-3.803369
1	2.105870	0.368173	-4.354058
1	2.345341	-1.324521	-4.827847

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me-TS(A-B)$_R$

Number of imaginary frequencies : 1 Electronic energy : HF=-1939.0677242
Zero-point correction= 0.579915 (Hartree/Particle)
Thermal correction to Energy= 0.618306
Thermal correction to Enthalpy= 0.619251
Thermal correction to Gibbs Free Energy= 0.506913
Sum of electronic and zero-point Energies= -1938.487810
Sum of electronic and thermal Energies= -1938.449418
Sum of electronic and thermal Enthalpies= -1938.448474
Sum of electronic and thermal Free Energies= -1938.560811

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Cartesian Coordinates

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46	-0.586590	-0.178532	-0.021253
7	1.213360	-1.089667	0.102323
7	0.667084	1.495093	-0.301303
8	4.412346	0.070546	-0.984441
8	4.013155	1.786460	0.894939
6	1.379017	-2.415715	0.156693
1	0.501212	-3.021622	0.331376
6	2.646595	-2.978204	-0.001608
1	2.758053	-4.053582	0.076966
6	3.725688	-2.169840	-0.331599
1	4.691616	-2.608654	-0.554690
6	3.536184	-0.782160	-0.442422
6	2.273409	-0.250209	-0.095705
6	1.963910	1.174748	-0.052978
6	2.888827	2.185106	0.293913
6	2.514130	3.521663	0.094796

1	3.223093	4.317176	0.294941
6	1.207960	3.810244	-0.288959
1	0.882591	4.835138	-0.428506
6	0.282542	2.773543	-0.416888
1	-0.766580	2.956216	-0.607785
6	6.500302	0.453051	-2.056322
1	6.195677	-0.215811	-2.864431
1	7.589041	0.415496	-1.965837
1	6.211400	1.472537	-2.327971
6	5.858333	0.033250	-0.743325
1	6.156347	-0.990632	-0.494871
6	6.183183	0.961764	0.439778
1	7.247431	1.215276	0.397136
1	6.018810	0.442879	1.390336
6	5.348196	2.244515	0.478894
1	5.252513	2.689975	-0.517658
6	5.867187	3.257446	1.487643
1	5.219228	4.135897	1.543458
1	6.867780	3.592835	1.200661
1	5.923328	2.809792	2.483797
6	-1.447773	-1.064857	2.428381
6	-1.680317	-2.453646	1.977234
8	-0.806817	-3.297315	2.022435
8	-2.903411	-2.627842	1.440114
6	-2.989025	-3.741839	0.501605
1	-2.690182	-4.668073	0.995354
1	-4.048146	-3.788896	0.242560
6	-2.114677	-3.426111	-0.690020
6	-2.202493	-2.144979	-1.275608
6	-1.201503	-4.343502	-1.202680
6	-1.372146	-1.796507	-2.357457
1	-2.999275	-1.479390	-0.961659
6	-0.377874	-3.995608	-2.285566
1	-1.123933	-5.332434	-0.760469
6	-0.448406	-2.724302	-2.853705
1	-1.494227	-0.833965	-2.845446
1	0.318596	-4.727668	-2.682647
1	0.184862	-2.465222	-3.695832
7	-2.319571	0.863502	-0.234864
6	-3.317531	1.444064	-0.379170
6	-4.529299	2.153084	-0.580118
6	-4.924305	2.473850	-1.897077
6	-5.316782	2.524785	0.530191
6	-6.111189	3.169537	-2.092007
1	-4.308984	2.178771	-2.740659
6	-6.499862	3.220308	0.310438
1	-5.001148	2.266200	1.534486
6	-6.894999	3.541334	-0.993314
1	-6.428035	3.422219	-3.098173
1	-7.116395	3.512064	1.153888
1	-7.821096	4.083958	-1.154722
7	-2.547815	-0.317096	2.566694
7	-3.458996	0.344384	2.652563
6	-0.271625	-0.733614	3.325627
1	-0.008174	0.324514	3.266178
1	-0.478957	-0.993798	4.368739
1	0.572173	-1.334251	2.984868

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me-TS(A-B)$_S$

Number of imaginary frequencies : 1 Electronic energy : HF=-1939.0678402
Zero-point correction= 0.579879 (Hartree/Particle)
Thermal correction to Energy= 0.618328
Thermal correction to Enthalpy= 0.619273
Thermal correction to Gibbs Free Energy= 0.507162
Sum of electronic and zero-point Energies= -1938.487961
Sum of electronic and thermal Energies= -1938.449512
Sum of electronic and thermal Enthalpies= -1938.448568
Sum of electronic and thermal Free Energies= -1938.560678

Cartesian Coordinates

46	-0.390225	-0.198806	-0.070259
7	1.346467	-1.239030	-0.088741
7	0.971987	1.410812	-0.112524
8	4.573530	-0.190839	-1.177941
8	4.386598	1.299481	0.906016
6	1.438225	-2.578293	-0.120240
1	0.524794	-3.136077	0.043923
6	2.661142	-3.203261	-0.358655
1	2.714323	-4.286015	-0.356109
6	3.775624	-2.435083	-0.676205
1	4.704348	-2.914339	-0.963874
6	3.669245	-1.034867	-0.678262
6	2.452901	-0.456343	-0.238132
6	2.253233	0.970768	0.001739
6	3.266911	1.855296	0.433947
6	2.981057	3.228658	0.457409
1	3.756816	3.936850	0.725981
6	1.680913	3.656312	0.208496
1	1.425178	4.709474	0.243881
6	0.675457	2.712424	-0.010933
1	-0.367737	2.986374	-0.102767
6	6.620184	0.211520	-2.318451
1	6.232383	-0.328908	-3.184876
1	7.707754	0.103128	-2.299906
1	6.380501	1.271808	-2.439655
6	6.026409	-0.341552	-1.032681
1	6.271341	-1.404469	-0.938743
6	6.470398	0.402359	0.238396
1	7.546912	0.589218	0.169309
1	6.313608	-0.224936	1.122582
6	5.732708	1.720917	0.487220
1	5.628269	2.302823	-0.435297
6	6.366668	2.550824	1.593026
1	5.789150	3.455816	1.797656
1	7.376575	2.853329	1.302044
1	6.431072	1.969822	2.517242
6	-1.238548	-1.259706	2.379229
6	-2.378405	-1.850692	1.655533
8	-3.470474	-1.322865	1.613283
8	-2.035840	-2.973581	0.975637
6	-2.946638	-3.304852	-0.115759
1	-3.962708	-3.402455	0.269295
1	-2.594911	-4.276129	-0.468095
6	-2.847622	-2.239047	-1.181484
6	-3.963928	-1.521499	-1.602004
6	-1.587201	-1.943698	-1.754620
6	-3.844798	-0.546881	-2.602320

1	-4.931936	-1.722231	-1.154215
6	-1.471506	-0.957301	-2.755429
1	-0.750805	-2.608197	-1.568438
6	-2.603473	-0.254792	-3.172166
1	-4.730008	-0.011973	-2.932073
1	-0.511373	-0.785551	-3.232388
1	-2.523108	0.493534	-3.953762
7	-2.069812	0.911293	-0.017078
6	-3.163241	1.303182	-0.011391
6	-4.495413	1.786125	0.005109
6	-5.422614	1.201897	0.893388
6	-4.872172	2.822561	-0.874346
6	-6.731967	1.670796	0.892762
1	-5.107146	0.397860	1.547893
6	-6.186530	3.273525	-0.856247
1	-4.144559	3.256730	-1.552173
6	-7.111988	2.700576	0.024699
1	-7.458678	1.234052	1.569572
1	-6.492319	4.071017	-1.525029
1	-8.136300	3.059678	0.033357
7	-0.212665	-2.070976	2.631933
7	0.683843	-2.733068	2.827494
6	-1.428936	-0.070704	3.294640
1	-1.826565	-0.374262	4.268580
1	-0.490373	0.467235	3.445091
1	-2.150003	0.596089	2.821776

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me-TS(C_1-D)

Number of imaginary frequencies : 1 Electronic energy : HF=-1947.4116736
Zero-point correction= 0.653735 (Hartree/Particle)
Thermal correction to Energy= 0.694119
Thermal correction to Enthalpy= 0.695064
Thermal correction to Gibbs Free Energy= 0.576723
Sum of electronic and zero-point Energies= -1946.773097
Sum of electronic and thermal Energies= -1946.732712
Sum of electronic and thermal Enthalpies= -1946.731768
Sum of electronic and thermal Free Energies= -1946.850108

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Cartesian Coordinates

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46	-0.444265	-0.718750	-0.003471
7	1.237459	-1.996464	0.564885
7	1.169409	0.577282	-0.332162
8	4.486262	-1.682436	-0.902794
8	4.555800	0.274505	0.788205
6	1.207862	-3.297217	0.890746
1	0.262830	-3.698460	1.241923
6	2.338641	-4.107146	0.796342
1	2.286199	-5.145904	1.102937
6	3.502271	-3.584072	0.241729
1	4.367350	-4.216211	0.072923
6	3.523286	-2.240270	-0.156880
6	2.398102	-1.437955	0.139527
6	2.376606	0.020764	-0.046434
6	3.505576	0.846046	0.180007
6	3.398240	2.214870	-0.105128
1	4.249244	2.872352	0.033059
6	2.170335	2.732552	-0.498442

1	2.046722	3.791277	-0.697045
6	1.057767	1.896398	-0.559668
1	0.069207	2.284113	-0.764645
6	6.599644	-2.721403	-1.542982
1	7.665473	-2.795132	-1.308281
1	6.496734	-2.351998	-2.567302
1	6.175168	-3.727933	-1.499835
6	5.911475	-1.782092	-0.562084
1	5.985940	-2.163656	0.462433
6	6.428531	-0.342722	-0.658676
1	6.113439	0.047914	-1.632656
1	7.523815	-0.345500	-0.661055
6	5.950292	0.588772	0.469998
1	6.013760	1.627640	0.130068
6	6.717931	0.435587	1.775411
1	6.308252	1.095912	2.543394
1	7.768087	0.697451	1.620541
1	6.671479	-0.591647	2.148700
6	-2.045902	0.148754	-0.623975
6	-2.724323	1.230812	0.184963
8	-3.616660	1.049151	0.987385
8	-2.189048	2.396164	-0.159486
6	-2.726583	3.628685	0.504388
1	-2.736105	3.432990	1.577697
1	-3.752892	3.741745	0.149853
6	-1.844374	4.773138	0.123723
6	-2.068999	5.474515	-1.069945
6	-0.781929	5.153984	0.956311
6	-1.241638	6.537974	-1.427898
1	-2.901164	5.196862	-1.711897
6	0.044137	6.220691	0.600023
1	-0.616927	4.630785	1.895215
6	-0.184465	6.911267	-0.593405
1	-1.428602	7.084276	-2.346917
1	0.849316	6.527093	1.260857
1	0.449042	7.750211	-0.864602
6	-4.729260	-2.310381	0.045642
6	-3.483857	-2.432922	-0.593088
6	-3.419744	-3.008563	-1.861306
6	-4.612927	-3.413040	-2.469328
6	-5.847389	-3.248971	-1.826646
6	-5.926893	-2.698264	-0.544121
6	-3.218049	-1.596560	1.570389
6	-2.471480	-1.911973	0.349467
1	-2.470340	-3.151550	-2.368591
1	-4.582312	-3.867060	-3.454267
1	-6.756927	-3.568767	-2.323768
1	-6.881548	-2.597905	-0.039660
1	-1.603270	-2.559170	0.525525
7	-4.507460	-1.810570	1.357929
6	-5.603078	-1.527767	2.286807
1	-5.205612	-1.284530	3.269412
1	-6.179202	-0.678634	1.910047
1	-6.246390	-2.406246	2.364571
6	-2.645262	-1.172887	2.878193
1	-1.555029	-1.158173	2.824119
1	-2.986493	-0.167541	3.142279
1	-2.944027	-1.857575	3.679257
6	-2.468982	0.101391	-2.045375
1	-2.023029	-0.711116	-2.616686

1	-3.560785	0.083139	-2.154906
1	-2.135272	1.060688	-2.473768

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me-TS(C-D)

Number of imaginary frequencies : 1 Electronic energy : HF=-2271.9514683
Zero-point correction= 0.753923 (Hartree/Particle)
Thermal correction to Energy= 0.802134
Thermal correction to Enthalpy= 0.803079
Thermal correction to Gibbs Free Energy= 0.662884
Sum of electronic and zero-point Energies= -2271.195745
Sum of electronic and thermal Energies= -2271.147534
Sum of electronic and thermal Enthalpies= -2271.146590
Sum of electronic and thermal Free Energies= -2271.286784

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Cartesian Coordinates

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46	0.339682	-0.634913	-0.071266
7	2.014914	-1.957259	0.275407
7	1.922038	0.647940	-0.516928
8	5.166092	-1.642761	-1.391857
8	5.373055	0.251000	0.360035
6	1.975123	-3.265437	0.558399
1	1.040033	-3.651963	0.944774
6	3.084382	-4.088200	0.362056
1	3.033062	-5.136483	0.634421
6	4.218654	-3.565538	-0.249908
1	5.058603	-4.205641	-0.497396
6	4.240754	-2.208848	-0.602970
6	3.153408	-1.399853	-0.206641
6	3.139858	0.064406	-0.336338
6	4.294835	0.863696	-0.151817
6	4.194080	2.244818	-0.367520
1	5.062672	2.883446	-0.252961
6	2.952740	2.796410	-0.658257
1	2.832916	3.864971	-0.794717
6	1.826947	1.978936	-0.684587
1	0.839198	2.398572	-0.819081
6	7.219960	-2.690119	-2.188715
1	8.296519	-2.786798	-2.020609
1	7.062349	-2.286193	-3.192883
1	6.782059	-3.691126	-2.152164
6	6.605644	-1.773411	-1.139423
1	6.735202	-2.189402	-0.133940
6	7.141008	-0.339605	-1.221000
1	6.772739	0.088147	-2.160114
1	8.233894	-0.358337	-1.291384
6	6.747878	0.559804	-0.034947
1	6.804379	1.608587	-0.344504
6	7.594590	0.354030	1.213253
1	7.243436	0.993037	2.026926
1	8.636607	0.607796	1.000560
1	7.556555	-0.684440	1.555042
6	-1.038728	0.646111	-0.637517
6	-1.515379	1.597951	0.418637
8	-1.693035	1.265451	1.575292
8	-1.616352	2.835550	-0.083514
6	-1.848402	3.948380	0.866934
1	-2.391147	3.548076	1.722993

1	-2.482943	4.632226	0.302000
6	-0.544529	4.582848	1.261025
6	0.016532	5.593486	0.466981
6	0.125125	4.167875	2.421573
6	1.229086	6.182657	0.828012
1	-0.506887	5.934600	-0.422832
6	1.337472	4.757460	2.782269
1	-0.312678	3.394487	3.046541
6	1.889992	5.764455	1.986825
1	1.644222	6.982116	0.221607
1	1.840617	4.444897	3.692198
1	2.822774	6.237169	2.279582
6	-5.574355	0.640161	-1.980834
6	-4.654849	-0.299910	-1.430029
6	-4.051490	-1.243011	-2.292327
6	-4.394382	-1.238552	-3.652431
6	-5.307745	-0.309139	-4.160191
6	-5.913994	0.645561	-3.327833
6	-5.368479	1.098568	0.211935
6	-4.527164	0.015159	-0.051002
1	-3.396334	-2.014335	-1.895930
1	-3.955484	-1.974538	-4.318358
1	-5.561219	-0.327368	-5.214837
1	-6.622860	1.358575	-3.736361
1	-3.945892	-0.499686	0.699491
7	-5.999577	1.472378	-0.948913
6	-6.993649	2.526717	-1.112270
1	-6.653736	3.261772	-1.847777
1	-7.945633	2.103515	-1.445752
1	-7.153524	3.032528	-0.161598
6	-5.610329	1.772321	1.522421
1	-4.916959	1.381623	2.269105
1	-5.465845	2.856624	1.461061
1	-6.630466	1.599148	1.885097
7	-1.096071	-1.964135	0.563280
6	-1.842565	-2.702296	1.060648
6	-2.750971	-3.604910	1.681219
6	-3.253398	-4.703892	0.954880
6	-3.127488	-3.386676	3.022701
6	-4.134333	-5.579370	1.579491
1	-2.953113	-4.861512	-0.075699
6	-4.009188	-4.275168	3.628092
1	-2.729321	-2.538124	3.569015
6	-4.510341	-5.366173	2.910127
1	-4.527690	-6.428938	1.031500
1	-4.304966	-4.119712	4.660175
1	-5.197226	-6.055608	3.390808
6	-1.505127	0.698301	-2.002054
1	-2.367337	-0.032845	-2.112975
1	-1.929579	1.668878	-2.278950
1	-0.766621	0.341845	-2.726613

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me-TS(C-D_2)

Number of imaginary frequencies : 1 Electronic energy : HF=-2476.6092276
Zero-point correction= 0.757740 (Hartree/Particle)
Thermal correction to Energy= 0.808150
Thermal correction to Enthalpy= 0.809095
Thermal correction to Gibbs Free Energy= 0.668826

Sum of electronic and zero-point Energies= -2475.851487
Sum of electronic and thermal Energies= -2475.801077
Sum of electronic and thermal Enthalpies= -2475.800133
Sum of electronic and thermal Free Energies= -2475.940402

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Cartesian Coordinates

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6	1.036909	-0.001104	-1.275648
6	1.746619	-0.828121	-0.236985
8	2.078686	-0.374655	0.839838
8	1.813326	-2.095229	-0.637932
6	2.091300	-3.123868	0.406730
1	2.731477	-2.664978	1.157164
1	2.653390	-3.885800	-0.128273
6	3.676614	1.652375	-1.184022
6	4.307771	0.470231	-1.771431
8	4.171403	0.228838	-2.967604
8	4.965779	-0.284531	-0.890023
6	5.657268	-1.478931	-1.380244
1	6.712245	-1.197194	-1.458125
1	5.287332	-1.721678	-2.377552
7	3.808539	1.820060	0.119615
7	3.889629	1.938778	1.242457
6	5.449476	-2.606629	-0.405521
6	5.288293	-3.911713	-0.885778
6	5.478218	-2.380382	0.977234
6	5.161404	-4.981043	0.005039
1	5.274718	-4.096096	-1.957061
6	5.334604	-3.446432	1.866168
1	5.605386	-1.370295	1.353722
6	5.177328	-4.748957	1.382356
1	5.052781	-5.991652	-0.376798
1	5.359268	-3.263661	2.936165
1	5.080147	-5.578711	2.075545
46	-0.490201	0.970647	-0.528897
7	-2.338016	1.867331	0.106110
7	-1.788821	-0.641427	-0.822638
8	-5.582854	0.775916	-0.934146
8	-4.969617	-1.098611	0.744338
6	-2.548859	3.156671	0.402475
1	-1.675447	3.758949	0.615610
6	-3.835604	3.693170	0.424559
1	-3.980180	4.733573	0.693305
6	-4.911780	2.905643	0.031085
1	-5.904022	3.334907	-0.047344
6	-4.688393	1.567443	-0.323934
6	-3.382815	1.046347	-0.162555
6	-3.044791	-0.365766	-0.367724
6	-3.927745	-1.416159	-0.034207
6	-3.605697	-2.718421	-0.433611
1	-4.290878	-3.533750	-0.231493
6	-2.368145	-2.952355	-1.018355
1	-2.060776	-3.952397	-1.295953
6	-1.458120	-1.906848	-1.139676
1	-0.448232	-2.097137	-1.467832
6	-7.729376	0.349168	-1.852666
1	-7.529417	1.083659	-2.636023
1	-8.806868	0.318160	-1.671166
1	-7.410996	-0.632216	-2.216031
6	-6.999447	0.725015	-0.572453

1	-7.326733	1.716925	-0.243241
6	-7.185548	-0.278705	0.577469
1	-8.245467	-0.547648	0.633624
1	-6.924195	0.186450	1.534339
6	-6.335613	-1.545323	0.447575
1	-6.349534	-1.929944	-0.578540
6	-6.729462	-2.626912	1.442119
1	-6.064227	-3.491731	1.373713
1	-7.750303	-2.966622	1.245912
1	-6.682568	-2.239654	2.463828
7	0.614192	2.608460	0.005578
6	1.143783	3.539652	0.453135
6	1.821500	4.670438	0.979744
6	2.368763	4.604942	2.278204
6	1.950867	5.831563	0.188486
6	3.047515	5.711572	2.776411
1	2.263877	3.701853	2.869531
6	2.634494	6.925360	0.707308
1	1.521174	5.865379	-0.807414
6	3.179968	6.865127	1.995194
1	3.474664	5.676055	3.772847
1	2.742613	7.825070	0.111032
1	3.712287	7.723661	2.392297
6	0.788980	-3.624817	0.959790
6	0.270036	-4.858061	0.546701
6	0.077214	-2.856605	1.896202
6	-0.938489	-5.325969	1.068620
1	0.823470	-5.463393	-0.166451
6	-1.136776	-3.317044	2.405223
1	0.491130	-1.911653	2.236351
6	-1.644003	-4.553792	1.994477
1	-1.319935	-6.295701	0.763263
1	-1.674286	-2.725694	3.140470
1	-2.576324	-4.923557	2.410920
6	3.230009	2.807432	-2.050217
1	2.196582	2.690891	-2.390285
1	3.309468	3.754921	-1.512402
1	3.872308	2.850547	-2.932355
6	1.249386	-0.169520	-2.700642
1	0.505439	0.324324	-3.325585
1	2.273321	0.171633	-2.995899
1	1.328183	-1.243836	-2.927989

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me-TS(C-P_{el})

Number of imaginary frequencies : 1 Electronic energy : HF=-1939.0574435
Zero-point correction= 0.573540 (Hartree/Particle)
Thermal correction to Energy= 0.614128
Thermal correction to Enthalpy= 0.615072
Thermal correction to Gibbs Free Energy= 0.493394
Sum of electronic and zero-point Energies= -1938.483903
Sum of electronic and thermal Energies= -1938.443315
Sum of electronic and thermal Enthalpies= -1938.442371
Sum of electronic and thermal Free Energies= -1938.564050

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Cartesian Coordinates

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46	-0.004266	0.860243	-0.438554
7	-1.144293	-0.851269	-0.427559

7	-1.830875	1.686212	0.148434
8	-4.368344	-1.317243	1.050931
8	-5.026196	0.385800	-0.767938
6	-0.679989	-2.111450	-0.493841
1	0.364755	-2.248137	-0.727202
6	-1.506180	-3.197791	-0.218300
1	-1.107028	-4.202140	-0.305022
6	-2.800468	-2.983141	0.239486
1	-3.419229	-3.818415	0.546992
6	-3.264969	-1.667416	0.381532
6	-2.439977	-0.610259	-0.074554
6	-2.842322	0.797074	-0.036715
6	-4.164226	1.251273	-0.225277
6	-4.448508	2.595525	0.059579
1	-5.466433	2.960658	-0.020420
6	-3.404235	3.457405	0.378058
1	-3.591646	4.505106	0.584624
6	-2.091006	2.984215	0.354218
1	-1.238590	3.636932	0.493524
6	-6.267948	-1.932655	2.342801
1	-5.606541	-2.378731	3.088973
1	-7.221648	-2.466626	2.359262
1	-6.449746	-0.891721	2.625195
6	-5.649510	-2.024121	0.956596
1	-5.465260	-3.073170	0.702023
6	-6.490271	-1.369523	-0.152699
1	-7.537753	-1.651283	-0.003676
1	-6.193717	-1.755299	-1.134069
6	-6.369064	0.155656	-0.215916
1	-6.401228	0.600144	0.785331
6	-7.400372	0.794428	-1.132940
1	-7.246976	1.873531	-1.214860
1	-8.407545	0.622836	-0.742725
1	-7.338216	0.363389	-2.136080
6	1.709750	-0.057248	-1.165807
6	2.750873	-0.320381	-0.105498
8	3.732728	0.383983	0.010833
8	2.387934	-1.361797	0.624361
6	3.346458	-1.858840	1.658525
1	3.989164	-1.021916	1.933607
1	2.703035	-2.131840	2.494522
6	4.101017	-3.025034	1.099224
6	3.742988	-4.333512	1.442033
6	5.149111	-2.807649	0.190889
6	4.424095	-5.416893	0.884199
1	2.938063	-4.506276	2.151941
6	5.824165	-3.890329	-0.370862
1	5.440853	-1.790627	-0.058547
6	5.461194	-5.195741	-0.025325
1	4.150162	-6.429920	1.161055
1	6.641614	-3.719335	-1.064448
1	5.993166	-6.038361	-0.455738
7	1.120705	2.557198	-0.245861
6	1.959107	3.342379	-0.059774
6	3.003045	4.271397	0.171138
6	2.747182	5.657488	0.118767
6	4.293132	3.769503	0.450725
6	3.794553	6.540354	0.350942
1	1.749786	6.023530	-0.100568
6	5.323541	4.673855	0.679876

1	4.463279	2.698394	0.480076
6	5.076005	6.050486	0.630814
1	3.615986	7.609610	0.314424
1	6.321384	4.307758	0.896728
1	5.887786	6.748088	0.811350
7	2.340760	-3.657070	-1.763234
7	2.363310	-4.743090	-1.559698
6	1.909884	-0.594168	-2.427862
1	2.776195	-1.215356	-2.663335
1	2.078277	0.824823	-1.896581
1	1.235745	-0.345940	-3.247131

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me-TS(D-F)

Number of imaginary frequencies : 1 Electronic energy : HF=-1947.5549167
Zero-point correction= 0.654882 (Hartree/Particle)
Thermal correction to Energy= 0.693870
Thermal correction to Enthalpy= 0.694814
Thermal correction to Gibbs Free Energy= 0.583538
Sum of electronic and zero-point Energies= -1946.899717
Sum of electronic and thermal Energies= -1946.860728
Sum of electronic and thermal Enthalpies= -1946.859784
Sum of electronic and thermal Free Energies= -1946.971061

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Cartesian Coordinates

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46	-0.981906	-0.579754	-0.196946
7	0.408739	-1.999540	0.532093
7	0.856322	0.137318	-1.116547
8	3.790313	-2.562162	-0.501428
8	4.021658	-0.185368	0.505564
6	0.106360	-3.154261	1.152979
1	-0.923955	-3.296299	1.451124
6	1.075504	-4.123870	1.390180
1	0.806074	-5.037414	1.908250
6	2.362880	-3.938361	0.896986
1	3.104138	-4.723429	0.993452
6	2.671366	-2.755527	0.213106
6	1.680648	-1.744207	0.137728
6	1.919294	-0.438755	-0.493222
6	3.162489	0.219117	-0.442584
6	3.376639	1.310922	-1.293900
1	4.340423	1.805946	-1.311421
6	2.316858	1.779753	-2.057308
1	2.438182	2.631218	-2.715968
6	1.053844	1.210393	-1.891955
1	0.184974	1.636250	-2.367944
6	5.900529	-3.292300	-1.307615
1	5.401103	-4.088905	-1.863614
1	6.907850	-3.627670	-1.047275
1	5.984052	-2.420256	-1.962503
6	5.122367	-2.957079	-0.044341
1	5.041879	-3.850627	0.583785
6	5.727537	-1.808858	0.781217
1	6.809184	-1.965476	0.850069
1	5.337218	-1.828983	1.804749
6	5.438550	-0.415465	0.216328
1	5.572209	-0.396467	-0.871213
6	6.255597	0.680974	0.883131

1	5.968012	1.666785	0.507538
1	7.321516	0.536151	0.686424
1	6.097471	0.667544	1.965506
6	-2.455535	0.870686	-0.872807
6	-2.197699	2.240980	-0.270210
8	-1.225794	2.881415	-0.910063
8	-2.840473	2.679542	0.665476
6	-0.733155	4.154656	-0.357325
1	-1.429880	4.476760	0.418798
1	-0.762747	4.861136	-1.187868
6	0.664990	3.950130	0.164607
6	1.713717	4.761027	-0.279933
6	0.924873	2.955571	1.119014
6	3.003203	4.591563	0.232575
1	1.523373	5.536134	-1.017547
6	2.212733	2.771501	1.616153
1	0.113019	2.328385	1.479024
6	3.255033	3.594874	1.175761
1	3.806207	5.238911	-0.105991
1	2.408256	1.995108	2.349448
1	4.255383	3.463108	1.576788
6	-5.336478	-0.874219	0.338795
6	-4.308149	-0.896363	-0.611885
6	-4.511281	-1.571289	-1.812435
6	-5.749384	-2.191481	-2.026868
6	-6.767768	-2.132797	-1.070314
6	-6.574855	-1.465780	0.145862
6	-3.636683	0.243507	1.359727
6	-3.204451	-0.056743	-0.063444
1	-3.731673	-1.651637	-2.558505
1	-5.917048	-2.731878	-2.952374
1	-7.719077	-2.615703	-1.265966
1	-7.360799	-1.423327	0.891295
1	-2.151601	-1.286207	0.557334
7	-4.865948	-0.193029	1.504465
6	-5.688332	-0.112067	2.718447
1	-5.897579	-1.123657	3.074474
1	-5.174377	0.457004	3.488304
1	-6.625947	0.387472	2.465887
6	-2.816378	0.717992	2.512046
1	-3.229694	1.632838	2.942210
1	-2.794480	-0.061644	3.282396
1	-1.795499	0.924357	2.200469
6	-2.573674	0.851049	-2.388216
1	-1.970758	1.648286	-2.819273
1	-2.257551	-0.094738	-2.828960
1	-3.616736	1.027297	-2.679545

$me\text{-}TS(E\text{-}P)_{2wat}$

Number of imaginary frequencies : 1 Electronic energy : HF=-2424.9979799
Zero-point correction= 0.807572 (Hartree/Particle)
Thermal correction to Energy= 0.858654
Thermal correction to Enthalpy= 0.859598
Thermal correction to Gibbs Free Energy= 0.719780
Sum of electronic and zero-point Energies= -2424.188580
Sum of electronic and thermal Energies= -2424.137498
Sum of electronic and thermal Enthalpies= -2424.136554
Sum of electronic and thermal Free Energies= -2424.276372

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Cartesian Coordinates

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46	-0.691708	-0.334686	-0.219053
7	-2.389511	-1.747574	-0.203530
7	-2.300500	0.959309	-0.640972
8	-5.519515	-0.670171	1.165034
8	-5.697660	0.053711	-1.356381
6	-2.341896	-3.036924	0.155895
1	-1.414405	-3.561067	-0.037889
6	-3.437257	-3.663388	0.749860
1	-3.385533	-4.717549	0.999214
6	-4.565365	-2.913620	1.071994
1	-5.389183	-3.368708	1.609820
6	-4.599105	-1.553788	0.735567
6	-3.515898	-1.027406	-0.001800
6	-3.504333	0.325018	-0.573506
6	-4.651875	0.876941	-1.181108
6	-4.589518	2.183600	-1.678600
1	-5.470152	2.641080	-2.115424
6	-3.361612	2.833427	-1.684349
1	-3.255582	3.826255	-2.106298
6	-2.229028	2.173789	-1.210700
1	-1.250127	2.613321	-1.308015
6	-7.516844	-0.030475	2.266844
1	-7.017161	-0.179859	3.226741
1	-8.585483	-0.219261	2.397959
1	-7.383901	1.014009	1.970352
6	-6.947085	-0.975018	1.219152
1	-7.085226	-2.009562	1.552337
6	-7.563375	-0.806213	-0.178539
1	-8.651689	-0.752665	-0.069331
1	-7.349547	-1.684802	-0.797152
6	-7.057529	0.416568	-0.950138
1	-6.993423	1.298494	-0.302248
6	-7.886544	0.712548	-2.191323
1	-7.469646	1.548595	-2.758550
1	-8.911443	0.969794	-1.909051
1	-7.915294	-0.162662	-2.846487
6	2.406770	0.629205	-0.489642
6	3.337642	-0.149678	0.293001
8	3.593120	0.016458	1.500384
8	4.061234	-1.020874	-0.452894
6	5.406187	-1.307543	0.041872
1	5.756382	-2.109107	-0.610704
1	5.351876	-1.669408	1.069703
6	6.242159	-0.057423	-0.076496
6	6.467960	0.504321	-1.343859
6	6.705917	0.612920	1.059331
6	7.148586	1.719554	-1.468610
1	6.110524	-0.011135	-2.231561
6	7.394313	1.823309	0.938263
1	6.510145	0.197041	2.042637
6	7.614424	2.380740	-0.322366
1	7.334082	2.139499	-2.452700
1	7.745785	2.334469	1.828395
1	8.148438	3.320841	-0.418324
6	0.000331	3.048423	0.919639
6	0.794592	2.588244	-0.149317
6	1.070356	3.456392	-1.214690

6	0.497993	4.729421	-1.210414
6	-0.328705	5.146803	-0.154502
6	-0.588351	4.311160	0.933750
6	0.661628	0.949771	1.483763
6	1.250598	1.230708	0.173921
1	1.719440	3.155312	-2.027619
1	0.701351	5.409925	-2.030479
1	-0.762237	6.141350	-0.175176
1	-1.215957	4.645494	1.752049
1	3.434658	1.826520	-0.521522
7	-0.048339	2.041868	1.892581
6	-0.935697	2.104588	3.048421
1	-1.958080	1.835748	2.759748
1	-0.590978	1.430454	3.830042
1	-0.931737	3.118941	3.449715
6	0.903739	-0.159346	2.465831
1	1.483911	0.227577	3.310778
1	-0.038707	-0.561915	2.848228
1	1.477483	-0.963773	2.025886
8	4.163518	2.674389	-0.446556
7	0.680696	-1.881936	-0.117911
6	1.396951	-2.790197	-0.228663
6	2.270261	-3.904466	-0.361315
6	2.104362	-5.020286	0.482509
6	3.276802	-3.881308	-1.347394
6	2.952892	-6.112288	0.333821
1	1.326242	-5.022160	1.238868
6	4.112316	-4.984672	-1.481780
1	3.397063	-3.004781	-1.972343
6	3.951562	-6.095306	-0.645631
1	2.836768	-6.976746	0.978772
1	4.888098	-4.982978	-2.240338
1	4.608017	-6.952388	-0.758026
8	4.268265	2.539707	2.034380
1	3.990659	1.590911	2.081217
1	4.273833	2.769137	0.591654
1	3.683468	3.061809	2.596912
1	5.024335	2.391490	-0.822683
6	2.280736	0.330668	-1.982360
1	3.250705	0.349383	-2.484689
1	1.843446	-0.661414	-2.153368
1	1.624838	1.049961	-2.475508

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me-TS(F-F_1)

Number of imaginary frequencies : 1 Electronic energy : HF=-1947.5476771
Zero-point correction= 0.654203 (Hartree/Particle)
Thermal correction to Energy= 0.693851
Thermal correction to Enthalpy= 0.694795
Thermal correction to Gibbs Free Energy= 0.581313
Sum of electronic and zero-point Energies= -1946.893474
Sum of electronic and thermal Energies= -1946.853826
Sum of electronic and thermal Enthalpies= -1946.852882
Sum of electronic and thermal Free Energies= -1946.966364

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Cartesian Coordinates

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46	-1.135071	-0.194246	-0.254926
7	0.137401	-1.775022	0.542921

7	0.876690	0.203840	-1.251885
8	3.395018	-2.797940	-0.528271
8	3.901312	-0.451209	0.542242
6	-0.314239	-2.865323	1.187188
1	-1.344212	-2.844228	1.522555
6	0.510274	-3.963942	1.408320
1	0.128797	-4.825862	1.944331
6	1.804172	-3.961910	0.893132
1	2.433445	-4.838896	0.993455
6	2.262913	-2.839964	0.191216
6	1.414559	-1.708158	0.106790
6	1.830272	-0.459369	-0.557616
6	3.131959	0.058899	-0.434806
6	3.494922	1.144738	-1.241530
1	4.501202	1.543967	-1.192149
6	2.527319	1.740851	-2.041826
1	2.768464	2.597031	-2.660720
6	1.212205	1.281772	-1.973556
1	0.410429	1.787578	-2.494320
6	5.436284	-3.715418	-1.315401
1	4.870805	-4.438353	-1.907623
1	6.397703	-4.161053	-1.047183
1	5.623219	-2.836449	-1.938743
6	4.667975	-3.343290	-0.056574
1	4.479650	-4.246019	0.535006
6	5.369337	-2.296930	0.825149
1	6.418551	-2.590571	0.936239
1	4.932106	-2.293481	1.829853
6	5.284475	-0.863020	0.293315
1	5.459588	-0.831909	-0.787975
6	6.214087	0.097826	1.019357
1	6.071180	1.122429	0.665076
1	7.258305	-0.180470	0.851931
1	6.017849	0.077045	2.095390
6	-2.545091	1.283137	-0.921796
6	-2.234720	2.660101	-0.360344
8	-1.019328	3.044521	-0.755184
8	-3.007919	3.296570	0.319868
6	-0.447318	4.279602	-0.202550
1	-1.108111	4.629489	0.594313
1	-0.447248	5.016819	-1.008079
6	0.942228	3.965951	0.284871
6	2.032928	4.736742	-0.128309
6	1.152587	2.910581	1.184148
6	3.314277	4.466090	0.361006
1	1.882777	5.559082	-0.822734
6	2.430345	2.627046	1.659808
1	0.308269	2.307723	1.511826
6	3.515151	3.410830	1.251199
1	4.151119	5.081799	0.046243
1	2.586376	1.801377	2.347222
1	4.509361	3.202034	1.634498
6	-4.902665	-1.240348	0.375506
6	-4.080519	-0.797314	-0.672917
6	-4.167534	-1.448509	-1.908884
6	-5.066253	-2.512321	-2.046309
6	-5.873715	-2.926651	-0.981854
6	-5.804387	-2.287360	0.261726
6	-3.696735	0.458951	1.283807
6	-3.279511	0.327878	-0.141745

1	-3.563508	-1.157109	-2.756339
1	-5.140344	-3.020805	-3.001668
1	-6.566656	-3.749743	-1.119208
1	-6.433770	-2.602822	1.086106
1	-1.010821	0.313824	1.136744
7	-4.638477	-0.441198	1.519267
6	-5.367966	-0.655728	2.775371
1	-5.113299	-1.639036	3.178498
1	-5.124788	0.117433	3.498567
1	-6.438254	-0.616733	2.562424
6	-3.217531	1.372742	2.363582
1	-3.946538	2.173260	2.528705
1	-3.077749	0.820601	3.296557
1	-2.279387	1.853733	2.106010
6	-2.602266	1.277352	-2.444457
1	-3.641953	1.374019	-2.777862
1	-2.035374	2.119666	-2.839502
1	-2.192778	0.367870	-2.892316

S_3

Number of imaginary frequencies : 0 Electronic energy : HF=-647.0161564
Zero-point correction= 0.186760 (Hartree/Particle)
Thermal correction to Energy= 0.199828
Thermal correction to Enthalpy= 0.200772
Thermal correction to Gibbs Free Energy= 0.144762
Sum of electronic and zero-point Energies= -646.829396
Sum of electronic and thermal Energies= -646.816328
Sum of electronic and thermal Enthalpies= -646.815384
Sum of electronic and thermal Free Energies= -646.871394

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Cartesian Coordinates

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6	2.590287	-0.298219	-0.343095
6	1.465584	0.006387	0.539389
6	2.781324	-1.594378	-1.090507
1	3.666944	-1.550268	-1.729143
1	1.909410	-1.802153	-1.717781
8	0.629991	-1.060642	0.592404
8	1.300916	1.055002	1.141310
6	-0.573416	-0.895321	1.393540
1	-0.806365	-1.905396	1.737067
1	-0.337856	-0.260935	2.250803
6	-1.703633	-0.321553	0.576783
6	-1.827524	1.065476	0.412708
6	-2.626940	-1.168747	-0.047216
6	-2.861202	1.591229	-0.362368
1	-1.099876	1.717929	0.884374
6	-3.662489	-0.643075	-0.821347
1	-2.534946	-2.245243	0.076308
6	-3.780618	0.739149	-0.979841
1	-2.950952	2.667084	-0.483146
1	-4.375620	-1.309894	-1.297662
1	-4.586740	1.150939	-1.580522
7	3.471758	0.662103	-0.466559
7	4.237364	1.499169	-0.573985
1	2.896652	-2.431531	-0.394481

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