Supporting Information

Facile H/D Exchange at (Hetero)Aromatic Hydrocarbons Catalyzed by a Stable Trans-Dihydride N-Heterocyclic Carbene (NHC) Iron Complex

Subhash Garhwal,† Alexander Kaushansky, † Natalia Fridman, † Linda J. W. Shimon,∥ and Graham de Ruiter†*

†Schulich Faculty of Chemistry, Technion – Israel Institute of Technology; Technion City, Haifa 3200003, Israel. †Department of Chemical Research Support, Weizmann Institute of Science, Rehovot, 7610001, Israel

E-mail: graham@technion.ac.il
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**General Information**

All reactions were performed at room temperature either by using standard Schlenk techniques or by using an N₂-filled M. Braun Glovebox unless otherwise specified. Glassware was oven dried at 140 °C for at least 2h prior to use, and allowed to cool under vacuum. All reagents were used as received unless mentioned otherwise. Anhydrous iron chloride (FeCl₂·1.5THF)¹ and 2,10-Di-tert-butyldipyrido[1,2-c;2',1'-e]imidazol-6-thione² were synthesized according to published procedures.¹⁻² Ter-butyl lithium (1.7 M in pentane) and chlorodiisopropylphosphine were purchased from Sigma Aldrich and Alfa Aesar respectively. Anhydrous unstabilized tetrahydrofuran (THF) and diethyl ether (Et₂O) were purchased from Sigma Aldrich and used as received. The ¹H, ¹³C{¹H} spectra were recorded on Bruker AVANCE III 200, 300, 400, and 500 NMR spectrometers at room temperature unless mentioned otherwise. All chemical shifts (δ) are reported in ppm, and coupling constants (J) are in Hz. The ¹H and ¹³C{¹H} NMR spectra were referenced using residual solvent peaks in the deuterated solvent. The ³¹P chemical shifts are reported relative to the internal lock signal. Deuterated solvents (CDCl₃, and C₆D₆) were purchased from Cambridge Isotope Laboratories, dried over calcium hydride, degassed by three freeze-pump-thaw cycles and vacuum-transferred prior to use. Atmospheric positive electrospray ionization time-of-flight mass spectrometry (TOF MS ES⁺) and high-resolution mass spectrometry (HRMS) were performed on a Waters QTOFMS Xevo G2 spectrometer in the positive ion mode.

**Physical Methods**

**Single-crystal X-ray diffraction.** For compounds A1 and 1 low temperature (100K) diffraction data were collected using a Bruker SMART APEX II diffractometer coupled to an APEX II CCD detector with graphite monochromatic MoKα (λ = 0.71073 Å) radiation. All diffractometer manipulations, including data collection, integration, and scaling were carried out using the Bruker APEXII software.³ Absorption corrections were applied using SADABS.⁴ For compound 2, low temperature (100K) diffraction data was collected on a Rigaku XtaLAB AFC12 (RINC) with a Kappa single CCD detector and a micro-focus sealed X-ray tube with monochromatic CuKα (λ = 1.54184 Å) radiation. All diffractometer manipulations, including data collection and integration were carried out using CrysAlisPro (Rigaku Oxford Diffraction, 2020). Absorption corrections were applied using CrysAlisPro (Rigaku Oxford Diffraction, 2020), with numerical absorption correction based on gaussian integration over a multifaceted crystal model. Empirical absorption correction were applied using spherical harmonics, implemented in the SCALE3 ABSPACK scaling algorithm. All structures were solved by direct methods using SHELXS⁵ and refined against F² on all data by full-matrix least squares with SHELXL-2014 or SHELXL-2018⁶ using established refinement techniques.⁷ All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement
parameters of all hydrogen atoms were fixed to 1.2 times the $U$ value of the atoms they are linked to (1.5 times for methyl groups). All air- and moisture-sensitive manipulations were carried out using standard Schlenk and cannula techniques or in an MBraun inert atmosphere drybox containing an atmosphere of purified nitrogen.

**Synthetic Procedures**

**Synthesis of pro-ligand A1.** In the glovebox, to a solution of 2,10-Di-tert-butyldipyrido[1,2-c;2′,1′-e]imidazol-6-thione (5 g, 16 mmol) in THF (400 mL) was added t-BuLi (1.7 M in pentane, 28.2 mL, 48 mmol) at −78 °C. The reaction mixture was stirred at −78 °C for 2.5 h, where after $\text{P}_2\text{PCl}$ (8.91 mL, 56 mmol) was added dropwise and the resulting solution stirred for another 3 h at −78 °C. Next, iodomethane (MeI; 6.5 mL, 100 mmol) was added at −78 °C and the solution was allowed to warm to room temperature and stirred for an additional 2 h. Hereafter, all volatiles were removed under reduced pressure and the remaining crude solid was re-dissolved in 250 mL of anhydrous methanol. To the resulting solution sodiumborohydride (NaBH₄; 1.8 g, 48 mmol) was added in small portions and stirred for 2 h at room temperature. Hereafter, the volatiles were removed under reduced pressure and the remaining solid re-dissolved in DCM (100 mL) and subsequently filtered through a pad of @celite. The remaining solvent was removed under vacuum and the crude red solid was washed with hexane (4×100 mL), and subsequently purified by column chromatography (DCM/Hexane (1:5)) to yield the title compound as a brown-red solid. Yield: 5.1 g (50%). $^1$H NMR (400 MHz, CDCl₃): δ (ppm) 10.37 (t, $^3\text{J}_{\text{H}-\text{H}} = 3.5$ Hz, 1H, NCHN), 9.17 (d, $J = 1.6$ Hz, 2H, m-bpy-H), 7.50 (d, $J = 1.6$ Hz, 2H, m-bpy-H), 2.36 (hept, $J = 6.8$ Hz, 4H, (CH₃)₂CH), 1.52 (s, 18H, t-Bu), 1.19 (dd, $J = 16.6, 7.1$ Hz, 12H, (CH₃)₂CH), 1.08 (dd, $J = 12.4, 6.9$ Hz, 12H (CH₃)₂CH). $^{13}$C $^1$H NMR (101 MHz, CDCl₃): δ (ppm) 146.37 (p-bpy-C), 131.70 (d, $J = 32.6$ Hz, o-bpy-C), 127.20 (d, $^3\text{J}_{\text{C}-\text{C}} = 3.9$ Hz, m-bpy-C), 124.61 (o-bpy-C), 116.59 (m-bpy-C), 111.51 (t, $^3\text{J}_{\text{C}-\text{C}} = 29.2$ Hz, NCHN), 35.87 (q, Bu-C), 30.82 (t, Bu-C), 23.78 (d, $J = 11.0$ Hz, (CH₃)₂CH), 19.82 (d, $J = 17.6$ Hz, (CH₃)₂CH), 18.57 (d, $J = 7.8$ Hz, (CH₃)₂CH). $^{31}$P $^1$H NMR (162 MHz, CDCl₃): δ (ppm) -3.34 (s). HRMS (TOF MS ES⁺, positive ion; m/z): calcd. for [C₅H₁₅N₂P₂]$^+$: 513.3527; found: 513.3516.

**Synthesis of free carbene A2.** In the glovebox, to a stirred suspension of A1 (5.0 g, 7.8 mmol) in THF (400 mL) was added – drop wise – a solution of potassium tert-butoxide (KO'Bu; 0.9 g, 7.8 mmol) in THF (50 mL). Upon addition of KO'Bu the color gradually changed from dark red suspension to light yellow solution. The reaction mixture was stirred for another 5 h, where after the solvent was removed under reduced pressure. The crude solid was extracted with hexane (150 mL) and filtered through a pad of Celite. The remaining solvent was evaporated under reduced pressure to yield the title compound as yellow-brown solid, which was used without further purification. Yield: 3.6 g (90%). $^1$H NMR (400 MHz, C₅D₅): δ (ppm) 7.49 (d, $J = 1.9$ Hz, 2H, m-bpy-H), 7.46 (dd, $J = 9.8, 2.0$ Hz, 2H, m-bpy-H), 3.61...
- 3.47 (m, 4H, (CH₃)₁CH), 1.37 (dd, J = 15.5, 7.0 Hz, 12 H, (CH₃)₂CH), 1.20 (s, 18H, Bu), 1.10 (dd, J = 13.3, 7.0 Hz, 6H, (CH₃)₂CH). ¹³C [¹H] NMR (101 MHz, CDCl₃): δ (ppm) 199.29 (t, Jₚ,C = 7.8 Hz, NCN), 139.79 (dd, J = 24.0, 13.2 Hz, o-bpy-C), 125.85 (d, Jₚ,C = 36.9 Hz, m-bpy-C), 123.20 (p-bpy-C), 112.43 (m-bpy-C), 34.38 (q-Bu-C), 30.28 (Bu-C), 23.54 (d, J = 11.0 Hz, (CH₃)₂CH), 21.33 (d, J = 23 Hz, (CH₃)₂CH), 21.24 (d, J = 13.2 Hz, (CH₃)₂CH). ³¹P [¹H] NMR (162 MHz, CDCl₃): δ (ppm) 24.18 (s). HRMS (TOF MS ES⁺, positive ion; m/z): calcd for [C₃₁H₅₀N₅P₂Fe²⁺]: 603.2487; found: 603.2497.

Synthesis of [(PC₅H₄P)FeCl₂] (1). In the glovebox, a solution of FeCl₂·1.5THF (0.5 g, 2.12 mmol, in THF (100 mL) was added – drop wise – to a stirred suspension of A2 (1.1 g, 2.14 mmol) in THF (150 mL). The reaction mixture was stirred for 16 h at room temperature, where after the solvent was removed under reduced pressure. The remaining yellow/brown solid (1) was washed with hexane (2×20mL) and recrystallized by slow vapor diffusion of pentane into concentrated toluene solution of 1 to yield the title compound as a yellow/brown solid. Yield 1.2 g (88 %). ¹H NMR (300 MHz, C₆D₆): δ (ppm) 160.30 (br), 21.94 (s), 13.15(s), 6.71 (s), 6.29 (br), 3.60(s), 1.42 (s), 0.96 (s). HRMS (TOF MS ES⁺, positive ion; m/z): calcd for [C₃₁H₅₀Cl₁N₁P₁Fe²⁺]: 603.2487; found 603.2497.

Synthesis of [(PC₅H₄P)Fe(H)₂N₂] (2). In the glovebox, to a frozen suspension of 1 (639.4 mg, 1.0 mmol) in THF (50 mL) was added – drop wise – a solution of sodium triethylborohydride (NaBHEt₃; 1.0 mL, 1.0 mmol, 1 M in THF). The resulting reaction mixture was stirred for 2h at −78 °C and for an additional 15 h at room temperature. Hereafter, the solvent was removed under reduced pressure and the remaining crude solid was re-dissolved in pentane (30 mL) and filtered through a pad of Celite. The pentane was removed under a flow of N₂ and the title compound was obtained as purple crystals upon recrystallization from a concentrated pentane solution −35 °C. Yield 419 mg (70 %). ¹H NMR (300 MHz, C₆D₆): δ (ppm) 6.98 (s, 2H, m-bpy-H), 6.81 (s, 2H, m-bpy-H), 2.44 (hept, J = 6.8 Hz, 4H, (CH₃)₂CH), 1.53 (dd, J = 15.5, 7.0 Hz, 12H, (CH₃)₂CH), 1.34 (dd, J = 13.7, 6.9 Hz, 12H, (CH₃)₂CH), 1.17 (s, 18H, Bu), -8.79 (t, J = 43.0 Hz, 2H, Fe-H). ¹³C [¹H] NMR (101 MHz, C₆D₆): δ (ppm) 141.15, 139.90 (t, J = 14.2 Hz), 119.36, 115.50, 111.89, 34.96, 30.47, 20.12, 19.24 (t, J = 3.3 Hz) (carbene carbon not observed). ³¹P [¹H] NMR (162 MHz, C₆D₆): δ (ppm) 133.02 (s). Due to reactivity of complex 1 and the lability of the dinitrogen ligand, reliable combustion analysis or high-resolution mass spectrometry could not be obtained.

Deuterium exchange experiment of [(PC₅H₄P)Fe(H)₂N₂] (2). from C₆D₆: Inside a glovebox, an oven-dried 4 mL vial was charged with [(PC₅H₄P)Fe(H)₂N₂] (2; 59.8 mg, 0.1 mmol) and 500 µL C₆D₆ was added. The resulting solution was transferred to a J-Young tube and its ¹H NMR spectrum was recoded within 5 minutes. Initially, the ¹H NMR showed a triplet at -8.79 ppm (Jₚ,H = 43.0 Hz),
while the $^1\text{H}^{\{31\text{P}\}}$ shows a broad singlet at -8.79 ppm. After 15 min $^1\text{H}^{\{31\text{P}\}}$ NMR shows triplet at -8.79 ppm ($^2J_{D,H} = 21.1$ Hz) which might indicate the formation a non-classical Fe-(HD) intermediate. During the course of 6 hours the intensity of the hydride resonance disappears and the $^{31}\text{P}^{\{1\text{H}\}}$ NMR spectrum shows a quintet at 133.27 ppm ($^2J_{D,P} = 6.2$ Hz) which indicates formation of di-deuteride. Analysis of the reaction mixture by $^2\text{H}$ NMR (after dissolution in benzene) showed a characteristic triplet at -8.68 ppm ($^2J_{P,D} = 6.6$ Hz). Similar, after keeping the dideuteride in benzene for 24 hours, resulted in the clean formation of 2.

![Figure S1](image1.png)

**Figure S1.** Hydride region of the $^1\text{H}^{\{31\text{P}\}}$ NMR spectrum (300 MHz) of complex 2 in $\text{C}_6\text{D}_6$.

![Figure S2](image2.png)

**Figure S2.** Hydride region of the $^1\text{H}$ NMR spectrum (300 MHz) of complex 2 in $\text{C}_6\text{D}_6$. 
Figure S3. $^2$H NMR spectrum (46.07 MHz) of the complex 2 in C$_6$H$_6$/C$_6$D$_6$ after 6h.

Figure S4. $^{31}$P{$^1$H} NMR spectrum (121.49 MHz) of the complex 2 in C$_6$D$_6$ after 6h.
Substrate scope for alkyne hydroboration

**General procedure for the HIE using C₆D₆ as deuterium source:** Inside a glovebox, an oven-dried 4 mL vial was charged with substrate (0.1 mmol) and a stock solution of catalyst 2 in C₆D₆ (0.5 mL, 0.005 mmol, 5 mol%) with tetraethylsilane (0.01 mmol, 50 μL from 0.2 mM stock solution) as internal standard. The reaction mixture was transferred to J-Young tube and heated at the specified temperature. The amount of deuteration was determined by ¹H NMR spectroscopy, by integrating the product peaks with respect to internal standard. The same procedure was repeated without internal standard. After the after specified time, the solution was filtered through sort plug of alumina to remove the iron catalyst. The alumina was washed with an additional 400 μL of C₆D₆ to collect all the organic products. The yield and selectivity was determined via a combination of ¹H and ¹³C NMR spectroscopy. The stock solution of catalyst 2 was prepared by dissolving 2 (149.6 mg, 0.25 mmol) in C₆D₆ (25 mL).

**Compound [d₃]-4.** Prepared according to general procedure (80°C, 8h). ¹H NMR (400 MHz, C₆D₆): δ (ppm) 7.02 (m, labeled, 1.5 H), 2.09 (m, labeled, 1.5 H). ¹³C ¹H} NMR (101 MHz, C₆D₆): δ (ppm) 137.87, 129.22, 128.34 (t, labeled, merging with C₆D₆), 125.19 (t, labelled), 21.44 (m, labeled).

**Compound [d₁]-5.** Prepared according to general procedure (80°C, 5h). ¹H NMR (400 MHz, C₆D₆): δ (ppm) 6.90 (m, 2 H), 6.85 (s, 1 H), 2.14 (m, labeled, 4 H). ¹³C ¹H} NMR (101 MHz, C₆D₆): δ (ppm) 137.77, 130.24, 128.41 (m, labeled, merging with C₆D₆), 126.34, 21.38, 21.10 (m, labeled).

**Compound [d₆]-6.** Prepared according to general procedure (50°C, 3h). ¹H NMR (400 MHz, C₆D₆): δ (ppm) 7.16 (residual peak of C₆D₆) ¹³C ¹H} NMR (101 MHz, C₆D₆): δ (ppm) 163.30 (t), 129.73 (m, labeled), 123.60 (m, labeled), 115.15 (m, labeled).

**Compound [d₁]-7.** Prepared according to general procedure (50°C, 3h). ¹H NMR (400 MHz, C₆D₆): δ (ppm) 7.11 (m, 2H), 7.60 (m, 2H). ¹³C ¹H} NMR (101 MHz, C₆D₆): δ (ppm) 134.23, 129.55, 128.45 (m), 126.03 (t, labeled).

**Compound [d₆]-8.** Prepared according to general procedure (80°C, 3h). ¹H NMR (400 MHz, C₆D₆): δ (ppm) 7.16 (residual peak of C₆D₆) ¹³C ¹H} NMR (101 MHz, C₆D₆): δ (ppm) 159.79 (s), 128.94 (m, labeled), 120.05 (m, labeled), 113.62 (m, labeled), 53.63 (m, labeled).
Compound [d2]-9. Prepared according to general procedure (50°C, 8h). $^1$H NMR (400 MHz, C$_6$D$_6$): $\delta$ (ppm) 6.51 (m, labeled, 0.7 H), 3.18 (labeled, 1.4 H). $^{13}$C ($^1$H) NMR (101 MHz, C$_6$D$_6$): $\delta$ (ppm) 158.78, 156.32 (d), 115.8 (m, labeled), 114.96 (m, labeled), 54.87 (m, labeled).

Compound [ds]-10. Prepared according to general procedure (50°C, 3h). $^1$H NMR (400 MHz, C$_6$D$_6$): $\delta$ (ppm) 7.31 (m, labeled 1.4H). $^{13}$C ($^1$H) NMR (101 MHz, C$_6$D$_6$): $\delta$ (ppm) 130.73 (m, labeled), 128.15 (m, labeled, merging with C$_6$D$_6$), 124.94 (m, labeled), 124.71 (d).

Compound [d3]-11. Prepared according to general procedure (50°C, 3h). $^1$H NMR (400 MHz, C$_6$D$_6$): $\delta$ (ppm) 6.64 (m, 2H), 2.52 (s, 6H). $^{13}$C ($^1$H) NMR (101 MHz, C$_6$D$_6$): $\delta$ (ppm) 151.06, 128.96 (m, labeled), 116.60 (m, labeled), 112.97, 40.27.

Compound [d2]-12. Prepared according to general procedure (50°C, 3h). $^1$H NMR (400 MHz, C$_6$D$_6$): $\delta$ 7.92 (m, 2H), 6.65 (m, labeled, 0.8H), 4.07 (q, J = 7.1 Hz, 2H), 0.99 (t, J = 7.1 Hz, 2H). $^{13}$C ($^1$H) NMR (101 MHz, C$_6$D$_6$): $\delta$ (ppm) 165.88 (d, J = 252.8), 165.22, 132.30 (m, labeled), 127.36 (d, J = 3.0 Hz), 115.53 (d, J = 21.9 Hz), 60.90, 14.23.

Compound [ds]-13. Prepared according to general procedure (50°C, 3h). $^1$H NMR (400 MHz, C$_6$D$_6$): $\delta$ (ppm) 7.32 (m, 2H), 2.76 (s, labeled 3H), 2.32 (s, labeled 3H). $^{13}$C ($^1$H) NMR (101 MHz, CDCl$_3$): $\delta$ (ppm) 171.64, 136.37, 129.00 (m, labeled), 127.88 (m, labeled), 39.54, 35.32.

Compound [d0]-14. Prepared according to general procedure (50°C, 3h). Only starting material was recovered.

Compound [d1]-15. Prepared according to general procedure (50°C, 3h). $^1$H NMR (400 MHz, C$_6$D$_6$): $\delta$ (ppm) 6.57 (s, 2H), 2.42 (s, 6H). $^{13}$C ($^1$H) NMR (101 MHz, C$_6$D$_6$): $\delta$ (ppm) 158.04, 135.77 (m, labeled), 119.77, 110.37, 24.57.
**Compound [d2]-16.** Prepared according to general procedure (50°C, 4h). $^1$H NMR (400 MHz, C$_6$D$_6$): δ (ppm) 6.34 (s, labeled, 0.4H), 6.31 (s, 2H), 2.86 (s, 3H). $^{13}$C {$^1$H} NMR (101 MHz, C$_6$D$_6$): δ (ppm) 121.52, 108.62 (m, labeled), 35.25.

**Compound [d3]-17.** Prepared according to general procedure (50°C, 3h). $^1$H NMR (400 MHz, C$_6$D$_6$): δ 2.61 (m, labeled, 3H). $^{13}$C {$^1$H} NMR (101 MHz, C$_6$D$_6$): δ (ppm) 137.72 (m, labeled), 129.56 (m, labeled), 119.40 (m, labeled), 32.02.

**Compound [d3]-18.** Prepared according to general procedure (50°C, 1.5h). $^1$H NMR (400 MHz, C$_6$D$_6$): δ (ppm) 2.52 (s, labeled, 1.5H). $^{13}$C {$^1$H} NMR (101 MHz, C$_6$D$_6$): δ (ppm) 151.96, 140.69 (m, labeled), 110.11 (m, labeled), 105.47 (m, labeled), 13.03 (m, labeled).

**Compound [d2]-19.** Prepared according to general procedure (50°C, 3h). $^1$H NMR (400 MHz, C$_6$D$_6$): δ (ppm) 5.77 (s, labeled, 0.35H), 2.05 (s, 6H). $^{13}$C {$^1$H} NMR (101 MHz, C$_6$D$_6$): δ (ppm) 149.85, 105.93 (m, labeled), 13.06 (labeled).

**Compound [d4]-20.** Prepared according to general procedure A. $^1$H NMR (400 MHz, CDCl$_3$): δ (ppm) 7.85 (s, 4H), 7.48 (s, labeled 0.6H). $^{13}$C {$^1$H} NMR (101 MHz, CDCl$_3$): δ (ppm) 133.53, 127.84, 125.60 (m, labeled).

**Compound [d7]-21.** Prepared according to general procedure A. $^1$H NMR (400 MHz, C$_6$D$_6$): δ (ppm) 8.78 (s, labeled, 0.04H), 8.32 (s, labeled, 0.40H), 7.52 (s, labeled, 0.08H), 7.38 (s, labeled, 0.40H), 7.34 (m, labeled, 0.21 H), 7.14 (m, labeled, 0.19H), 6.76 (m, labeled, 0.08H). $^{13}$C {$^1$H} NMR (101 MHz, CDCl$_3$): δ (ppm) 150.08 (m, labeled), 148.25, 135.81 (m, labeled), 129.30 (m, labeled), 128.20 (m, labeled), 127.70 (m, labeled), 126.35 (m, labeled), 120.79 (m, labeled).
$^1$H NMR and high-resolution mass spectra of selected compounds

**Figure S5.** $^1$H NMR spectrum (400 MHz) of A1 in CDCl$_3$.

**Figure S6.** $^{13}$C {$^1$H} NMR spectrum (101 MHz) of A1 in CDCl$_3$. 
Figure S7 HMQC NMR spectrum (400 MHz) of A1 in C₆D₆.

Figure S8. ³¹P NMR spectrum (162 MHz) of A1 in CDCl₃.
Figure S9. High resolution mass spectrum of A1

Figure S10. $^1$H NMR spectrum (400 MHz) of A2 in C$_6$D$_6$. 
Figure S11. $^{13}$C ($^1$H) NMR spectrum (101 MHz) of A2 in C$_6$D$_6$.

Figure S12. HMQC NMR spectrum (400 MHz) of A2 in C$_6$D$_6$. 
Figure S13. $^{13}$C DEPT NMR spectrum (101 MHz) of A2 in C$_6$D$_6$.

Figure S14. $^{31}$P NMR spectrum (162 MHz) of A2 in C$_6$D$_6$. 
Figure S15. High resolution mass spectrum of A2

Figure S16. $^1$H NMR spectrum (300 MHz) of 1 in CD$_6$. 
Figure S17. High resolution mass spectrum of 1

Figure S13. $^1$H NMR spectrum (300 MHz) of 2 in C$_6$D$_6$. 
Figure S18. $^{13}$C {$^1$H} NMR spectrum (101 MHz) of 2 in C$_6$D$_6$.

Figure S19. $^{31}$P NMR spectrum (162 MHz) of 2 in C$_6$D$_6$. 
Figure S20. Crude $^1$H NMR spectrum of [d3]-4 in C₆D₆. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 4. (Middle) After 3 h (300 MHz) with tetraethylsilane (internal standard). (Bottom) After 8 h (300 MHz) with tetraethylsilane (internal standard).
Figure S21. $^1$H NMR spectrum (400 MHz) of [d3]-4 in C$_6$D$_6$.

Figure S22. $^{13}$C {$^1$H} NMR spectrum (101 MHz) of [d3]-4 in C$_6$D$_6$. (Top) natural abundance. (Bottom) Labeled.
Figure S23. Crude $^1$H NMR spectrum of [d$_1$]-5 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 5. (Middle) After 3 h (300 MHz) with tetraethylsilane (internal standard). (Bottom) After 8 h (300 MHz) with tetraethylsilane (internal standard).

Figure S24. $^1$H NMR spectrum (400 MHz) of [d$_1$]-5 in C$_6$D$_6$. 

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Figure S25. $^{13}$C {$^1$H} NMR spectrum (101 MHz) of [d$_1$]-5 in C$_6$D$_6$. (Top) natural abundance. (Bottom) Labeled.

Figure S26. Crude $^1$H NMR spectrum of [d$_5$]-6 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 6. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).
**Figure S27.** $^1$H NMR spectrum (400 MHz) of [d$_5$]-6 in C$_6$D$_6$.

**Figure S28.** $^{13}$C {$^1$H} NMR spectrum (101 MHz) of [d$_1$]-6 in C$_6$D$_6$. (Top) natural abundanced. (Bottom) labeled.
**Figure S29.** Crude $^1$H NMR spectrum of [d$_1$]-7 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 7. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).

**Figure S30.** $^1$H NMR spectrum (400 MHz) of [d$_1$]-7 in C$_6$D$_6$. 
Figure S31. $^{13}$C {$^1$H} NMR spectrum (101 MHz) of [d$_1$]-7 in C$_6$D$_6$. (Top) natural abundance. (Bottom) labeled.

Figure S32. Crude $^1$H NMR spectrum of [d$_3$]-8 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 8. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).
Figure S33. $^1$H NMR spectrum (400 MHz) of [d$_8$]-8 in C$_6$D$_6$.

Figure S34. $^{13}$C {$^1$H} NMR spectrum (101 MHz) of [d$_8$]-8 in C$_6$D$_6$. (Top) natural abundance. (Bottom) labeled.
Figure S35. Crude $^1$H NMR spectrum of [d$_2$]-9 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 9. (Middle) After 3 h (300 MHz) with tetraethylsilane (internal standard). (Bottom) After 8 h (300 MHz) with tetraethylsilane (internal standard).

Figure S36. $^1$H NMR spectrum (400 MHz) of [d$_2$]-9 in C$_6$D$_6$. 
Figure S37. $^{13}$C \{H\} NMR spectrum (101 MHz) of [d$_2$]-9 in C$_6$D$_6$. (Top) natural abundance. (Bottom) labeled.

Figure S38. Crude $^1$H NMR spectrum of [d$_5$]-10 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 8. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).
Figure S39. $^1$H NMR spectrum (400 MHz) of [d$_5$]-10 in C$_6$D$_6$.

Figure S40. $^{13}$C {$^1$H} NMR spectrum (101 MHz) of [d$_5$]-10 in C$_6$D$_6$. (Top) natural abundance. (Bottom) labeled ii) Natural abundance
Figure S41. Crude $^1$H NMR spectrum of [d$_3$]-11 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 11. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).

Figure S42. $^1$H NMR spectrum (400 MHz) of [d$_3$]-11 in C$_6$D$_6$. 
Figure S43. $^{13}$C {\textsuperscript{1}H} NMR spectrum (101 MHz) of [d$\text{$_3$}$]-11 in C$_6$D$_6$. (Top) natural abundance. (Bottom) labeled.

Figure S44. Crude $^1$H NMR spectrum of [d$\text{$_2$}$]-12 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 12. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).
Figure S45. $^1$H NMR spectrum (400 MHz) of [d$_2$]-12 in C$_6$D$_6$.

Figure S46. $^{13}$C \{$^1$H\} NMR spectrum (101 MHz) of [d$_2$]-12 in C$_6$D$_6$. (Top) natural abundance. (Bottom) labeled.
Figure S47. Crude $^1$H NMR spectrum of [d₃]-13 in C₆D₆. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 13. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).

Figure S48. $^1$H NMR spectrum (400 MHz) of [d₃]-13 in C₆D₆.
Figure S49. $^{13}$C {$^1$H} NMR spectrum (101 MHz) of [d$_3$]-13 in C$_6$D$_6$. (Top) natural abundance. (Bottom) labeled.

Figure S50. Crude $^1$H NMR spectrum of [d$_1$]-15 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 15. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).
Figure S51. $^1\text{H}$ NMR spectrum (400 MHz) of $[d_1]$-15 in $\text{C}_6\text{D}_6$.

Figure S52. $^{13}\text{C} \{^1\text{H}\}$ NMR spectrum (101 MHz) $[d_1]$-15 in $\text{C}_6\text{D}_6$. (Top) natural abundance. (Bottom) labeled.
**Figure S53.** Crude $^1$H NMR spectrum of [d$_2$]-16 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 16. (Bottom) After 4 h (300 MHz) with tetraethylsilane (internal standard).

**Figure S54.** $^1$H NMR spectrum (400 MHz) of [d$_2$]-16 in C$_6$D$_6$. 
Figure S55. $^{13}$C $\{^1\text{H}\}$ NMR spectrum (101 MHz) of [d$_3$]-16 in C$_6$D$_6$. (Top) natural abundance. (Bottom) labeled.

Figure S56. Crude $^1$H NMR spectrum of [d$_3$]-17 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 17. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).
**Figure S57.** $^1$H NMR spectrum (400 MHz) of [d₃]-17 in C₆D₆.

**Figure S58.** $^{13}$C ($^1$H) NMR spectrum (101 MHz) of [d₃]-17 in C₆D₆. (Top) natural abundance. (Bottom) labeled
Figure S59. Crude $^1$H NMR spectrum of [d$_3$]-18 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 18. (Bottom) After 1.5 h (300 MHz) with tetraethylsilane (internal standard).

Figure S60. $^1$H NMR spectrum (400 MHz) of [d$_3$]-18 in C$_6$D$_6$. 
Figure S61. $^{13}$C {$^{1}$H} NMR spectrum (101 MHz) of [d$_{3}$]-18 in C$_{6}$D$_{6}$. (Top) natural abundance. (Bottom) labeled

Figure S62. Crude $^{1}$H NMR spectrum of [d$_{3}$]-19 in C$_{6}$D$_{6}$. (Top) Natural abundance (400 MHz) $^{1}$H NMR spectrum of 19. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).
Figure S63. $^1$H NMR spectrum (400 MHz) of [d$_2$]-19 in C$_6$D$_6$.

Figure S64. $^{13}$C {${}^1$H} NMR spectrum (101 MHz) of [d$_2$]-19 in C$_6$D$_6$. (Top) natural abundance. (Bottom) labeled
Figure S65. Crude $^1$H NMR spectrum of [d₄]-20 in C₆D₆. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 20. (Bottom) After 3 h (300 MHz) with tetramethylsilane (internal standard).

Figure S66. $^1$H NMR spectrum (400 MHz) [d₄]-20 in C₆D₆.
Figure S67. $^{13}$C $^{1}$H NMR spectrum (101 MHz) of [d4]-20 in CDCl$_3$. (Top) natural abundance. (Bottom) labeled.

Figure S68. Crude $^1$H NMR spectrum of [d7]-21 in C$_6$D$_6$. (Top) Natural abundance (400 MHz) $^1$H NMR spectrum of 21. (Bottom) After 3 h (300 MHz) with tetraethylsilane (internal standard).
Figure S69. $^1$H NMR spectrum (400 MHz) of [d$_7$]-21 in CDCl$_3$.

Figure S70. $^{13}$C {$^1$H} NMR spectrum (101 MHz) of [d$_7$]-21 in CDCl$_3$. (Top) natural abundance. (Bottom) labeled.
Figure S71. $^{19}$F NMR spectrum (188.2 MHz) of [d$_x$]-6 in C$_6$D$_6$. 
Figure S72. $^1$H NMR spectrum (300 MHz) of [d$_6$]-6 in C$_6$D$_6$. 
X-Ray Crystallography

Figure S73. Solid state structure of ligand A1. Ellipsoids are shown at the 30% probability level. Hydrogen atoms and co-crystallized solvent molecules are not shown for clarity.

Special Refinement Details for A1. Compound A1 crystallizes in the orthorhombic space group Pna2₁, with one molecule in the asymmetric unit along with one iodide (I⁻) counter ion. The C20–C21 and C20–C22 distances were refined with the help of enhanced rigid bond restraints on the 1,2- and 1,3-distances. No further special refinement conditions were necessary.
**Figure S74.** Solid state structure of [(PC\textsubscript{NHC}P)FeCl\textsubscript{2}] (1). Ellipsoids are shown at the 30% probability level. Hydrogen atoms and co-crystallized solvent molecules are not shown for clarity.

**Special Refinement Details for 1.** Compound 1 crystallizes in the monoclinic space group P2\(_1\)/c, with one molecule in the asymmetric unit and one co-crystallized toluene molecule. The toluene molecule was refined with the help of enhanced rigid bond restraints on the 1,2- and 1,3-distances, together with restrained C–C (~1.5 Å) bond distances for C32–C38. No further special refinement conditions were necessary.
Figure S75. Solid state structure of [(PC$_{3}$NHC)$_{2}$Fe(H)$_{2}$N$_{2}$] (2). Ellipsoids are shown at the 30% probability level. Hydrogen atoms and co-crystallized solvent molecules are not shown for clarity.

Special Refinement Details for 2. Compound 2 crystallizes in the tetragonal space group I-4, with one molecule in the asymmetric unit. No further special refinement conditions were necessary. However, the crystal was of poor quality and did not further to approximately 1Å, resulting in the CheckCif alerts reported and addressed in the CIF file.
Tables

Table S1. Selected bond angles and distances for A1 and complexes 1 and 2.

| Bond Distances (Å) | M = Fe |
|--------------------|--------|
|                    | A1     | 1      | 2      |
| Fe–C1              | -      | 2.061(6)| 1.828(8)|
| Fe–P1              | -      | 2.766(2)| 2.204(2)|
| Fe–P2              | -      | 2.782(2)| 2.212(2)|
| Fe–H1A             | -      | -      | 1.39(7) |
| Fe–H1B             | -      | -      | 1.64(7) |
| Fe–H1C             | -      | -      | -      |
| Fe–Cl1             | -      | 2.266(2)| -      |
| Fe–Cl1             | -      | 2.291(2)| -      |
| Fe–B1              | -      | -      | -      |
| Fe–N3              | -      | -      | 1.789(8)|

| Bond Angles (°)    |        |
|--------------------|--------|
| NCN                | 106(1) | 102.3(5)| 101.6(6)|
| PCN                | 115.8(8)| 114.7(4)| 106.0(5)|
| NCP                | 116.6(8)| 114.1(4)| 106.3(5)|
| PFeP               | 149.97(6)| 162.1(1)|

Table S2. Crystal and refinement data for A1 and complexes 1 and 2.

|                     | Ligand A1 | Complex 1 | Complex 2 |
|---------------------|-----------|-----------|-----------|
| CCDC                | 1994927   | 1994923   | 1994924   |
| Empirical formula   | C₃₁H₅₁IN₂P₂ | C₃₈H₆₈Cl₂FeN₂P₂ | C₃₁H₅₂FeNaP₂ |
| Formula weight (g/mol) | 640.58   | 730.85   | 598.55   |
| T (K)               | 100(2)    | 100(2)   | 100(2)   |
| Radiation           | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) | CuKα (λ = 1.54184) |
| a (Å)               | 18.189(8) | 12.651(5) | 25.1779(7) |
| b (Å)               | 16.524(9) | 16.879(6) | 25.1779(7) |
| c (Å)               | 11.802(6) | 19.442(8) | 11.7626(5) |
| α (deg)             | 90        | 90       | 90       |
| β (deg)             | 90        | 99.903(12)| 90       |
| γ (deg)             | 90        | 90       | 90       |
| V (Å³)              | 3547(3)   | 4090(3)  | 7456.6(5) |
| Z                   | 4         | 4        | 8        |
| Cryst. syst.        | orthorhombic | monoclinic | tetragonal |
| Space group         | Pna2₁     | P2₁/c    | I-4      |
| ρcalc (g/cm³)       | 1.200     | 1.187    | 1.066    |
| 2σ range (deg)      | 3.33 to 49.15 | 3.216 to 49.346 | 8.296 to 117.814 |
| Crystal size/mm     | 0.270×0.120×0.090 | 0.330×0.150×0.120 | 0.116×0.013×0.012 |
| μ (mm⁻¹)            | 1.012     | 0.600    | 4.213    |
| GOF                 | 0.990     | 0.968    | 0.954    |
| R1, wR₂ (I> 2σ (I))| R₁ = 0.0608, wR₂ = 0.0965 | R₁ = 0.0897, wR₂ = 0.1903 | R₁ = 0.0493, wR₂ = 0.1153 |
Computational Details

The calculations were performed using Gaussian 09 Rev. D.01. Geometry optimization, and frequency calculations of intermediates, transition structures and products were carried out at PBE0-D3/BS1 with dispersion correction GD3b level of theory, where BS1 denotes basis set: SDD with effective core potential (ECP) for Fe and 6-31G(d,p) for other elements. Wave function stability tests were performed using the keyword Stable=opt. Frequency calculations were performed to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and the thermal corrections at 298 K. All transition-state structures were confirmed to connect corresponding reactants and products by intrinsic reaction coordinate (IRC) calculations. Further, single point energies of optimized geometries were calculated at PBE0-D3/BS2 level of theory with the Polarizable Continuum Model (IEFPCM) method in benzene, where BS2 denotes basis set: SDD with ECP for Fe and 6-311+G(2d,2p) for other elements. The quoted energies include zero point, enthalpy, and entropic corrections determined from vibrational frequencies calculated at the PBE0-D3/BS1 level of theory.

![Figure S76](image-url) Plausible mechanistic pathway for H/D exchange at the benzene catalyzed by dideuteride complex 3, via σ-CAM at the equatorial (Path A) and the axial (Path B) position.

**Evaluation of energy barriers of C-H activation step at X-substituted benzenes (X = F, Me, Me₂N).**

In order to evaluate effects of substituents on Gibbs free energies of TS1_R we performed calculations for hydrogen substituted (dihydrides) transition states TS1_R. Specifically in these studies, we have opted to use the dihydride as the model system since, computationally, the only difference between hydrogen and deuterium atoms are in the vibrational modes. As a result, the respective potential energy surfaces (PESs) will be nearly identical except for their relative energies. Typically, PESs that include deuterium are slightly higher in energy (ca. 0.4 kcal/mol).

**The search of lowest energy isomers of R-substituted TS1.**

Possible isomers of TS1_R (R = F, Me, Me₂N, MeO) were found (Fig S77. and Fig S78) and their energies were compared (Table S3. and Table S4.) in order to choose the lowest Gibbs free energy isomers for further comparison (Table S5.).
**Fig S77.** TS1_X isomers (X = F, Me, Me2N).

**Table S3.** Relative energies: electronic, enthalpies and Gibbs free energies of X-substituted isomers relative to the energies of the isomers with the lowest Gibbs free energy (X = F, Me, Me2N).

| X     | [kcal/mol] | TS2_X_o1 | TS2_X_o2 | TS2_X_m1 | TS2_X_m2 | TS2_X_p |
|-------|------------|----------|----------|----------|----------|---------|
| F     | ΔE         | 0.6      | 0.0      | 1.2      | 1.1      | 2.5     |
|       | ΔH         | -0.5     | -1.0     | 0.2      | 0.0      | 1.2     |
|       | ΔG         | 0.3      | 0.6      | 0.8      | 0.0      | 1.5     |
| Me    | ΔE         | 2.3      | 1.9      | -0.5     | -0.5     | 0.0     |
|       | ΔH         | 2.6      | 2.5      | -0.4     | -0.3     | 0.0     |
|       | ΔG         | 5.2      | 5.4      | 1.0      | 0.6      | 0.0     |
| Me2N  | ΔE         | 3.2      | 3.9      | 0.0      | 0.0      | 1.2     |
|       | ΔH         | 3.5      | 3.9      | 0.3      | 0.0      | 1.6     |
|       | ΔG         | 6.1      | 6.8      | 1.2      | 0.0      | 2.3     |

**Fig S78.** Isomers of TS1_OMe_Z.

**Table S4.** Relative energies: electronic, enthalpies and Gibbs free energies of MeO-substituted isomers relative to the energies of the isomers with the lowest Gibbs free energy.

| Z     | p_D | p_U | m1_D | m1_U | m2_D | m2_U | o1_D | o2_U |
|-------|-----|-----|------|------|------|------|------|------|
| ΔE    | 0.8 | 0.7 | -0.3 | -0.5 | -0.9 | 0.0  | 0.3  | 0.2  |
| ΔH    | 0.1 | 0.7 | -0.2 | -0.3 | -0.8 | 0.0  | 0.2  | 0.4  |
| ΔG    | 3.2 | 1.2 | 1.0  | 1.2  | 0.5  | 0.0  | 1.1  | 2.7  |
Table S5. The energies ($\Delta G^\ddagger$) of the rate determining step of H/H exchange reaction relative to starting reagent A, the step of the reaction presented right to the table [kcal/mol].

| X       | Ortho | Meta | Para |
|---------|-------|------|------|
| H       | 25.2  | 25.2 | 25.2 |
| Me      | 30.4  | 25.9 | 25.2 |
| MeO     | 25.6  | 24.5 | 25.7 |
| Me$_2$N | 31.3  | 25.2 | 27.5 |
| F       | 23.9  | 23.6 | 25.1 |

$\Delta G^\ddagger$ & $\frac{L_3Fe}{PhX}$ & $\frac{N_2}{-N_2}$ & A & B

Table S6. Single point electronic energies at PBE0-D3/6-311g+(2d,2p) level of theory in benzene //PBE0-D3/6-31g(d,p) [Hartree]

| Path A | N2   | Ph   | A     | B     |
|--------|------|------|-------|-------|
|        | -109.4363204 | -232.0390742 | -2001.136543 | -1891.654664 |
| C      | -2123.711277  | -2123.698547  | -2123.712904 | -2123.712951  |
| E      | -2123.712904  | -2123.698547  | -2123.711277 |               |
| G      | -1891.654664  | -2001.136543  | -232.0390742 |               |
| Path B |                  |                  |               |       |
| L2B    | -1891.334286   | -1891.332432   | -2123.333455 |       |
| LTS1B  | -2123.320126   | -2123.343286   | -2123.342505 |       |
| L3B    | -1891.334286   | -1891.332432   | -2123.333455 |       |
| R4B    | -2123.343286   | -2123.320126   | -2123.33455  |       |
| RTS2B  | -2123.343286   | -2123.320126   | -2123.33455  |       |
| R3B    | -2123.343286   | -2123.320126   | -2123.33455  |       |
| RTS1B  | -1891.334286   | -1891.332432   | -2123.33455  |       |

Table S7. Single point electronic energies at PBE0-D3/6-311g+(2d,2p) level of theory of TS1-R //PBE0-D3/6-31g(d,p) [Hartree]

| X       | PhF      | TS2_F_m1 | TS2_NMe2_m1 | TS2_Me_m1 | TS2_MeO_m1_U | TS2_MeO_p_D |
|---------|----------|----------|-------------|-----------|--------------|-------------|
| H       | -331.2216457 | -2222.883718 | -2257.555329 | -2162.981396 | -2238.138454 | -2238.136394 |
| Me      | -271.3218005 | -2222.883839 | -2257.555369 | -2162.981374 | -2238.139202 | -2238.136519 |
| MeO     | -365.8959821 | -2222.884705 | -2257.550293 | -2162.97693  | -2238.137697 | -2162.980612 |
| Name       | Energy (Hartree) |
|------------|-----------------|
| PhOMe      | -346.4780305    |
| TS2_F\_o2  | -2222.885656    |
| TS2_NMe2\_o2 | -2257.549181  |
| TS2_Me\_o2  | -2162.977615    |
| TS2_MeO\_o1_D | -2238.137141  |
| TS2_F\_p   | -2222.881639    |
| TS2_NMe2\_p | -2257.553454  |
| TS2_MeO\_m1_D | -2238.138235  |
| TS2_MeO\_o2\_U | -2238.137428 |

**Figure S78.** Calculated charges by natural population analysis (NPA) of H₂ and carbon atoms of aromatic ring in TS1'.

**Geometries of intermediates and transition states involved in Path A and their thermal parameters.**

Name - A  
Zero-point correction= 0.607141 (Hartree/Particle)  
Thermal correction to Energy= 0.644701  
Thermal correction to Enthalpy= 0.645645  
Thermal correction to Gibbs Free Energy= 0.538748  
Sum of electronic and zero-point Energies= -2000.180771  
Sum of electronic and thermal Energies= -2000.143211  
Sum of electronic and thermal Enthalpies= -2000.142267  
Sum of electronic and thermal Free Energies= -2000.249164

Charge = 0  Multiplicity = 1

0 1
26 0.000000 1.282445 -0.000002
0 1
1 0.000169 1.264911 1.550017
1 2.182471 0.952131 -0.013066
15 -2.182472 0.952130 0.013069
7 1.053459 -1.407291 -0.006456
7 -1.053458 -1.407292 0.006463
6 0.000000 -0.559845 0.000004
6 2.333882 -0.906015 -0.026827
6 3.343215 -1.814606 -0.065757
1 4.374032 -1.478624 -0.105235
6 3.067821 -3.233271 -0.065877
6 1.771103 -3.684369 -0.033897
1 1.560628 -4.749316 -0.034552
6 0.697492 -2.764472 -0.007666
6 -0.697491 -2.764473 0.007667
6 -1.771102 -3.684370 0.033893
1 -1.560626 -4.749316 0.034545
6 -3.067820 -3.233273 0.065869
6 -3.343214 -1.814608 0.065750
1 -4.374032 -1.478627 0.105224
6 -2.333882 -0.906016 0.026827
|   |          |          |          |
|---|----------|----------|----------|
| 1 | -0.000170| 1.264889 | -1.550021|
| 6 | -3.205031| 1.457924 | -1.470782|
| 1 | -2.941697| 2.519221 | -1.583407|
| 6 | -3.238634| 1.424162 | 1.472156 |
| 1 | -4.256324| 1.063029 | 1.276288 |
| 6 | 3.238641 | 1.424165 | -1.472147|
| 1 | 2.941693 | 2.519217 | 1.583417 |
| 6 | -3.248466| 2.946736 | 1.592000 |
| 1 | -3.879839| 3.257209 | 2.431634 |
| 1 | -2.235696| 3.318852 | 1.775401 |
| 1 | -3.628655| 3.437104 | 0.689679 |
| 6 | -2.721596| 0.772602 | 2.749791 |
| 1 | -1.676282| 1.048872 | 2.918953 |
| 1 | -3.320161| 1.103418 | 3.606056 |
| 1 | -2.777718| -0.318948| 2.696857 |
| 6 | -4.717642| 1.332527 | -1.325246|
| 1 | -5.205522| 1.670019 | -2.246644|
| 1 | -5.016171| 0.290215 | -1.168990|
| 1 | -5.118658| 1.931706 | -0.503609|
| 6 | -2.709820| 0.717154 | -2.710685|
| 1 | -3.172316| 1.138153 | -3.609944|
| 1 | -1.622872| 0.795382 | -2.800406|
| 1 | -2.977985| -0.344237| -2.659339|
| 6 | 3.248481 | 2.946740 | -1.591985|
| 1 | 3.628667 | 3.437102 | -0.689660|
| 1 | 3.879858 | 3.257213 | -2.431615|
| 1 | 2.235713 | 3.318862 | -1.775390|
| 6 | 2.721606 | 0.772612 | -2.749787|
| 1 | 3.320175 | 1.103430 | -3.606049|
| 1 | 2.777722 | -0.318938| -2.696857|
| 1 | 1.676294 | 1.048887 | -2.918953|
| 6 | 2.709807 | 0.717147 | 2.710690 |
| 1 | 2.977970 | -0.344244| 2.659342 |
| 1 | 3.172300 | 1.138142 | 3.609951 |
| 1 | 1.622859 | 0.795378 | 2.800406 |
| 6 | 4.717636 | 1.332519 | 1.325260 |
| 1 | 5.118658 | 1.931700 | 0.503627 |
| 1 | 5.205513 | 1.670007 | 2.246661 |
| 1 | 5.016163 | 0.290207 | 1.169003 |
| 6 | -4.227351| -4.183134| 0.101456 |
| 1 | -4.840640| -4.025081| 0.996390 |
| 1 | -4.883393| -4.039262| -0.765116|
| 1 | -3.893149| -5.223411| 0.101693 |
| 6 | 4.227352 | -4.183131| -0.101471|
| 1 | 4.883399 | -4.039260| 0.765097 |
| 1 | 3.893151 | -5.223409| -0.101706|
| 1 | 4.840636 | -4.025078| -0.996408 |
| 7 | -0.000003| 3.086819 | -0.000015 |
|   |        |        |        |
|---|--------|--------|--------|
| 7 | -0.00006 | 4.206388 | -0.000023 |

---

**Name - B**

Zero-point correction= 0.597082 (Hartree/Particle)

Thermal correction to Energy= 0.632546

Thermal correction to Enthalpy= 0.633491

Thermal correction to Gibbs Free Energy= 0.532689

Sum of electronic and zero-point Energies= -1890.740880

Sum of electronic and thermal Energies= -1890.705416

Sum of electronic and thermal Enthalpies= -1890.704472

Sum of electronic and thermal Free Energies= -1890.805273

Charge = 0  Multiplicity = 1

0 1

| 26  | -0.000019 | -1.455529 | -0.000175 |
|-----|-----------|-----------|-----------|
| 1   | -0.011961 | -1.626116 | -1.559680 |
| 15  | 2.196261  | -1.156695 | -0.005624 |
| 15  | -2.196359 | -1.156568 | 0.005491  |

| 7   | 1.055161  | 1.198549  | 0.025322  |
|-----|-----------|-----------|-----------|
| 7   | -1.055055 | 1.198608  | -0.025374 |
| 6   | 0.000022  | 0.345379  | 0.000001  |
| 6   | 2.334869  | 0.700899  | 0.060330  |
| 6   | 3.343084  | 1.609512  | 0.122955  |
| 1   | 4.373754  | 1.274762  | 0.174493  |
| 6   | 3.064759  | 3.028295  | 0.128282  |
| 6   | 1.768410  | 3.477023  | 0.071385  |
| 1   | 1.556143  | 4.541704  | 0.071567  |
| 6   | 0.696511  | 2.555739  | 0.021213  |
| 6   | -0.696328 | 2.555782  | -0.021269 |
| 6   | -1.768181 | 3.477120  | -0.071391 |
| 1   | -1.555857 | 4.541789  | -0.071649 |
| 6   | -3.064558 | 3.028465  | -0.128243 |
| 6   | -3.342958 | 1.609698  | -0.122929 |
| 1   | -4.373640 | 1.275000  | -0.174516 |
| 6   | -2.334791 | 0.701028  | -0.060337 |
| 1   | 0.012187  | -1.626864 | 1.559265  |
| 6   | -3.203314 | -1.585366 | 1.527749  |
| 1   | -2.950917 | -2.643430 | 1.686481  |
| 6   | -3.280850 | -1.678691 | -1.415987 |
| 1   | -4.300950 | -1.327756 | -1.215880 |
| 6   | 3.280491  | -1.679050 | 1.415951  |
| 1   | 4.300765  | -1.328634 | 1.215813  |
| 6   | 3.203404  | -1.585408 | -1.527814 |
| 1   | 2.950751  | -2.643365 | -1.686875 |
| 6   | -3.266642 | -3.204410 | -1.482676 |
| 1   | -3.888056 | -3.557932 | -2.312724 |
| 1   | -2.244142 | -3.561162 | -1.651611 |
| 1   | -3.641784 | -3.667616 | -0.563703 |
|   |   |   |   |
|---|---|---|---|
| 6 | -2.791652 | -1.064109 | -2.722650 |
| 1 | -1.741876 | -1.323576 | -2.891862 |
| 1 | -3.391400 | -1.438872 | -3.560003 |
| 1 | -2.871634 | 0.026981  | -2.708086 |
| 6 | -4.715835 | -1.445967 | 1.403065  |
| 1 | -5.192319 | -1.719297 | 2.351394  |
| 1 | -5.000636 | -0.410536 | 1.187987  |
| 1 | -5.140317 | -2.087099 | 0.625767  |
| 6 | -2.671756 | -0.793985 | 2.720605  |
| 1 | -3.111032 | -1.172491 | 3.650075  |
| 1 | -1.582698 | -0.876151 | 2.782945  |
| 1 | -2.937023 | 0.265514  | 2.629821  |
| 6 | 3.265518  | -3.204767 | 1.482832  |
| 1 | 3.640276  | -3.668255 | 0.563841  |
| 1 | 3.886909  | -3.558506 | 2.312803  |
| 1 | 2.242853  | -3.560948 | 1.651962  |
| 6 | 2.791585  | -1.064072 | 2.722536  |
| 1 | 3.391046  | -1.439178 | 3.559942  |
| 1 | 2.872277  | 0.026961  | 2.707895  |
| 1 | 1.741651  | -1.322934 | 2.891714  |
| 6 | 2.672320  | -0.793553 | -2.720536 |
| 1 | 2.937870  | 0.265849  | -2.629467 |
| 1 | 3.111630  | -1.171963 | -3.650029 |
| 1 | 1.583245  | -0.875377 | -2.783050 |
| 6 | 4.715938  | -1.446509 | -1.402653 |
| 1 | 5.139967  | -2.088381 | -0.625719 |
| 1 | 5.192596  | -1.719278 | -2.351057 |
| 1 | 5.001037  | -0.411344 | -1.186686 |
| 6 | 4.221638  | 3.979743  | -0.192683 |
| 1 | -4.815645 | 3.819069  | -1.100165 |
| 1 | -4.896885 | 3.840346  | 0.659877  |
| 1 | -3.886054 | 5.019625  | -0.189685 |
| 6 | 4.221882  | 3.979503  | 0.193003  |
| 1 | 4.898518  | 3.838546  | -0.658183 |
| 1 | 3.886466  | 5.019430  | 0.187706  |
| 1 | 4.814358  | 3.820287  | 1.101754  |

Name - L_3B_
Zero-point correction= 0.699965 (Hartree/Particle)
Thermal correction to Energy= 0.740324
Thermal correction to Enthalpy= 0.741269
Thermal correction to Gibbs Free Energy= 0.630685
Sum of electronic and zero-point Energies= -3262.141876
Sum of electronic and thermal Energies= -3262.101517
Sum of electronic and thermal Enthalpies= -3262.100573
Sum of electronic and thermal Free Energies= -3262.211157

Charge = 0 Multiplicity = 1
0 1
26  0.069015  -0.984175  0.719682
  1 -0.141907  -2.462771  -0.202216
  1  0.250907  -2.156011   1.747448
 15  2.100972 -0.176493   0.893448
 15 -2.120831 -0.947631   0.765293
  7  0.671844   1.596185  -0.434468
  7 -1.371394   1.105979  -0.672297
  6 -0.197906   0.566357  -0.244770
  6  1.942794   1.514265   0.089311
  1  2.726208   2.617080  -0.041364
  1  3.728666   2.620084   0.374591
  6  2.238750   3.805789  -0.702894
  6  0.943979   3.859083  -2.076031
  1  0.559724   4.763579  -1.617201
  6  0.086430   2.746704  -0.984114
  6 -1.258750   2.419415  -1.154151
  6 -2.454833   3.006736  -1.631753
  1 -2.423194   3.996878  -2.076031
  6 -3.647293   2.335204  -1.517992
  6 -3.694080  1.057030  -0.842353
  1 -4.658113   0.593889  -0.655943
  6 -2.558350   0.459404  -0.396823
  6  0.545942  -2.582731  -1.083074
  6  1.589951  -3.494244  -0.930215
  1  1.809543  -3.871455   0.064302
  1 -0.066085  -0.217767   1.969501
  6  0.224696  -2.095961  -2.351159
  6  0.967944  -2.497690  -3.458220
  1  0.727626  -2.108328  -4.443532
  6  2.019717  -3.399277  -3.301942
  1  2.596172  -3.714921  -4.167041
  6  2.329943  -3.899191  -2.038396
  1 -0.597441  -1.396013  -2.462778
  1  3.146560  -4.605943  -1.919241
  6 -2.861493  -0.287125   2.363555
  1 -2.381857  -0.928320   3.114585
  6 -3.310843  -2.286443   0.256070
  1 -4.329652  -1.894539   0.366639
  6  2.762950   0.257209   2.580819
  1  3.729130   0.754070   2.429000
  6  3.614342  -0.849823   0.004008
  1  3.545611  -1.927606   0.200776
  6 -3.120673  -3.478950   1.192064
  1 -3.782066  -4.302516   0.901067
  1 -2.085469  -3.834083   1.152295
  1 -3.336101  -3.226147   2.234968
  6 -3.105871  -2.689284  -1.200723
  1 -2.114169  -3.120544  -1.360546
  1 -3.845284  -3.446338  -1.485651
Name - C
Zero-point correction= 0.700433 (Hartree/Particle)
Thermal correction to Energy= 0.741458
Thermal correction to Enthalpy= 0.742402
Thermal correction to Gibbs Free Energy= 0.628161
Sum of electronic and zero-point Energies= -2122.642078
Sum of electronic and thermal Energies= -2122.601053
Sum of electronic and thermal Enthalpies= -2122.600108
Sum of electronic and thermal Free Energies= -2122.714349

Charge = 0  Multiplicity = 1

0 1
26 0.427206 -0.647958 -0.085971
1 0.547963 -0.803556 1.455464
|   |    |    |    |
|---|----|----|----|
| 1 | 1.179255 | -2.203220 | -0.520361 |
| 15 | -1.368173 | -1.929675 | -0.051776 |
| 15 | 1.809835 | 1.093998 | 0.004490 |
| 7 | -2.170932 | 0.554088 | -0.010725 |
| 7 | -0.644566 | 2.009663 | 0.013872 |
| 6 | -0.818237 | 0.664266 | -0.013433 |
| 6 | -2.755086 | -0.688094 | -0.054307 |
| 6 | -4.112380 | -0.727215 | -0.094569 |
| 1 | -4.626938 | -1.680613 | -0.153733 |
| 6 | -4.891057 | 0.490717 | -0.071792 |
| 6 | -4.261422 | 1.709649 | -0.018024 |
| 1 | -4.842370 | 2.626698 | -0.002721 |
| 6 | -2.849235 | 1.782744 | 0.007063 |
| 6 | -1.840979 | 2.743831 | 0.032471 |
| 6 | -1.704050 | 4.150394 | 0.083970 |
| 1 | -2.593985 | 4.771975 | 0.100164 |
| 6 | -0.456546 | 4.721792 | 0.121676 |
| 6 | 0.724044 | 3.888341 | 0.099488 |
| 1 | 1.699774 | 4.359283 | 0.148724 |
| 6 | 0.625010 | 2.534602 | 0.033017 |
| 6 | 2.258451 | -2.275551 | -0.236412 |
| 6 | 3.209614 | -2.027542 | -1.224805 |
| 1 | 2.884674 | -1.589492 | -2.163766 |
| 1 | 0.407909 | -0.611643 | -1.649357 |
| 6 | 2.636074 | -2.873215 | 0.965810 |
| 6 | 3.974025 | -3.183709 | 1.193544 |
| 1 | 4.273748 | -3.637438 | 2.134010 |
| 6 | 4.931565 | -2.901601 | 0.219845 |
| 1 | 5.976029 | -3.138438 | 0.402483 |
| 6 | 4.549859 | -2.327306 | -0.991153 |
| 1 | 1.882765 | -3.063512 | 1.722861 |
| 1 | 5.295305 | -2.120115 | -1.754047 |
| 6 | 2.952605 | 1.516087 | -1.419786 |
| 1 | 3.577610 | 0.615176 | -1.485813 |
| 6 | 2.839387 | 1.499721 | 1.506109 |
| 1 | 3.240726 | 2.510369 | 1.355432 |
| 6 | -1.866144 | -3.037639 | -1.467112 |
| 1 | -2.860791 | -3.442177 | -1.239514 |
| 6 | -1.743390 | -2.960776 | 1.469490 |
| 1 | -0.828802 | -3.561791 | 1.577226 |
| 6 | 3.989808 | 0.504565 | 1.623482 |
| 1 | 4.614257 | 0.749497 | 2.490112 |
| 1 | 3.603498 | -0.508965 | 1.759620 |
| 1 | 4.634475 | 0.494412 | 0.738979 |
| 6 | 1.977187 | 1.499619 | 2.763182 |
| 1 | 1.483570 | 0.530301 | 2.881595 |
| 1 | 2.599568 | 1.695603 | 3.643882 |
| 1 | 1.199999 | 2.269019 | 2.718397 |
| 6 | 3.864747 | 2.724471 | -1.238891 |
| 1 | 4.509861 | 2.830867 | -2.118699 |
| 1  | 3.285961 | 3.650063 | -1.155611 |
|----|----------|----------|-----------|
| 1  | 4.514976 | 2.642938 | -0.364210 |
| 6  | 2.141702 | 1.633238 | -2.707661 |
| 1  | 2.810457 | 1.686204 | -3.574161 |
| 1  | 1.466716 | 0.780351 | -2.822096 |
| 1  | 1.534094 | 2.545627 | -2.696943 |
| 6  | -0.866930 | -4.187800 | -1.578587 |
| 1  | -0.790668 | -4.773590 | -0.656474 |
| 1  | -1.162480 | -4.870227 | -2.382972 |
| 1  | 0.131861  | -3.807887 | -1.818496 |
| 6  | -1.939987 | -2.244918 | -2.767416 |
| 1  | -2.173961 | -2.915055 | -3.602592 |
| 1  | -2.713778 | -1.472719 | -2.722766 |
| 1  | -0.984598 | -1.748237 | -2.963477 |
| 6  | -1.852549 | -2.048384 | 2.688656 |
| 1  | -2.774422 | -1.457367 | 2.645245 |
| 1  | -1.879775 | -2.646078 | 3.606408 |
| 1  | -1.001642 | -1.362841 | 2.733332 |
| 6  | -2.945883 | -3.893419 | 1.378441 |
| 1  | -2.860183 | -4.627265 | 0.572686 |
| 1  | -3.055991 | -4.447810 | 2.317444 |
| 1  | -3.871972 | -3.327184 | 1.231265 |
| 6  | -0.275956 | 6.208655  | 0.186505  |
| 1  | 0.281027  | 6.500382  | 1.084778  |
| 1  | 0.293413  | 6.576172  | -0.675454 |
| 1  | -1.236744 | 6.728967  | 0.202218  |
| 6  | -6.385787 | 0.380531  | -0.108792 |
| 1  | -6.762179 | -0.192344 | 0.747045  |
| 1  | -6.860704 | 1.364498  | -0.089928 |
| 1  | -6.722077 | -0.139364 | -1.013716 |

Name - D
Zero-point correction= 0.698984 (Hartree/Particle)
Thermal correction to Energy= 0.739941
Thermal correction to Enthalpy= 0.740885
Thermal correction to Gibbs Free Energy= 0.628496
Sum of electronic and zero-point Energies= -2122.641953
Sum of electronic and thermal Energies= -2122.600997
Sum of electronic and thermal Enthalpies= -2122.600052
Sum of electronic and thermal Free Energies= -2122.712442
Charge = 0 Multiplicity = 1

0 1
26 -0.539454 -0.551802 0.360132
1 0.412917 -0.381992 -1.126736
1 -0.984389 -1.147680 1.776884
15 1.193320 -1.893978 0.200342
15 -1.849864 1.203671 0.191186
| 7  | 2.121476 | 0.567241 | 0.220856 |
| 7  | 0.640863 | 2.072671 | 0.140555 |
| 6  | 0.785532 | 0.742461 | 0.345689 |
| 6  | 2.645102 | -0.708897 | 0.174384 |
| 6  | 3.993271 | -0.802429 | 0.031631 |
| 1  | 4.467078 | -1.777995 | -0.000444 |
| 6  | 4.814689 | 0.378004 | -0.111958 |
| 6  | 4.230481 | -0.708897 | 0.174384 |
| 1  | 4.837749 | 2.505349 | -0.327060 |
| 6  | 2.828327 | 1.751483 | -0.039017 |
| 6  | 1.512056 | 3.972509 | -0.478065 |
| 1  | -1.650730 | 4.397312 | -0.486291 |
| 6  | -0.686337 | 3.927509 | -0.322418 |
| 1  | -1.512056 | 4.629210 | -0.478065 |
| 6  | -2.958375 | -2.316466 | 0.828569 |
| 6  | -2.943329 | -1.931330 | 1.850320 |
| 1  | -0.521873 | -0.469147 | 1.971949 |
| 6  | -2.098873 | -2.453251 | -1.375157 |
| 6  | -3.120423 | -3.334526 | -1.728573 |
| 1  | -3.170247 | -3.721864 | -2.744830 |
| 6  | -4.081390 | -3.712519 | -0.793889 |
| 1  | -4.882932 | -4.394854 | -1.063922 |
| 6  | -3.990075 | -3.194178 | 0.494730 |
| 1  | -1.384613 | -2.169797 | -2.146117 |
| 1  | -4.727507 | -3.471350 | 1.245941 |
| 6  | -2.856681 | 1.781874 | 1.661412 |
| 1  | -3.506923 | 0.918044 | 1.859994 |
| 6  | -2.990835 | 1.485487 | -1.249776 |
| 1  | -3.289259 | 2.542085 | -1.212580 |
| 6  | 1.657666 | -3.067025 | 1.567633 |
| 1  | 2.623972 | -3.520253 | 1.311839 |
| 6  | 1.435225 | -2.899488 | -1.354588 |
| 1  | 0.475706 | -3.430492 | -1.425551 |
| 6  | -4.232158 | 0.601608 | -1.124289 |
| 1  | -4.906645 | 0.794997 | -1.965911 |
| 1  | -3.957274 | -0.456297 | -1.141303 |
| 1  | -4.790743 | 0.788593 | -0.202169 |
| 6  | -2.268424 | 1.228574 | -2.567884 |
| 1  | -1.974512 | 0.178436 | -2.639114 |
| 1  | -2.934963 | 1.463182 | -3.405641 |
| 1  | -1.366808 | 1.841113 | -2.666302 |
| 6  | -3.719294 | 3.019394 | 1.436640 |
| 1  | -4.289065 | 3.245817 | 2.345094 |
| 1  | -3.096908 | 3.894464 | 1.220787 |
| 1  | -4.436411 | 2.896501 | 0.621485 |
| 6  | -1.943941 | 1.987593 | 2.868506 |
|   | -2.540937 | 2.202839 | 3.761322 |
|---|-----------|----------|----------|
| 1 | -1.329702 | 1.108373 | 3.075307 |
| 1 | -1.271195 | 2.836959 | 2.704178 |
| 6 | 0.586636  | -4.153709| 1.656667 |
| 1 | 0.523702  | -4.750446| 0.741642 |
| 1 | 0.803616  | -4.834434| 2.487281 |
| 1 | -0.402577 | -3.712766| 1.819249 |
| 6 | 1.812416  | -2.323192| 2.890281 |
| 1 | 2.114572  | -3.021170| 3.678875 |
| 1 | 2.569002  | -1.534866| 2.826943 |
| 1 | 0.868849  | -1.862659| 3.196463 |
| 6 | 1.557333  | -1.978079| -2.565933|
| 1 | 2.515156  | -1.445753| -2.554434|
| 1 | 1.509557  | -2.565848| -3.488951|
| 1 | 0.756220  | -1.234428| -2.580750|
| 6 | 2.573552  | -3.913645| -1.331415|
| 1 | 2.471769  | -4.652539| -0.532657|
| 1 | 2.599680  | -4.459954| -2.281066|
| 1 | 3.545667  | -3.420537| -1.222853|
| 6 | 0.365564  | 6.180450 | -0.783746|
| 1 | -0.215644 | 6.335776 | -1.700235|
| 1 | -0.163602 | 6.702236 | 0.022330 |
| 1 | 1.337589  | 6.661973 | -0.914854|
| 6 | 6.298330  | 0.202743 | -0.238428|
| 1 | 6.549283  | -0.448182| -1.084152|
| 1 | 6.803725  | 1.159909 | -0.387758|
| 1 | 6.719102  | -0.264220| 0.659883 |

Name - Ph
Zero-point correction= 0.101360 (Hartree/Particle)
Thermal correction to Energy= 0.105744
Thermal correction to Enthalpy= 0.106688
Thermal correction to Gibbs Free Energy= 0.073904
Sum of electronic and zero-point Energies= -231.881288
Sum of electronic and thermal Energies= -231.876904
Sum of electronic and thermal Enthalpies= -231.875960
Sum of electronic and thermal Free Energies= -231.908745

Charge = 0 Multiplicity = 1

|   |       |        |        |        |
|---|-------|--------|--------|--------|
| 6 | -1.284202 | -0.538607 | 0.000000 |
| 6 | -1.108517 | 0.842759  | -0.000033|
| 6 | 0.175590  | 1.381326  | 0.000014 |
| 6 | 1.284221  | 0.538561  | -0.000006|
| 6 | 1.108547  | -0.842719 | -0.000016|
| 6 | -0.175639 | -1.381321 | 0.000024 |
| 1 | -2.285771 | -0.958758 | 0.000009 |
| 1 | -1.973248 | 1.499993  | 0.000020 |
|   |   |   |   |
|---|---|---|---|
| 1 | 0.312432 | 2.458815 | 0.000061 |
| 1 | 2.285737 | 0.958838 | 0.000025 |
| 1 | 1.973198 | -1.500058 | -0.000033 |
| 1 | -0.312347 | -2.458826 | 0.000024 |

Name – TS2
Zero-point correction= 0.698883 (Hartree/Particle)
Thermal correction to Energy= 0.739077
Thermal correction to Enthalpy= 0.740022
Thermal correction to Gibbs Free Energy= 0.628994

Sum of electronic and zero-point Energies= -2122.641620
Sum of electronic and thermal Energies= -2122.601425
Sum of electronic and thermal Enthalpies= -2122.600481
Sum of electronic and thermal Free Energies= -2122.711509

1 imaginary frequency.
Charge = 0 Multiplicity = 1

0 1
26 -0.708537 -0.307068 0.365145
1 -0.498521 -0.187442 -1.115872
1 -0.940727 -0.871343 1.856901
15 0.421984 -2.169842 0.169233
15 -1.289449 1.790730 0.157474
7 2.182379 -0.220052 0.301773
7 1.346345 1.719235 0.222014
6 0.997558 0.425427 0.433927
6 2.204475 -1.596016 0.196277
6 3.424177 -2.171545 0.030363
1 3.506353 -3.250369 -0.051224
6 4.620880 -1.369322 0.008163
6 4.527872 0.000462 -0.103815
1 5.414745 0.608979 0.157474
6 3.268903 0.628804 0.039574
6 2.715424 1.907536 -0.023279
6 3.121939 3.232922 -0.303514
1 4.176033 3.448989 -0.447716
6 2.184310 4.226857 -0.436684
6 0.779042 3.913911 -0.314366
1 0.048655 4.689071 -0.523005
6 0.362031 2.662738 0.013104
6 -2.500655 -1.080572 -0.061900
6 -3.528145 -1.202352 0.900528
1 -3.337105 -0.883538 1.926622
1 -1.169848 -0.063031 1.889570
6 -2.867129 -1.522391 -1.352925
6 -4.129049 -2.031227 -1.661919
1 -4.348742 -2.349966 -2.679571
6 -5.110418 -2.124526 -0.678113
1 -6.097192 -2.515471 -0.911565
|   |    |    |    |   |
|---|----|----|----|---|
| 6 | -4.797339 | -1.704038 | 0.611955 |
| 1 | -2.137422 | -1.448241 | -2.158474 |
| 1 | -5.546643 | -1.765076 | 1.399455 |
| 6 | -2.065055 | 2.695174 | 1.603865 |
| 1 | -2.973637 | 2.106960 | 1.796247 |
| 6 | -2.212409 | 2.453453 | -1.313148 |
| 1 | -2.123500 | 3.547592 | -1.274477 |
| 6 | 0.410367  | -3.474949 | 1.495807 |
| 1 | 1.143171  | -4.241684 | 1.213922 |
| 6 | 0.296103  | -3.146205 | -1.417972 |
| 1 | -0.791485 | -3.277202 | -1.506863 |
| 6 | -3.687351 | 2.057905 | -1.230077 |
| 1 | -4.227356 | 2.471815 | -2.088994 |
| 1 | -3.796593 | 0.970121  | -1.247760 |
| 6 | -4.173305 | 2.429427 | -0.322923 |
| 1 | -1.586368 | 1.958301 | -2.612259 |
| 1 | -1.681711 | 0.872183 | -2.686970 |
| 6 | -2.099879 | 2.413801 | -3.466578 |
| 1 | -0.523431 | 2.210789 | -2.676820 |
| 6 | -2.447338 | 4.150063 | 1.352156 |
| 1 | -2.910832 | 4.573011 | 2.250617 |
| 1 | -1.559959 | 4.750471 | 1.133560 |
| 6 | -3.156465 | 4.269379 | 0.529831 |
| 1 | -1.156045 | 2.600288 | 2.828311 |
| 1 | -1.669421 | 2.998885 | 3.709908 |
| 1 | -0.855401 | 1.572873 | 3.048762 |
| 6 | -0.244691 | 3.189423 | 2.677100 |
| 1 | -0.984477 | -4.095374 | 1.565244 |
| 1 | -1.265978 | -4.592224 | 0.631916 |
| 1 | -1.028295 | -4.839249 | 2.368448 |
| 1 | -1.743726 | -3.30291 | 1.759395 |
| 6 | 0.830204  | -2.889965 | 2.840412 |
| 1 | 0.843637  | -3.677798 | 3.601582 |
| 1 | 1.827991  | -2.442570 | 2.796288 |
| 1 | 0.129691  | -2.118867 | 3.176190 |
| 6 | 0.768746  | -2.304204 | -2.600303 |
| 1 | 1.854901  | -2.162321 | -2.569786 |
| 1 | 0.521044  | -2.808976 | -3.540272 |
| 1 | 0.296874  | -1.318206 | -2.597193 |
| 6 | 0.971009  | -4.513709 | -1.423521 |
| 1 | 0.584308  | -5.184000 | -0.652040 |
| 1 | 0.803842  | -4.999534 | -2.391442 |
| 1 | 2.055175  | -4.427171 | -1.293184 |
| 6 | 5.938760  | -2.069564 | -0.224686 |
| 1 | 5.934494  | -2.749265 | -1.084870 |
| 6 | 6.757696  | -1.358969 | -0.359775 |
| 1 | 6.161772  | -2.676475 | 0.660747 |
| 6 | 2.576036  | 5.639145 | -0.752057 |
| 1 | 2.103428  | 5.982302 | -1.679815 |
| 1 | 2.256569  | 6.324640 | 0.041715 |
Name - L_TS1_
Zero-point correction= 0.706342 (Hartree/Particle)
Thermal correction to Energy= 0.751219
Thermal correction to Enthalpy= 0.752163
Thermal correction to Gibbs Free Energy= 0.627416
Sum of electronic and zero-point Energies= -2232.033467
Sum of electronic and thermal Energies= -2231.988591
Sum of electronic and thermal Enthalpies= -2231.987647
Sum of electronic and thermal Free Energies= -2232.112393
1 imaginary frequency.
Charge = 0 Multiplicity = 1

0 1
26 0.151661 -0.609941 0.388369
  1 0.579334 -0.879620 -1.091012
  1 2.302251 -2.733941 -0.479003
  15 1.569614 1.102399 0.514748
  15 -1.634966 -1.889618 0.100017
  7 -0.815058 2.040397 -0.043597
  7 -2.349886 0.605776 -0.249335
  6 -1.022530 0.700579 0.014015
  6 0.437587 2.549058 0.200269
  6 0.564195 3.901570 0.171185
  1 1.524897 4.361080 0.377816
  6 -0.570446 4.748002 -0.121321
  6 -1.801345 4.191545 -0.366264
  1 -2.656280 4.824395 -0.583520
  6 -1.969355 2.787787 -0.325816
  6 -2.981305 1.840614 -0.469029
  6 -4.364079 1.783058 -0.759744
  1 -4.909526 2.704536 -0.938498
  6 -5.009020 0.572547 -0.819583
  6 -4.279485 -0.651849 -0.576961
  1 -4.805352 -1.598326 -0.640952
  6 -2.953499 -0.627919 -0.281152
  6 3.249191 -2.319358 -0.808155
  6 4.299296 -2.145217 0.089420
  1 4.184146 -2.443405 1.127402
  1 -0.104009 -0.532321 1.930911
  6 3.395227 -1.930834 -2.137627
  6 4.592249 -1.367833 -2.570708
  1 4.704914 -1.061173 -3.606797
  6 5.640433 -1.180417 -1.670474
  1 6.571083 -0.731230 -2.005652
  6 5.494254 -1.569439 -0.340743
  1 2.560361 -2.044993 -2.821881
  1 6.310671 -1.424235 0.361228
|   |       |       |        |
|---|-------|-------|--------|
| 6 | -2.376515 | -2.865318 | 1.518439 |
| 1 | -1.529489 | -3.485158 | 1.842812 |
| 6 | -1.800824 | -3.038020 | -1.360315 |
| 1 | -2.818444 | -3.447596 | -1.349119 |
| 6 | 2.387722  | 1.624234  | 2.105546  |
| 1 | 2.902538  | 2.574315  | 1.914634  |
| 6 | 2.904845  | 1.334167  | -0.774128 |
| 1 | 1.842812  | -0.372298 | 0.820077  |
| 7 | 1.131735  | -3.463333 | 1.819388  |
| 7 | 1.737328  | -2.837600 | 2.496038  |
Name – TS1
Zero-point correction=  0.696675 (Hartree/Particle)
Thermal correction to Energy=  0.737227
Thermal correction to Enthalpy=  0.738172
Thermal correction to Gibbs Free Energy=  0.625668
Sum of electronic and zero-point Energies= -2122.630737
Sum of electronic and thermal Energies= -2122.590185
Sum of electronic and thermal Enthalpies= -2122.589241
Sum of electronic and thermal Free Energies= -2122.701745
1 imaginary frequency.
Charge =  0 Multiplicity = 1

0 1
26 -0.531791 -0.578571  0.199853
  1 -0.556515 -0.565113 -1.326749
  1 -1.223230 -1.489274  1.78568
 15  1.199682 -1.953240  0.091716
 15 -1.795005  1.228972  0.055885
  7  2.149099  0.488676  0.110742
  7  0.705508  2.024420  0.047605
  6  0.809648  0.678274  0.150694
  6  2.659761 -0.789096  0.114744
  6  4.013954 -0.902090  0.102975
  1  4.476777 -1.882871  0.127558
  6  4.859411  0.269101  0.052037
  6  4.299184  1.521171  0.011407
  1  4.930335  2.402366 -0.072063
  6  2.893391  1.673353  0.002933
  6  1.937992  2.688142 -0.049878
  6  1.875455  4.093928 -0.190004
  1  2.796429  4.665481 -0.250134
  6  0.659142  4.725684 -0.270057
  6 -0.562970  3.956783 -0.211648
  1 -1.511799  4.470707 -0.322354
  6 -0.537210  2.608461 -0.043307
  6 -2.177766 -1.892181  0.167829
  6 -3.317822 -1.839805  0.989903
  1 -3.285689 -1.225302  1.889344
  1 -0.593547 -0.663149  1.765811
  6 -2.259921 -2.759403 -0.939785
  6 -3.422702 -3.463471 -1.238828
  1 -3.453875 -4.095216 -2.123821
  6 -4.548555 -3.357173 -0.422162
  1 -5.455195 -3.907216 -0.658397
  6 -4.485498 -2.546898  0.705460
  1 -1.412891 -2.839421 -1.612530
  1 -5.343696 -2.463970  1.368244
  6 -2.873656  1.771416  1.487083
|   |        |        |        |
|---|--------|--------|--------|
| 1 | -3.541849 | 0.909309 | 1.614241 |
| 6 | -2.845406 | 1.591514 | -1.439218 |
| 1 | -3.212226 | 2.620051 | -1.324197 |
| 6 | 1.616187  | -3.114514 | 1.486747 |
| 1 | 2.594271  | -3.561853 | 1.268418 |
| 6 | 1.521529  | -2.982424 | -1.439723 |
| 1 | 0.603322  | -3.580903 | -1.516244 |
| 6 | -4.031308 | 0.629658  | -1.484047 |
| 1 | -4.669621 | 0.866325  | -2.342702 |
| 1 | -3.686609 | -0.403237 | -1.586343 |
| 1 | -4.650029 | 0.681204  | -0.582882 |
| 6 | -2.023151 | 1.512900  | -2.720463 |
| 1 | -1.600072 | 0.511538  | -2.838988 |
| 1 | -2.660695 | 1.733975  | -3.584032 |
| 1 | -1.195326 | 2.228906  | -2.716167 |
| 6 | -3.724202 | 3.017993  | 1.271458 |
| 1 | -4.329622 | 3.209662  | 2.164732 |
| 1 | -3.098772 | 3.902801  | 1.113349 |
| 1 | -4.410086 | 2.922904  | 0.425709 |
| 6 | -2.017009 | 1.903493  | 2.743864 |
| 1 | -2.653447 | 2.048827  | 3.623615 |
| 1 | -1.400192 | 1.013864  | 2.897847 |
| 1 | -1.349802 | 2.769678  | 2.666393 |
| 6 | 0.555959  | -4.213075 | 1.543900 |
| 1 | 0.519273  | -4.805312 | 0.624033 |
| 1 | 0.762812  | -4.897420 | 2.373966 |
| 1 | -0.440055 | -3.784913 | 1.697952 |
| 6 | 1.713436  | -2.360773 | 2.808920 |
| 1 | 1.951459  | -3.058427 | 3.619771 |
| 1 | 2.494482  | -1.594803 | 2.779026 |
| 1 | 0.767705  | -1.864082 | 3.043211 |
| 6 | 1.602334  | -2.073210 | -2.662938 |
| 1 | 2.522984  | -1.478733 | -2.640384 |
| 1 | 1.612351  | -2.672840 | -3.579570 |
| 1 | 0.752935  | -1.385173 | -2.694430 |
| 6 | 2.715634  | -3.928768 | -1.383212 |
| 1 | 2.648486  | -4.653555 | -0.567703 |
| 1 | 2.780318  | -4.494382 | -2.319620 |
| 1 | 3.654740  | -3.375574 | -1.278855 |
| 6 | 0.557201  | 6.212762  | -0.431715 |
| 1 | 0.013508  | 6.474334  | -1.347137 |
| 1 | 0.010972  | 6.665054  | 0.404432 |
| 1 | 1.544092  | 6.679210  | -0.480764 |
| 6 | 6.346026  | 0.074105  | 0.050996 |
| 1 | 6.663903  | -0.543782 | -0.797108 |
| 1 | 6.875087  | 1.028187  | -0.010272 |
| 1 | 6.678358  | -0.438093 | 0.961674 |
|   | x   | y   | z   |
|---|-----|-----|-----|
| 26 | -0.000382 | -0.810256 | 0.338502 |
| 1  | -0.279832  | -1.362509  | -1.024467  |
| 1  | 0.022647   | -1.615439  | 1.602116   |
| 15 | 2.181157   | -0.491793  | 0.352445   |
| 15 | -2.197844  | -0.457761  | 0.345398   |
| 7  | 1.080880   | 1.785631   | -0.353588  |
| 7  | -1.028643  | 1.773684   | -0.465240  |
| 6  | 0.023205   | 0.935473   | -0.311248  |
| 6  | 2.328712   | 1.338850   | 0.024505   |
| 6  | 3.315018   | 2.271108   | 0.096463   |
| 1  | 4.310193   | 1.979350   | 0.416037   |
| 6  | 3.057905   | 3.657694   | -0.213510  |
| 6  | 1.782704   | 4.066553   | -0.516895  |
| 1  | 1.571178   | 5.114659   | -0.704652  |
| 6  | 0.723913   | 3.130024   | -0.536181  |
| 6  | -0.666866  | 3.121180   | -0.626360  |
| 6  | -1.728789  | 4.036119   | -0.805591  |
| 1  | -1.506171  | 5.082062   | -0.992704  |
| 6  | -3.029503  | 3.604696   | -0.722752  |
| 6  | -3.309919  | 2.227744   | -0.390636  |
| 1  | -4.341378  | 1.926507   | -0.243876  |
| 6  | -2.309813  | 1.320378   | -0.231154  |
| 6  | 0.017303   | -2.712243  | -0.439015  |
| 6  | -0.721198  | -3.690823  | 0.270096   |
| 1  | -1.309020  | -3.382745  | 1.128496   |
| 1  | 0.060267   | 0.035767   | 1.573194   |
| 6  | 0.754029   | -3.217094  | -1.530490  |
| 6  | 0.807034   | -4.572241  | -1.857744  |
| 1  | 1.400981   | -4.891142  | -2.711422  |
| 6  | 0.091457   | -5.503577  | -1.116878  |
| 1  | 0.125975   | -6.560623  | -1.364646  |
| 6  | -0.682115  | -5.043645  | -0.052089  |
| 1  | 1.282662   | -2.521664  | -2.173977  |
| 1  | -1.252584  | -5.748200  | 0.549453   |
| 6  | -3.146623  | -0.465769  | 1.957718   |
| 1  | -3.083154  | -1.525972  | 2.243425   |
| 6  | -3.409094  | -1.211892  | -0.865573  |
| 1  | -4.278137  | -0.539770  | -0.856326  |
|     |         |         |         |         |         |
|-----|---------|---------|---------|---------|---------|
| 6   | 3.146559| -0.745129| 1.918218|
| 1   | 4.166902| -0.378600| 1.748478|
| 6   | 3.321364| -1.151532| -0.979885|
| 1   | 3.092477| -2.224220| -0.995184|
| 6   | -3.869460| -2.613006| -0.472688|
| 1   | -4.648740| -2.949830| -1.165722|
| 1   | -3.041965| -3.324205| -0.525894|
| 1   | -4.287386| -2.652733| 0.537751|
| 6   | -2.815350| -1.204076| -2.271602|
| 1   | -1.962157| -1.885703| -2.336891|
| 1   | -3.568953| -1.534327| -2.995425|
| 1   | -2.477472| -0.205617| -2.566561|
| 6   | -4.614081| -0.055348| 1.894471|
| 1   | -5.086380| -0.225457| 2.868559|
| 1   | -4.709131| 1.012904| 1.676641|
| 1   | -5.188099| -0.613082| 1.149969|
| 6   | -2.403422| 0.349876| 3.011065|
| 1   | -2.901055| 0.250672| 3.982167|
| 1   | -1.367751| 0.017928| 3.105923|
| 1   | -2.397000| 1.413301| 2.744695|
| 6   | 3.178266| -2.246871| 2.202455|
| 1   | 3.678632| -2.812483| 1.409956|
| 1   | 3.707245| -2.444245| 3.141244|
| 1   | 2.156790| -2.631535| 2.290333|
| 6   | 2.534232| 0.024538| 3.082560|
| 1   | 3.127747| -0.140940| 3.988937|
| 1   | 2.502595| 1.100928| 2.886960|
| 1   | 1.511507| -0.314807| 3.268141|
| 6   | 2.913968| -0.543335| -2.323008|
| 1   | 3.268360| 0.490537| -2.396749|
| 1   | 3.356626| -1.109459| -3.149747|
| 1   | 1.827668| -0.529357| -2.456274|
| 6   | 4.815709| -0.965787| -0.742912|
| 1   | 5.171087| -1.484706| 0.151012|
| 1   | 5.375764| -1.363497| -1.597122|
| 1   | 5.076751| 0.094346| -0.653382|
| 6   | 4.201018| 4.626081| -0.158277|
| 1   | 4.979655| 4.360537| -0.882966|
| 1   | 3.873526| 5.645735| -0.374984|
| 1   | 4.672112| 4.624623| 0.831648|
| 6   | -4.182757| 4.542299| -0.918527|
| 1   | -4.832288| 4.561526| -0.035471|
| 1   | -3.841374| 5.562725| -1.108694|
| 1   | -4.805171| 4.232046| -1.766125|

Name - N2_
Zero-point correction= 0.005689 (Hartree/Particle)
Thermal correction to Energy= 0.008049
Thermal correction to Enthalpy= 0.008993
Thermal correction to Gibbs Free Energy= -0.012756
Sum of electronic and zero-point Energies= -109.394943
Sum of electronic and thermal Energies= -109.392583
Sum of electronic and thermal Enthalpies= -109.391639
Sum of electronic and thermal Free Energies= -109.413388

Charge =  0 Multiplicity = 1
0 1
7  0.000000  0.000000  0.551304
7  0.000000  0.000000  -0.551304

Name - H
Zero-point correction= 0.609246 (Hartree/Particle)
Thermal correction to Energy= 0.646573
Thermal correction to Enthalpy= 0.647517
Thermal correction to Gibbs Free Energy= 0.540986
Sum of electronic and zero-point Energies= -2000.178666
Sum of electronic and thermal Energies= -2000.141339
Sum of electronic and thermal Enthalpies= -2000.140395
Sum of electronic and thermal Free Energies= -2000.246926

Charge =  0 Multiplicity = 1
0 1
26 0.000000 1.282445 -0.000002
1  0.000169 1.264911  1.550017
15 2.182471 0.952131 -0.013066
15 -2.182472 0.952130  0.013069
7  1.053459 -1.407291 -0.006456
7  -1.053458 -1.407292  0.006463
6  0.000000 -0.559845  0.000004
6  2.333882 -0.906015 -0.026827
6  3.343215 -1.814606 -0.065757
1  4.374032 -1.478624 -0.105235
6  3.067821 -3.233271 -0.065877
6  1.771103 -3.684369 -0.033897
1  1.560628 -4.749316 -0.034552
6  0.697492 -2.764472 -0.007666
6  -0.697491 -2.764473  0.007667
6  -1.771102 -3.684370  0.033893
1 -1.560626 -4.749316  0.034545
6 -3.067820 -3.233273  0.065869
6 -3.343214 -1.814608  0.065750
1 -4.374032 -1.478627  0.105224
6 -2.333882 -0.906016  0.026827
1 -0.000170  1.264889 -1.550021
6 -3.205031  1.457924 -1.470782
1 -2.941697  2.519221 -1.583407
|    |       |       |       |
|----|-------|-------|-------|
| 6  | -3.238634 | 1.424162 | 1.472156 |
| 1  | -4.256324  | 1.063029  | 1.276288  |
| 6  | 3.238641   | 1.424165  | -1.472147 |
| 1  | 4.256329   | 1.063027  | -1.276277 |
| 6  | 3.205024   | 1.457920  | 1.470790  |
| 1  | 2.941693   | 2.519217  | 1.583417  |
| 6  | -3.248466  | 2.946736  | -1.592000 |
| 1  | -1.676282  | 1.048872  | 2.918953  |
| 1  | -3.320161  | 1.103418  | 3.606056  |
| 1  | -2.777718  | -0.318948 | 2.696857  |
| 6  | -4.717642  | 1.332527  | -1.325246 |
| 1  | -5.205522  | 1.670019  | -2.246644 |
| 1  | -5.016171  | 0.290215  | -1.168990 |
| 1  | -5.118658  | 1.931706  | -0.503609 |
| 6  | -2.709820  | 0.717154  | -2.710685 |
| 1  | -3.172316  | 1.138153  | -3.609944 |
| 1  | -1.622872  | 0.795382  | -2.800406 |
| 1  | -2.977985  | -0.344237 | -2.659339 |
| 6  | 3.248481   | 2.946740  | -1.591985 |
| 1  | 3.628667   | 3.437102  | -0.689660 |
| 1  | 3.879858   | 3.257213  | -2.431615 |
| 1  | 2.235713   | 3.18862   | -1.775390 |
| 6  | 2.721606   | 0.772612  | -2.749787 |
| 1  | 3.320175   | 1.103430  | -3.606049 |
| 1  | 2.777722   | -0.318938 | -2.696857 |
| 1  | 1.676294   | 1.048887  | -2.918953 |
| 6  | 2.709807   | 0.717147  | 2.710690  |
| 1  | 2.977970   | -0.344244 | 2.659342  |
| 1  | 3.172300   | 1.138142  | 3.609951  |
| 1  | 1.622859   | 0.795378  | 2.800406  |
| 6  | 4.717636   | 1.332519  | 1.325260  |
| 1  | 5.118658   | 1.931700  | 0.503627  |
| 1  | 5.205513   | 1.670007  | 2.246661  |
| 1  | 5.016163   | 0.290207  | 1.169003  |
| 6  | -4.227351  | -4.183134 | 0.101456  |
| 1  | -4.840640  | -4.025081 | 0.996390  |
| 1  | -4.883393  | -4.039262 | -0.765116 |
| 1  | -3.893149  | -5.223411 | 0.101693  |
| 6  | 4.227352   | -4.183131 | -0.101471 |
| 1  | 4.883399   | -4.039260 | 0.765097  |
| 1  | 3.893151   | -5.223409 | -0.101706 |
| 1  | 4.840636   | -4.025078 | -0.996408 |
| 7  | -0.000003  | 3.086819  | -0.000015 |
| 7  | -0.000006  | 4.206388  | -0.000023 |
Name - G

Zero-point correction= 0.599034 (Hartree/Particle)
Thermal correction to Energy= 0.634262
Thermal correction to Enthalpy= 0.635206
Thermal correction to Gibb's Free Energy= 0.534816
Sum of electronic and zero-point Energies= -1890.738928
Sum of electronic and thermal Energies= -1890.703701
Sum of electronic and thermal Enthalpies= -1890.702756
Sum of electronic and thermal Free Energies= -1890.803146

Charge = 0  Multiplicity = 1

| 0  | 1 |
|----|---|
| 26 | -0.000019 | -1.455529 | -0.000175 |
| 1  | -0.011961  | -1.626116 | -1.559680 |
| 15 |  2.196261  | -1.156695 | -0.005624 |
| 15 | -2.196359  | -1.156568 |  0.005491 |
|  7 |  1.055161  |  1.198549 |  0.025322 |
|  7 | -1.055055  |  1.198608 | -0.025374 |
|  6 |  0.000022  |  0.345379 |  0.000001 |
|  6 |  2.334869  |  0.700899 |  0.060330 |
|  6 |  3.343084  |  1.609512 |  0.122955 |
|  1 |  4.373754  |  1.274762 |  0.174493 |
|  6 |  3.064759  |  3.028295 |  0.128282 |
|  6 |  1.768410  |  3.477023 |  0.071385 |
|  1 |  1.556143  |  4.541704 |  0.071567 |
|  6 |  0.696511  |  2.555739 |  0.021213 |
|  6 | -0.696328  |  2.555782 | -0.021269 |
|  6 | -1.768181  |  3.477120 | -0.071391 |
|  1 | -1.555857  |  4.541789 | -0.071649 |
|  6 | -3.064558  |  3.028465 | -0.128243 |
|  6 | -3.342958  |  1.609698 | -0.122929 |
|  1 | -4.373640  |  1.275000 | -0.174516 |
|  6 | -2.334791  |  0.701028 | -0.060337 |
|  1 |  0.012187  | -1.626864 |  1.559265 |
|  6 | -3.203314  | -1.585366 |  1.527749 |
|  1 | -2.950917  | -2.643430 |  1.686481 |
|  6 | -3.280850  | -1.678691 | -1.415987 |
|  1 | -4.300950  | -1.327756 | -1.215880 |
|  6 |  3.280491  | -1.679050 |  1.415951 |
|  1 |  4.300765  | -1.328634 |  1.215813 |
|  6 |  3.203404  | -1.585408 | -1.527814 |
|  1 |  2.950751  | -2.643365 | -1.686875 |
|  6 | -3.266642  | -3.204410 | -1.482676 |
|  1 | -3.888056  | -3.557932 | -2.312724 |
|  1 | -2.244142  | -3.561162 | -1.651611 |
|  1 | -3.641784  | -3.667616 | -0.563703 |
|  6 | -2.791652  | -1.064109 | -2.722650 |
|  1 | -1.741876  | -1.323576 | -2.891862 |
|  1 | -3.391400  | -1.438872 | -3.560003 |
|   |       |       |       |
|---|-------|-------|-------|
| 1 | -2.871634 | 0.026981 | -2.708086 |
| 6 | -4.715835 | -1.445967 | 1.403065 |
| 1 | -5.192319 | -1.719297 | 2.351394 |
| 1 | -5.000636 | -0.410536 | 1.187987 |
| 1 | -5.140317 | -2.087099 | 0.625767 |
| 6 | -2.671756 | -0.793985 | 2.720605 |
| 1 | -3.111032 | -1.172491 | 3.650075 |
| 1 | -1.582698 | -0.876151 | 2.782945 |
| 1 | -2.937023 | 0.265514   | 2.629821 |
| 6 | 3.265518  | -3.204767 | 1.482832 |
| 1 | 3.640276  | -3.668255 | 0.563841 |
| 1 | 3.886909  | -3.558506 | 2.312803 |
| 1 | 2.242853  | -3.560948 | 1.651962 |
| 6 | 2.791585  | -1.064072 | 2.722536 |
| 1 | 3.391046  | -1.439178 | 3.559942 |
| 1 | 2.872277  | 0.026961  | 2.707895 |
| 1 | 1.741651  | -1.322934 | 2.891714 |
| 6 | 2.672320  | -0.793553 | -2.720536|
| 1 | 2.937870  | 0.265849  | -2.629467|
| 1 | 3.111630  | -1.171963 | -3.650029|
| 1 | 1.583245  | -0.875377 | -2.783050|
| 6 | 4.715938  | -1.446509 | -1.402653|
| 1 | 5.139967  | -2.088381 | -0.625719 |
| 1 | 5.192596  | -1.719278 | -2.351057 |
| 1 | 5.001037  | -0.411344 | -1.186686 |
| 6 | -4.221638 | 3.979743  | -0.192683 |
| 1 | -4.815645 | 3.819069  | -1.100165 |
| 1 | -4.896885 | 3.840346  | 0.659877  |
| 1 | -3.886054 | 5.019625  | -0.189685 |
| 6 | 4.221882  | 3.979503  | 0.193003  |
| 1 | 4.898518  | 3.838546  | -0.658183 |
| 1 | 3.886466  | 5.019430  | 0.187706  |
| 1 | 4.814358  | 3.820287  | 1.101754  |

Name - F
Zero-point correction= 0.699256 (Hartree/Particle)
Thermal correction to Energy= 0.740161
Thermal correction to Enthalpy= 0.741105
Thermal correction to Gibbs Free Energy= 0.627056
Sum of electronic and zero-point Energies= -2122.643254
Sum of electronic and thermal Energies= -2122.602350
Sum of electronic and thermal Enthalpies= -2122.601406
Sum of electronic and thermal Free Energies= -2122.715454

Charge = 0 Multiplicity = 1
0 1
26  0.427206 -0.647958 -0.085971
1   0.547963 -0.803556  1.455464
|   | 1.179255 | -2.203220 | -0.520361 |
|---|----------|-----------|-----------|
| 15| -1.368173 | -1.929675 | -0.051776 |
| 15| 1.809835 | 1.093998  | 0.004490  |
| 7 | -2.170932 | 0.554088  | -0.010725 |
| 7 | -0.644566 | 2.009663  | 0.013872  |
| 6 | -0.818237 | 0.664266  | -0.013433 |
| 6 | -2.755086 | -0.688094 | -0.054307 |
| 6 | -4.112380 | -0.727215 | -0.094569 |
| 1 | -4.626938 | -1.680613 | -0.153733 |
| 6 | -4.891057 | 0.490717  | -0.071792 |
| 6 | -4.261422 | 1.709649  | -0.018024 |
| 1 | -4.842370 | 2.626698  | -0.002721 |
| 6 | -2.849235 | 1.782744  | 0.007063  |
| 6 | -1.840979 | 2.743831  | 0.032471  |
| 6 | -1.704050 | 4.150394  | 0.083970  |
| 1 | -2.593985 | 4.771975  | 0.100164  |
| 6 | -0.456546 | 4.721792  | 0.121676  |
| 6 | 0.724044  | 3.888341  | 0.099488  |
| 1 | 1.699774  | 4.359283  | 0.148724  |
| 6 | 0.625010  | 2.534602  | 0.033017  |
| 6 | 2.258451  | -2.275551 | -0.236412 |
| 6 | 3.209614  | -2.027542 | -1.224805 |
| 1 | 2.884674  | -1.589492 | -2.163766 |
| 1 | 0.407909  | -0.611643 | -1.649357 |
| 6 | 2.636074  | -2.873215 | 0.965810  |
| 6 | 3.974025  | -3.183709 | 1.193544  |
| 1 | 4.273748  | -3.637438 | 2.134010  |
| 6 | 4.931565  | -2.901601 | 0.219845  |
| 1 | 5.976029  | -3.138438 | 0.402483  |
| 6 | 4.549859  | -2.327306 | -0.991153 |
| 1 | 1.882765  | -3.063512 | 1.722861  |
| 1 | 5.295305  | -2.120115 | -1.754047 |
| 6 | 2.952605  | 1.516087  | -1.419786 |
| 1 | 3.577610  | 0.615176  | -1.485813 |
| 6 | 2.839387  | 1.499721  | 1.506109  |
| 1 | 3.240726  | 2.510369  | 1.355432  |
| 6 | -1.866144 | -3.037639 | -1.467112 |
| 1 | -2.860791 | -3.442177 | -1.239514 |
| 6 | -1.743390 | -2.960776 | 1.469490  |
| 1 | -0.828802 | -3.561791 | 1.577226  |
| 6 | 3.989808  | 0.504565  | 1.623482  |
| 1 | 4.614257  | 0.749497  | 2.490112  |
| 1 | 3.603498  | -0.508965 | 1.759620  |
| 1 | 4.634475  | 0.494412  | 0.738979  |
| 6 | 1.977187  | 1.496199  | 2.763182  |
| 1 | 1.483570  | 0.530301  | 2.881595  |
| 1 | 2.599568  | 1.695603  | 3.643882  |
| 1 | 1.199999  | 2.269019  | 2.718397  |
| 6 | 3.864747  | 2.724471  | -1.238891 |
| 1 | 4.509861  | 2.830867  | -2.118699 |
Name - E
Zero-point correction=          0.698964 (Hartree/Particle)
Thermal correction to Energy=       0.739916
Thermal correction to Enthalpy=      0.740860
Thermal correction to Gibbs Free Energy= 0.628470
Sum of electronic and zero-point Energies=     -2122.641973
Sum of electronic and thermal Energies=    -2122.601021
Sum of electronic and thermal Enthalpies=  -2122.600077
Sum of electronic and thermal Free Energies=  -2122.712467

Charge =  0 Multiplicity = 1

0 1
26  -0.539454   -0.551802    0.360132
  -0.412917   -0.381992   -1.126736
  -0.984389   -1.147680    1.776884
15   1.193320   -1.893978    0.200342
  -1.849864    1.203671    0.191186
|   |         |         |         |         |
|---|---------|---------|---------|---------|
| 7 | 2.121476 | 0.567241 | 0.220856 |         |
| 7 | 0.640863 | 2.072671 | 0.140555 |         |
| 6 | 0.785532 | 0.742461 | 0.345689 |         |
| 6 | 2.645102 | -0.708897 | 0.174384 |         |
| 6 | 3.993271 | -0.802429 | 0.031631 |         |
| 1 | 4.467078 | -1.777995 | 0.000444 |         |
| 6 | 4.814689 | 0.378004 | -0.111958 |         |
| 6 | 4.230481 | 1.619480 | -0.000444 |         |
| 1 | 4.837749 | 2.505349 | -0.375308 |         |
| 6 | 2.828327 | 1.751483 | -0.039017 |         |
| 6 | 1.849213 | 2.743904 | -0.103040 |         |
| 6 | 1.746477 | 4.127878 | -0.375308 |         |
| 1 | 2.649521 | 4.709668 | -0.531986 |         |
| 6 | 0.511925 | 4.719988 | -0.478065 |         |
| 6 | -0.686337 | 3.927509 | -0.322418 |         |
| 1 | -1.650730 | 4.397312 | -0.486291 |         |
| 6 | -0.622299 | 2.606064 | -0.011583 |         |
| 6 | -1.964139 | -1.893872 | -0.083796 |         |
| 6 | -2.958375 | -2.316466 | 0.828569 |         |
| 1 | -2.943329 | -1.931330 | 1.850320 |         |
| 6 | -0.521873 | -0.469147 | 1.971949 |         |
| 6 | -2.098873 | -2.453251 | -1.375157 |         |
| 6 | -3.120423 | -3.334526 | -1.728573 |         |
| 1 | -3.170247 | -3.721864 | -2.744830 |         |
| 6 | -4.081390 | -3.712519 | -0.793889 |         |
| 1 | -4.882932 | -4.394854 | -1.063922 |         |
| 6 | -3.990075 | -3.194178 | 0.494730 |         |
| 1 | -1.384613 | -2.169797 | -2.146117 |         |
| 1 | -4.727507 | -3.471350 | 1.245941 |         |
| 6 | -2.856681 | 1.781874 | 1.661412 |         |
| 1 | -3.506923 | 0.918044 | 1.859994 |         |
| 6 | -2.990835 | 1.485487 | -1.249776 |         |
| 1 | -3.289259 | 2.542085 | -1.212580 |         |
| 6 | 1.657666 | -3.067025 | 1.567633 |         |
| 1 | 2.623972 | -3.520253 | 1.311839 |         |
| 6 | 1.435225 | -2.899488 | -1.354588 |         |
| 1 | 0.475706 | -3.430492 | -1.425551 |         |
| 6 | -4.232158 | 0.601608 | -1.124289 |         |
| 1 | -4.906645 | 0.794997 | -1.965911 |         |
| 1 | -3.957274 | -0.456297 | -1.141303 |         |
| 1 | -4.790743 | 0.788593 | -0.202169 |         |
| 6 | -2.268424 | 1.228574 | -2.567884 |         |
| 1 | -1.974512 | 0.178436 | -2.639114 |         |
| 1 | -2.934963 | 1.463182 | -3.405641 |         |
| 1 | -1.366808 | 1.841113 | -2.666302 |         |
| 6 | -3.719294 | 3.019394 | 1.436640 |         |
| 1 | -4.259065 | 3.245817 | 2.345094 |         |
| 1 | -3.096908 | 3.894464 | 1.220787 |         |
| 1 | -4.436411 | 2.896501 | 0.621485 |         |
| 6 | -1.943941 | 1.987593 | 2.868506 |         |
1  -2.540937  2.202839  3.761322
1  -1.329702  1.108373  3.075307
1  -1.271195  2.836959  2.704178
6   0.586636  -4.153709  1.656667
1   0.523702  -4.750446  0.741642
1   0.803616  -4.834434  2.487281
1  -0.402577  -3.712766  1.819249
6   1.812416  -2.323192  2.890281
1   2.114572  -3.021170  3.678875
1   2.569002  -1.534866  2.826943
1   0.868849  -1.862659  3.196463
6   1.557333  -1.978079  2.569333
1   2.515156  -1.445753  2.554434
1   1.509557  -2.565848  -3.489511
1   0.756220  -1.234428  -2.580750
6   2.573552  -3.913645  -1.331415
1   2.471769  -4.652539  -0.532657
1   2.596480  -4.459954  -2.281066
1   3.545667  -3.420537  -1.222853
6   0.365564   6.180450  -0.783746
1  -0.215644   6.335776  -1.700235
1  -0.163602   6.702236   0.022330
1   1.337589   6.661973  -0.914854
6   6.298330   0.202743  -0.238428
1   6.549283  -0.448182  -1.084152
1   6.803725   1.159909  -0.387758
1   6.719102  -0.264220   0.659883

Name - R_Ph_
Zero-point correction=  0.098073 (Hartree/Particle)
Thermal correction to Energy=   0.102586
Thermal correction to Enthalpy=   0.103530
Thermal correction to Gibbs Free Energy=  0.070498
Sum of electronic and zero-point Energies=  -231.884576
Sum of electronic and thermal Energies=  -231.880062
Sum of electronic and thermal Enthalpies=  -231.879118
Sum of electronic and thermal Free Energies=  -231.912151

Charge =  0 Multiplicity = 1
Name - R_Ts1_
Zero-point correction= 0.705033 (Hartree/Particle)
Thermal correction to Energy= 0.749812
Thermal correction to Enthalpy= 0.750756
Thermal correction to Gibbs Free Energy= 0.626153
Sum of electronic and zero-point Energies= -2232.034776
Sum of electronic and thermal Energies= -2231.989998
Sum of electronic and thermal Enthalpies= -2231.989054
Sum of electronic and thermal Free Energies= -2232.113656
1 imaginary frequency.
Charge = 0 Multiplicity = 1
0 1
26 0.151661 -0.609941 0.388369
1 0.579334 -0.879620 -1.091012
1 2.302251 -2.733941 -0.479003
15 1.569614 1.102399 0.514748
15 -1.634966 -1.889618 0.100017
7 -0.815058 2.040397 -0.043597
7 -2.349886 0.605776 -0.249335
6 -1.022530 0.700579 0.014015
6 0.437587 2.549058 0.200269
6 0.564195 3.901570 0.171185
1 1.524897 4.361080 0.377816
6 -0.570446 4.748002 -0.121321
6 -1.801345 4.191545 -0.366264
6 -2.656280 4.824395 -0.583520
6 -1.969355 2.787787 -0.325816
6 -2.981305 1.840614 -0.469029
6 -4.364079 1.783058 -0.759744
1 -4.909526 2.704536 -0.938498
6 -5.009020 0.572547 -0.819583
6 -4.279485 -0.651849 -0.576961
1 -4.805352 -1.598326 -0.640952
6 -2.953499 -0.627919 -0.281152
6 3.249191 -2.319358 -0.808155
6 4.299296 -2.145217 0.089420
1 4.184146 -2.443405 1.127402
1 -0.104009 -0.532321 1.930911
6 3.395227 -1.930834 -2.137627
6 4.592249 -1.367833 -2.570708
1 4.704914 -1.061173 -3.606797
6 5.640433 -1.180417 -1.670474
1 6.571083 -0.731230 -2.005652
6 5.494254 -1.569439 -0.340743
1 2.560361 -2.044993 -2.821881
1 6.310671 -1.424235 0.361228
6 -2.376515 -2.865318 1.518439
1 -1.529489 -3.485158 1.842812
6 -1.800824 -3.038020 -1.360315
1 -2.818444 -3.447196 -2.105546
1 2.902538 2.574315 1.914634
6 2.904845 1.334167 -0.774128
1 3.459340 0.390267 -0.711329
6 -0.790158 -4.170742 -2.387722
1 -0.869655 -4.873781 -2.105546
1 0.227472 -3.765290 -1.201936
1 -0.929767 -4.735106 -0.276122
6 -1.586636 -2.284600 -2.668107
1 -0.612018 -1.786059 -2.659383
1 -1.625093 -2.982085 -3.512709
1 -2.354544 -1.520475 -2.82051
6 -3.549673 -3.778915 1.182401
1 -3.880813 -4.301943 2.086813
1 -4.406407 -3.205710 0.813075
1 -3.297394 -4.538564 0.437283
6 -2.725062 -1.911729 2.58626
1 -2.965479 -2.477988 3.565203
1 -1.888630 -1.238477 2.867849
1 -3.599495 -1.303932 2.399718
6 3.410670 0.561965 2.500720
1 4.164088 0.393098 1.724568
1 3.929952 0.857158 3.419401
1 2.907108 -0.391295 2.692129
6 1.353044 1.832080 3.205502
1 1.853861 2.076219 4.149433
1 0.667246 2.649346 2.962535
1 0.757710 0.923778 3.341412
6 2.263231 1.406055 -2.156551
1 1.738796 2.358849 -2.294215
1 3.035632 1.327958 -2.929299
1 1.546045 0.590872 -2.290183
6 3.876052 2.488110 -0.557569
1 4.422276 2.412788 0.386596
1 4.618088 2.492443 -1.364064
1 3.364402 3.456527 -0.585218
6 -6.472951 0.478642 -1.129909
1 -6.649688 -0.122539 -2.029696
1 -7.021096 -0.002965 -0.311400
1 -6.911840 1.465974 -1.293187
6 -0.362834 6.232686 -0.145942
1 0.381106 6.516156 -0.899883
1 -1.290901 6.763238 -0.372298
Name – TS3
Zero-point correction= 0.696748 (Hartree/Particle)
Thermal correction to Energy= 0.737181
Thermal correction to Enthalpy= 0.738125
Thermal correction to Gibbs Free Energy= 0.625806
Sum of electronic and zero-point Energies= -2122.630664
Sum of electronic and thermal Energies= -2122.590231
Sum of electronic and thermal Enthalpies= -2122.589287
Sum of electronic and thermal Free Energies= -2122.701606
1 imaginary frequency.
Charge = 0 Multiplicity = 1

|   |  X       |  Y       |  Z       |
|---|----------|----------|----------|
| 1 | 0.007180 | 6.596236 | 0.82077  |
| 7 | 1.131735 | -3.463333| 1.819388 |
| 7 | 1.737328 | -2.837600| 2.496038 |

S84
|   |     |     |     |
|---|-----|-----|-----|
| 1 | -1.28 | -2.39 | -1.61 |
| 1 | -5.34 | -2.46 | 1.36 |
| 6 | -2.87 | 1.77 | 1.48 |
| 1 | -3.54 | 0.91 | 1.61 |
| 6 | -2.85 | 1.59 | -1.43 |
| 1 | -3.21 | 2.62 | -1.32 |
| 6 | 1.61 | -3.11 | 1.48 |
| 1 | 2.59 | -3.56 | 1.26 |
| 6 | 1.52 | -2.98 | -1.43 |
| 1 | 0.60 | -3.58 | -1.51 |
| 6 | -4.03 | 0.63 | -1.48 |
| 1 | -4.67 | 0.86 | -2.34 |
| 1 | -3.68 | -0.40 | -1.58 |
| 1 | -4.65 | 0.68 | -0.58 |
| 6 | -2.02 | 1.51 | -2.72 |
| 1 | -1.60 | 0.51 | -2.83 |
| 1 | -2.66 | 1.73 | -3.58 |
| 1 | -1.19 | 2.22 | -2.71 |
| 6 | -3.72 | 3.01 | 1.27 |
| 1 | -4.33 | 3.21 | 2.16 |
| 1 | -3.09 | 3.90 | 1.11 |
| 1 | -4.41 | 2.92 | 0.42 |
| 6 | -2.01 | 1.90 | 2.74 |
| 1 | -2.65 | 2.05 | 3.62 |
| 1 | -1.40 | 1.01 | 2.89 |
| 1 | -1.34 | 2.76 | 2.66 |
| 6 | 0.56 | -4.21 | 1.54 |
| 1 | 0.52 | -4.80 | 0.62 |
| 1 | 0.76 | -4.89 | 2.37 |
| 1 | -0.44 | -3.78 | 1.69 |
| 6 | 1.71 | -2.36 | 2.81 |
| 1 | 1.95 | -3.05 | 3.62 |
| 1 | 2.49 | -1.59 | 2.78 |
| 1 | 0.77 | -1.86 | 3.04 |
| 6 | 1.60 | -2.07 | 2.66 |
| 1 | 2.52 | -1.47 | 2.64 |
| 1 | 1.61 | -2.67 | 3.58 |
| 1 | 0.75 | -1.39 | 2.69 |
| 6 | 2.71 | -3.93 | -1.38 |
| 1 | 2.64 | -4.65 | -0.57 |
| 1 | 2.78 | -4.49 | -2.32 |
| 1 | 3.65 | -3.38 | -1.27 |
| 6 | 0.56 | 6.21 | -0.43 |
| 1 | 0.01 | 6.47 | -1.34 |
| 1 | 0.01 | 6.66 | 0.40 |
| 1 | 1.54 | 6.67 | -0.48 |
| 6 | 6.34 | 0.07 | 0.05 |
| 1 | 6.66 | -0.54 | -0.79 |
| 1 | 6.87 | 1.03 | -0.01 |
| 1 | 6.67 | -0.43 | 0.96 |
Geometries of intermediates and transition states involved in Path B and their thermal parameters.

Name - L_2B_
Zero-point correction= 0.596581 (Hartree/Particle)
Thermal correction to Energy= 0.632473
Thermal correction to Enthalpy= 0.633418
Thermal correction to Gibbs Free Energy= 0.530820
Sum of electronic and zero-point Energies= -1890.737705
Sum of electronic and thermal Energies= -1890.701812
Sum of electronic and thermal Enthalpies= -1890.700868
Sum of electronic and thermal Free Energies= -1890.803465

Charge = 0 Multiplicity = 1

|   |     |     |     |     |
|---|-----|-----|-----|-----|
| 0 | 1   | 26  | 0.000921 | -1.444943 | 0.001864 |
| 1 | -0.013852 | -3.025479 | 0.196429 |
| 15| 2.157187   | -1.155875  | 0.046919 |
| 15| -2.160941  | -1.131402  | 0.036501 |
| 7 | 1.070875   | 1.228360   | -0.137058 |
| 7 | -1.043548  | 1.237886   | -0.188187 |
| 6 | 0.010176   | 0.379853   | -0.191425 |
| 6 | 2.339160   | 0.715513   | 0.019608 |
| 6 | 3.344701   | 1.619387   | 0.158000 |
| 1 | 4.363146   | 1.276564   | 0.310180 |
| 6 | 3.078908   | 3.040624   | 0.134852 |
| 6 | 1.790278   | 3.499638   | 0.015091 |
| 1 | 1.584300   | 4.565517   | 0.026115 |
| 6 | 0.717039   | 2.583853   | -0.091994 |
| 6 | -0.678436  | 2.590817   | -0.136933 |
| 6 | -1.745318  | 3.519754   | -0.142905 |
| 1 | -1.528114  | 4.583438   | -0.135413 |
| 6 | -3.044557  | 3.076030   | -0.148715 |
| 6 | -3.328463  | 1.658627   | -0.110755 |
| 1 | -4.362768  | 1.334182   | -0.072202 |
| 6 | -2.326096  | 0.740312   | -0.107379 |
| 1 | 0.012583   | -1.159605  | 1.454428 |
| 6 | -3.186550  | -1.549310  | 1.535937 |
| 1 | -3.015557  | -2.630493  | 1.627936 |
| 6 | -3.187715  | -1.692938  | -1.411821 |
| 1 | -4.164271  | -1.192916  | -1.377568 |
| 6 | 3.269202   | -1.636118  | 1.453642 |
| 1 | 4.253078   | -1.180190  | 1.278246 |
| 6 | 3.098483   | -1.660217  | -1.484645 |
| 1 | 3.050768   | -2.756815  | -1.445975 |
| 6 | -3.374296  | -3.206813  | -1.344882 |
| 1  | -3.888455 | -3.566429 | -2.243255 |
| 1  | -2.402229 | -3.707283 | -1.277846 |
| 1  | -3.965777 | -3.513290 | -0.476768 |
| 6  | -2.462791 | -1.282947 | -3.707283 |
| 1  | -1.472013 | -1.750458 | -2.737120 |
| 1  | -3.026287 | -1.606280 | -3.573944 |
| 1  | -2.327611 | -0.198597 | -2.753230 |
| 6  | -4.682742 | -1.281745 | 1.416621  |
| 1  | -5.195952 | -1.645272 | 2.314087  |
| 1  | -4.883967 | -0.208328 | 1.345381  |
| 1  | -5.138982 | -1.775311 | 0.554107  |
| 6  | -2.603422 | -0.870660 | 2.772569  |
| 1  | -3.128935 | -1.212580 | 3.671081  |
| 1  | -1.538988 | -1.093916 | 2.875174  |
| 1  | -2.719096 | 0.217448  | 2.708972  |
| 6  | 3.404757  | -3.157081 | 1.478351  |
| 1  | 3.913652  | -3.542537 | 0.589223  |
| 1  | 3.983727  | -3.469459 | 2.354454  |
| 1  | 2.415109  | -3.622969 | 1.530357  |
| 6  | 2.702759  | -1.107508 | 2.767940  |
| 1  | 3.356168  | -1.394091 | 3.599672  |
| 1  | 2.616207  | -0.016635 | 2.761919  |
| 1  | 1.705411  | -1.520915 | 2.943497  |
| 6  | 2.299645  | -1.196415 | -2.701622 |
| 1  | 2.266271  | -0.102357 | -2.756052 |
| 1  | 2.756410  | -1.563878 | -3.627172 |
| 1  | 1.267596  | -1.561910 | -2.663856 |
| 6  | 4.554476  | -1.221736 | -1.565643 |
| 1  | 5.145578  | -1.583786 | -0.719166 |
| 1  | 5.016804  | -1.611064 | -2.480059 |
| 1  | 4.632451  | -0.129919 | -1.598295 |
| 6  | 4.237163  | 3.983496  | 0.267159  |
| 1  | 4.952752  | 3.849468  | -0.552720 |
| 1  | 3.908842  | 5.025677  | 0.260009  |
| 1  | 4.785027  | 3.807809  | 1.200482  |
| 6  | -4.199723 | 4.031933  | -0.162171 |
| 1  | -4.843099 | 3.887059  | 0.713730  |
| 1  | -3.860890 | 5.070757  | -0.163449 |
| 1  | -4.827788 | 3.880697  | -1.048054 |

Name - L_3B_
Zero-point correction= 0.700332 (Hartree/Particle)
Thermal correction to Energy= 0.741575
Thermal correction to Enthalpy= 0.742519
Thermal correction to Gibbs Free Energy= 0.627690
Sum of electronic and zero-point Energies= -2122.633123
Sum of electronic and thermal Energies= -2122.591879
Sum of electronic and thermal Enthalpies= -2122.590935
Sum of electronic and thermal Free Energies= -2122.705765

| Charge | Multiplicity | 0 1 |
|--------|--------------|-----|
| 26     | -0.020925    | -1.014206 0.497957 |
| 1      | -0.293506    | -0.502949 1.866110 |
| 1      | -0.205414    | -1.977094 -0.980180 |
| 15     | -2.189963    | -1.094081 0.354767 |
| 15     | 1.994733     | -0.238520 0.875766 |
| 7      | -1.448599    | 1.292152 -0.480784 |
| 7      | 0.619606     | 1.693609 -0.275351 |
| 6      | -0.276714    | 0.678906 -0.170321 |
| 6      | -2.636678    | 0.613599 -0.308684 |
| 6      | -3.772973    | 1.321415 -0.544677 |
| 1      | -4.742041    | 0.859859 -0.386608 |
| 6      | -3.722977    | 2.705971 -0.958290 |
| 6      | -2.515682    | 3.351074 -1.059477 |
| 1      | -2.474722    | 4.401368 -1.331316 |
| 6      | -1.315869    | 2.657168 -0.776626 |
| 6      | 0.047814     | 2.920855 -0.645220 |
| 6      | 0.934985     | 4.018256 -0.739464 |
| 1      | 0.558296     | 4.984985 -1.059082 |
| 6      | 2.255938     | 3.862397 -0.401598 |
| 6      | 2.735440     | 2.587393 0.080805 |
| 1      | 3.756924     | 2.518036 0.438357 |
| 6      | 1.918860     | 1.501529 0.146063 |
| 6      | 0.727800     | -2.031042 -1.595948 |
| 6      | 0.986307     | -1.084285 -2.588296 |
| 1      | 0.380354     | -0.185131 -2.641051 |
| 1      | 0.171573     | -2.397563 1.220398 |
| 6      | 1.482258     | -3.201984 -1.534040 |
| 6      | 2.524161     | -3.405743 -2.435211 |
| 1      | 3.121781     | -4.311184 -2.378126 |
| 6      | 2.807412     | -2.442532 -3.402492 |
| 1      | 3.626266     | -2.597377 -4.099464 |
| 6      | 2.035228     | -1.283887 -3.481937 |
| 1      | 1.259092     | -3.927465 -0.758540 |
| 1      | 2.251301     | -0.537039 -4.240670 |
| 6      | -3.273271    | -1.168050 1.870462 |
| 1      | -4.315412    | -1.098603 1.530913 |
| 6      | -3.012305    | -2.208427 -0.913927 |
| 1      | -2.571640    | -1.831785 -1.848822 |
| 6      | 3.529153     | -0.965589 0.093488 |
| 1      | 3.198292     | -1.142889 -0.936454 |
| 6      | 2.480968     | 0.144794 2.644027 |
| 1      | 3.547276     | 0.409424 2.646103 |
| 6      | -2.555915    | -3.658543 -0.739790 |
| 1      | -2.774941    | -4.230790 -1.647949 |
| 1      | -1.485530    | -3.729108 -0.530392 |
| 1      | -3.082515    | -4.142902 0.087773 |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| 6 | -4.529179 | -2.120702 | -1.027235 |
| 1 | -4.883098 | -2.773597 | -1.833509 |
| 1 | -5.018316 | -2.452350 | -0.105221 |
| 1 | -4.869337 | -1.107472 | -1.254953 |
| 6 | 3.829406  | -2.324983 | 0.725982  |
| 1 | 2.916054  | -2.902757 | 0.895270  |
| 1 | 4.485154  | -2.902585 | 0.065445  |
| 1 | 4.347036  | -2.206827 | 1.683817  |
| 6 | 4.777333  | -0.092997 | 0.052014  |
| 1 | 5.093795  | 0.222548  | 1.053007  |
| 1 | 5.608530  | -0.660439 | -0.382879 |
| 1 | 4.630645  | 0.796635  | -0.564090 |
| 6 | -3.050040 | -2.495211 | 2.592493  |
| 1 | -1.982147 | -2.641343 | 2.785194  |
| 1 | -3.584901 | -2.495831 | 3.548950  |
| 1 | -3.406612 | -3.349628 | 2.011504  |
| 6 | -2.980470 | 0.006934  | 2.799387  |
| 1 | -1.938703 | -0.023876 | 3.131661  |
| 1 | -3.151600 | 0.969862  | 2.309390  |
| 1 | -3.629986 | -0.048128 | 3.680335  |
| 6 | 2.249054  | -1.092598 | 3.511900  |
| 1 | 2.868420  | -1.940833 | 3.216199  |
| 1 | 2.473498  | -0.856763 | 4.558703  |
| 1 | 1.204289  | -1.406903 | 3.429614  |
| 6 | 1.676724  | 1.317991  | 3.201625  |
| 1 | 1.875567  | 2.251969  | 2.670404  |
| 1 | 0.604515  | 1.105689  | 3.134348  |
| 1 | 1.927975  | 1.466437  | 4.257855  |
| 6 | -5.015630 | 3.412926  | -1.236155 |
| 1 | -5.556271 | 2.938967  | -2.064006 |
| 1 | -5.678613 | 3.382640  | -0.363378 |
| 1 | -4.851100 | 4.460897  | -1.498223 |
| 6 | 3.225600  | 5.003250  | -0.480598 |
| 1 | 3.687818  | 5.197193  | 0.494492  |
| 1 | 4.039840  | 4.782431  | -1.180913 |
| 1 | 2.737122  | 5.923020  | -0.811515 |

Name - L_4B_
Zero-point correction= 0.699624 (Hartree/Particle)
Thermal correction to Energy= 0.740352
Thermal correction to Enthalpy= 0.741297
Thermal correction to Gibbs Free Energy= 0.628925
Sum of electronic and zero-point Energies= -2122.643662
Sum of electronic and thermal Energies= -2122.602933
Sum of electronic and thermal Enthalpies= -2122.601989
Sum of electronic and thermal Free Energies= -2122.714360

Charge = 0 Multiplicity = 1
|   |   |   |   |   |
|---|---|---|---|---|
| 0 1 | 26 | -0.000065 | -0.958964 | 0.692670 |
| 1 | -0.000100 | -0.365806 | 2.133798 |
| 1 | -0.000168 | -2.542075 | 1.068314 |
| 15 | -2.198460 | -0.657635 | 0.619605 |
| 15 | 2.198358 | -0.657713 | 0.619730 |
| 7 | -1.054777 | 1.575447 | -0.156809 |
| 7 | 1.054793 | 1.575381 | -0.156825 |
| 6 | -0.000015 | 0.770451 | 0.099845 |
| 6 | -2.337034 | 1.109681 | 0.025172 |
| 6 | -3.340155 | 1.999382 | 0.199485 |
| 1 | -4.371034 | 1.701555 | -0.041897 |
| 6 | -3.062711 | 3.351392 | -0.624816 |
| 6 | -1.765419 | 3.767550 | -0.792561 |
| 1 | -1.549523 | 4.784664 | -1.104456 |
| 6 | -0.697314 | 2.874762 | -0.548359 |
| 6 | 0.697405 | 2.874716 | -0.548376 |
| 6 | 1.765561 | 3.767434 | -0.792609 |
| 1 | 1.549723 | 4.784559 | -1.104512 |
| 6 | 3.062831 | 3.351197 | -0.624885 |
| 6 | 3.340197 | 1.999181 | -0.199523 |
| 1 | 2.337024 | 1.109548 | 0.025164 |
| 6 | 0.000008 | -1.756294 | -1.158850 |
| 6 | -0.000071 | -0.968151 | -2.333259 |
| 1 | -0.000232 | 0.118387 | -2.249695 |
| 1 | -0.000118 | -2.114108 | 1.795413 |
| 6 | 0.000188 | -3.147950 | -1.410962 |
| 6 | 0.000314 | -3.703296 | -2.689980 |
| 1 | 0.000458 | -4.785463 | -2.806734 |
| 6 | 0.000250 | -2.881705 | -3.813516 |
| 1 | 0.000347 | -3.305660 | -4.814051 |
| 6 | 0.000046 | -1.502884 | -3.622245 |
| 1 | 0.000231 | -3.843230 | -0.570257 |
| 1 | -0.000019 | -0.834802 | -4.481701 |
| 6 | -3.216868 | -0.629087 | 2.189486 |
| 1 | -4.278799 | -0.629741 | 1.909569 |
| 6 | -3.221538 | -1.593174 | -0.630870 |
| 1 | -2.586321 | -1.521565 | -1.522716 |
| 6 | 3.221546 | -1.593384 | -0.630557 |
| 1 | 2.586276 | -1.522100 | -1.522389 |
| 6 | 3.216625 | -0.628988 | 2.189701 |
| 1 | 4.278582 | -0.630090 | 1.909883 |
| 6 | -3.300337 | -3.069006 | -0.243590 |
| 1 | -3.649482 | -3.654304 | -1.100662 |
| 1 | -2.322733 | -3.462022 | 0.046451 |
| 1 | -4.007948 | -3.230401 | 0.576626 |
| 6 | -4.601358 | -1.034773 | -0.953662 |
| 1 | -5.102568 | -1.691476 | -1.673913 |
| 1 | -5.244953 | -0.980383 | -0.067761 |
|   | X          | Y          | Z          |
|---|------------|------------|------------|
| 1 | -4.543949  | -0.041001  | -1.402699  |
| 6 | 3.300651   | -3.069112  | -0.242940  |
| 1 | 2.323188   | -3.462200  | 0.047466   |
| 1 | 3.649649   | -3.654565  | 0.577122   |
| 1 | 4.008507   | -3.230208  | 0.242940   |
| 6 | 4.601246   | -1.034800  | 3.009476   |
| 1 | -1.848117  | -1.864786  | 2.462810   |
| 1 | -3.514874  | -1.535278  | 2.524914   |
| 1 | -3.081464  | -2.808450  | 3.968500   |
| 6 | -2.908913  | 0.614794   | 1.847327   |
| 1 | 1.847327   | -1.863822  | 3.310562   |
| 1 | 2.909018   | 0.615285   | 3.206171   |
| 1 | 3.227953   | 1.535493   | 2.524345   |
| 1 | 3.514000   | -1.896883  | 3.917561   |
| 6 | 3.080456   | -2.808209  | 2.463805   |
| 1 | 4.878663   | 3.882105   | -1.652086  |
| 1 | 3.885016   | 5.266451   | -1.171856  |
| 1 | 4.832972   | 4.384264   | 0.036041   |
| 6 | -4.220480  | 4.272677   | -0.866771  |
| 1 | -3.884797  | 5.266680   | -1.171821  |
| 1 | -4.878600  | 3.882380   | -1.651871  |
| 1 | -4.832030  | 4.384638   | 0.036220   |

Name - L_TS1B
Zero-point correction= 0.595869 (Hartree/Particle)
Thermal correction to Energy= 0.631241
Thermal correction to Enthalpy= 0.632185
Thermal correction to Gibbs Free Energy= 0.531130
Sum of electronic and zero-point Energies= -1890.736563
Sum of electronic and thermal Energies= -1890.701191
Sum of electronic and thermal Enthalpies= -1890.700247
Sum of electronic and thermal Free Energies= -1890.801302
1 imaginary frequency.
Charge = 0 Multiplicity = 1

0 1
26 -0.002322 -1.437626 -0.073428
1 -0.025202 -2.941754 0.565808
|   |     |     |     |     |     |     |
|---|-----|-----|-----|-----|-----|-----|
| 15 | -2.167284 | -1.152773 | -0.049494 |
| 15 | 2.171416 | -1.137323 | -0.043402 |
| 7  | -1.067852 | 1.224252 | 0.003571 |
| 7  | 1.046365 | 1.232035 | 0.057778 |
| 6  | -0.007221 | 0.375569 | 0.028635 |
| 6  | -2.342260 | 0.714658 | -0.091248 |
| 6  | -3.351952 | 1.620063 | -0.178239 |
| 1  | -4.377790 | 1.280083 | -0.276804 |
| 6  | -3.081958 | 3.040787 | -0.151486 |
| 6  | -1.789994 | 3.497371 | -0.061593 |
| 1  | -1.584818 | 4.563376 | -0.050651 |
| 6  | -0.713625 | 2.580983 | -0.001598 |
| 6  | 0.681079  | 2.586499 | 0.045021  |
| 6  | 1.749139  | 3.512484 | 0.098471  |
| 1  | 1.533351  | 4.576382 | 0.111160  |
| 6  | 3.047326  | 3.067047 | 0.135712  |
| 6  | 3.332260  | 1.649694 | 0.096192  |
| 1  | 4.366560  | 1.323507 | 0.112435  |
| 6  | 3.329290  | 0.733831 | 0.041293  |
| 1  | -0.016081 | -1.103085 | -1.529626 |
| 6  | 3.255734  | -1.614606 | -1.485039 |
| 1  | 3.106729  | -2.701849 | -1.537521 |
| 6  | 3.140992  | -1.640015 | 1.462932  |
| 1  | 4.119107  | -1.142280 | 1.436552  |
| 6  | -3.338201 | -1.700762 | -1.380854 |
| 1  | -4.315938 | -1.242407 | -1.180852 |
| 6  | -3.030770 | -1.583669 | 1.545871  |
| 1  | -2.939355 | -2.677941 | 1.570360  |
| 6  | 3.321243  | -3.155668 | 1.466573  |
| 1  | 3.806066  | -3.475963 | 2.395440  |
| 1  | 2.344718  | -3.647479 | 1.397693  |
| 1  | 3.937275  | -3.504330 | 0.631683  |
| 6  | 2.372818  | -1.178467 | 2.698484  |
| 1  | 1.378007  | -1.637945 | 2.712846  |
| 1  | 2.901533  | -1.477060 | 3.610594  |
| 1  | 2.248443  | -0.091062 | 2.718837  |
| 6  | 4.743010  | -1.321377 | -1.320890 |
| 1  | 5.295316  | -1.715179 | -2.181629 |
| 1  | 4.925893  | -0.242769 | -1.288278 |
| 1  | 5.170781  | -1.771213 | -0.420819 |
| 6  | 2.712190  | -0.996743 | -2.770827 |
| 1  | 3.270722  | -1.374013 | -3.634577 |
| 1  | 1.652636  | -1.228199 | -2.902418 |
| 1  | 2.819851  | 0.093808  | -2.751709 |
| 6  | -3.469790 | -3.221874 | -1.332121 |
| 1  | -3.923513 | -3.569269 | -0.398892 |
| 1  | -4.097095 | -3.572951 | -2.158877 |
| 1  | -2.485808 | -3.694024 | -1.421849 |
| 6  | -2.836342 | -1.226387 | -2.741281 |
| 1  | -3.525575 | -1.549909 | -3.529341 |
|    |        |        |        |
|----|--------|--------|--------|
| 1  | -2.756006 | -0.135932 | -2.783981 |
| 1  | -1.845554 | -1.641111 | -2.948539 |
| 6  | -2.200886 | -1.021270 | 2.697750  |
| 1  | -2.209823 | 0.074949  | 2.690855  |
| 1  | -2.605340 | -1.353368 | 3.660205  |
| 1  | -1.161012 | -1.356721 | 2.625328  |
| 6  | -4.497210 | -1.188237 | 1.656489  |
| 1  | -5.109773 | -1.620998 | 0.859518  |
| 1  | -4.908541 | -1.533698 | 2.611808  |
| 1  | -4.612314 | -0.099602 | 1.627440  |
| 6  | -4.243174 | 3.986283  | -0.227423 |
| 1  | -4.932587 | 3.834633  | 0.611576  |
| 1  | -3.914079 | 5.028057  | -0.208392 |
| 1  | -4.820139 | 3.830547  | -1.146635 |
| 6  | 4.201768  | 4.021435  | 0.203870  |
| 1  | 4.871005  | 3.894937  | -0.655396 |
| 1  | 3.863165  | 5.060240  | 0.216995  |
| 1  | 4.803188  | 3.850907  | 1.104612  |

Name - L_TS2B
Zero-point correction= 0.696910 (Hartree/Particle)
Thermal correction to Energy= 0.737393
Thermal correction to Enthalpy= 0.738337
Thermal correction to Gibbs Free Energy= 0.627102
Sum of electronic and zero-point Energies= -2122.623541
Sum of electronic and thermal Energies= -2122.583059
Sum of electronic and thermal Enthalpies= -2122.582115
Sum of electronic and thermal Free Energies= -2122.693349
1 imaginary frequency.
Charge = 0 Multiplicity = 1

|    |        |        |        |        |
|----|--------|--------|--------|--------|
| 0  | 1      |        |        |        |
| 26 | 0.003825 | -1.049506 | -0.517370 |
| 1  | 0.039812 | -0.625213 | -1.968870 |
| 1  | 0.138661 | -2.393310 | 0.148431 |
| 15 | 2.178970 | -0.776573 | -0.601955 |
| 15 | -2.145681 | -0.586630 | -0.700771 |
| 7  | 1.150363 | 1.472647 | 0.281709 |
| 7  | -0.959436 | 1.564681 | 0.245832 |
| 6  | 0.063041 | 0.703236 | 0.040215 |
| 6  | 2.413578 | 0.964141 | 0.063599 |
| 6  | 3.450911 | 1.812871 | 0.287342 |
| 1  | 4.469206 | 1.486194 | 0.106492 |
| 6  | 3.227624 | 3.170003 | 0.732035 |
| 6  | 1.947982 | 3.640888 | 0.891498 |
| 1  | 1.774511 | 4.667426 | 1.199149 |
| 6  | 0.843666 | 2.794175 | 0.640611 |
| 6  | -0.549839 | 2.855189 | 0.613872 |
| 6  | -1.580768 | 3.802137 | 0.811494 |
|   |     |     |     |
|---|-----|-----|-----|
| 1 | -1.328048 | 4.810538 | 1.123976 |
| 6 | -2.888016  | 3.448630  | 0.588763  |
| 6 | -3.213295  | 2.114952  | 0.138945  |
| 1 | -4.245376  | 1.884627  | -0.099109 |
| 6 | -2.250653  | 1.168027  | -0.024735 |
| 6 | -0.155550  | -1.903918 | 1.429899  |
| 6 | 0.485012   | -2.888016 | 3.448630  |
| 1 | 1.133126   | -0.341409 | 2.203117  |
| 1 | -0.031383  | -2.500118 | -1.101656 |
| 6 | -0.961640  | -2.974676 | 1.857513  |
| 1 | 0.696059   | -2.738467 | 5.239989  |
| 6 | 0.284487   | -1.462279 | 3.800689  |
| 1 | -1.438042  | -3.601095 | 1.106293  |
| 1 | 0.779676   | -0.854944 | 4.554982  |
| 6 | 3.047087   | -0.626463 | -2.246454 |
| 1 | 4.103005   | -0.412009 | -2.038049 |
| 6 | 3.345320   | -1.776818 | 0.475651  |
| 1 | 3.106243   | -1.413171 | 1.483089  |
| 6 | -3.476540  | -1.490391 | 0.251459  |
| 1 | -2.997904  | -1.632157 | 1.228212  |
| 6 | -2.868121  | -0.351976 | -2.415276 |
| 1 | -3.957688  | -0.260025 | -2.307004 |
| 6 | 2.984526   | -3.261672 | 0.433979  |
| 1 | 3.624187   | -3.813847 | 1.131682  |
| 1 | 1.945998   | -3.428445 | 0.725102  |
| 6 | 3.130612   | -3.691669 | -0.561316 |
| 6 | 4.833868   | -1.566286 | 0.219662  |
| 1 | 5.419289   | -2.109154 | 0.970310  |
| 1 | 5.130758   | -1.950097 | -0.761845 |
| 1 | 5.127514   | -0.514771 | 0.276152  |
| 6 | -3.702238  | -2.872562 | -0.363814 |
| 1 | -2.764540  | -3.354399 | -0.656100 |
| 1 | -4.210395  | -3.521942 | 0.357437  |
| 1 | -4.340484  | -2.806941 | -1.251254 |
| 6 | -4.805262  | -0.774004 | 0.460047  |
| 1 | -5.269126  | -0.480821 | -0.489232 |
| 1 | -5.508839  | -1.444705 | 0.966949  |
| 1 | -4.693811  | 0.115197  | 1.083365  |
| 6 | 2.926716   | -1.948657 | -3.000456 |
| 1 | 1.872486   | -2.228115 | -3.098718 |
| 1 | 3.356841   | -1.850902 | -4.003546 |
| 1 | 3.447803   | -2.765826 | -2.493484 |
| 6 | 2.468264   | 0.522013  | -3.066864 |
| 1 | 1.400892   | 0.360062  | -3.244046 |
| 1 | 2.588566   | 1.485580  | -2.562727 |
| 1 | 2.979450   | 0.578481  | -4.034518 |
| 6 | -2.533152  | -1.565008 | -3.283787 |
|   |   |   |   |
|---|---|---|---|
| 1 | -2.962259 | -2.494015 | -2.904484 |
| 1 | -2.913061 | -1.407597 | -4.299833 |
| 1 | -1.447402 | -1.694200 | -3.326820 |
| 6 | -2.321141 | 0.912793 | -3.074314 |
| 1 | -2.623716 | 1.822126 | -2.549393 |
| 1 | -1.226676 | 0.877626 | -3.099840 |
| 1 | -2.683405 | 0.977546 | -4.106368 |
| 6 | -4.008370 | 4.426542 | 0.780007 |
| 1 | -4.583449 | 4.554651 | -0.14568 |
| 1 | -4.710093 | 4.077987 | 1.546883 |
| 1 | -3.636548 | 5.407740 | 1.084861 |
| 6 | 4.421321 | 4.041142 | 0.985577 |
| 1 | 5.053992 | 3.624764 | 1.778329 |
| 1 | 5.046923 | 4.126087 | 0.089169 |
| 1 | 4.125065 | 5.048964 | 1.286362 |

Name - L_TS3B_
Zero-point correction= 0.699145 (Hartree/Particle)
Thermal correction to Energy= 0.739244
Thermal correction to Enthalpy= 0.740188
Thermal correction to Gibbs Free Energy= 0.630148
Sum of electronic and zero-point Energies= -2122.643359
Sum of electronic and thermal Energies= -2122.603261
Sum of electronic and thermal Enthalpies= -2122.602317
Sum of electronic and thermal Free Energies= -2122.712357
1 imaginary frequency.
Charge = 0 Multiplicity = 1
0 1
26 0.000112 -0.954802 0.664665
1 -0.001841 -0.404622 2.126994
1 0.419868 -2.388142 1.296750
15 -2.181754 -0.643350 0.617862
15 2.181574 -0.638691 0.619649
7 -1.056705 1.580251 -0.182011
7 1.052294 1.582132 -0.182211
6 -0.001459 0.774438 0.074963
6 -2.337219 1.117249 0.011535
6 -3.342261 2.005368 -0.209840
1 -4.372088 1.709705 -0.042128
6 -3.066658 3.355002 -0.644333
6 -1.770086 3.770652 -0.818653
1 -1.555661 4.786668 -1.134994
6 -0.700519 2.879449 -0.574646
6 0.693699 2.880678 -0.574828
6 1.761601 3.773765 -0.819225
1 1.545282 4.789334 -1.135710
6 3.058954 3.360460 -0.645156
6 3.337054 2.011479 -0.210246
|   | 4.367414  | 1.717783  | -0.042393  |
|---|-----------|-----------|------------|
| 6 | 2.333665  | 1.121572  | 0.011465   |
| 6 | 0.003262  | -1.779726 | -1.167801  |
| 6 | 0.001243  | -1.024695 | -2.362323  |
|   | -0.002930 | 0.064304  | -2.305981  |
|   | -0.418071 | -2.394559 | 1.283021   |
| 6 | 0.008382  | -3.177567 | -1.374363  |
| 6 | 0.011569  | -3.770191 | -2.636535  |
|   | 0.015599  | -4.855320 | -2.722981  |
|   | 0.009554  | -3.165029 | -0.611481  |
| 6 | 0.012004  | -3.435479 | -4.771157  |
| 6 | 0.004243  | -1.597182 | -3.635210  |
|   | 0.010208  | -3.844952 | -0.511644  |
|   | 0.002451  | -0.955979 | -4.514950  |
|   | -3.165029 | -0.611481 | 2.208174   |
|   | -4.231621 | -0.621688 | 1.946994   |
| 6 | -3.219358 | -1.596264 | -0.609845  |
|   | -2.597360 | -1.532450 | -1.508798  |
| 6 | 3.223254  | -1.591135 | -0.602068  |
|   | 2.601635  | -1.532014 | -1.504432  |
| 6 | 3.162929  | -0.601865 | 2.211138   |
|   | 4.229789  | -0.609338 | 1.950933   |
| 6 | -3.295086 | -3.068749 | -0.207573  |
|   | -3.673040 | -3.656257 | -1.050799  |
| 6 | -2.311825 | -3.468033 | 0.053227   |
|   | -3.979036 | -3.221475 | 0.633935   |
| 6 | -4.604052 | -1.039487 | -0.912812  |
|   | -5.116524 | -1.702034 | -1.619534  |
|   | -5.233713 | -0.977367 | -0.017457  |
|   | -4.553229 | -0.049754 | -1.371173  |
| 6 | 3.303914  | -3.062192 | -0.198367  |
|   | 2.322222  | -3.463637 | 0.064989   |
| 6 | 3.682586  | -3.651118 | -1.040271  |
|   | 3.989314  | -3.210265 | 0.642801   |
| 6 | 4.606189  | -1.030420 | -0.908629  |
|   | 5.234929  | -0.963129 | -0.012985  |
| 6 | 5.121566  | -1.693460 | -1.612775  |
|   | 4.552151  | -0.042392 | -1.370269  |
| 6 | -2.822096 | -1.853459 | 3.030925   |
|   | -1.758845 | -1.833780 | 3.291837   |
| 6 | -3.405159 | -1.858907 | 3.958661   |
|   | -3.024461 | -2.787211 | 2.501449   |
| 6 | -2.849367 | 0.641260  | 3.021881   |
|   | -1.769124 | 0.710147  | 3.191475   |
| 6 | -3.177995 | 1.556211  | 2.523185   |
|   | -3.346931 | 0.585145  | 3.996560   |
| 6 | 2.823062  | -1.843590 | 3.035537   |
|   | 3.028195  | -2.777579 | 2.507570   |
| 6 | 3.405815  | -1.846048 | 3.963491   |
|   | 1.759705  | -1.826479 | 3.296225   |
Name - R_2B_
Zero-point correction= 0.598364 (Hartree/Particle)
Thermal correction to Energy= 0.634000
Thermal correction to Enthalpy= 0.634944
Thermal correction to Gibbs Free Energy= 0.532823
Sum of electronic and zero-point Energies= -1890.735922
Sum of electronic and thermal Energies= -1890.700286
Sum of electronic and thermal Enthalpies= -1890.699342
Sum of electronic and thermal Free Energies= -1890.801463

Charge = 0 Multiplicity = 1

0 1
26 0.000921 -1.444943 0.001864
1 -0.013852 -3.025479 0.196429
15 2.157187 -1.155875 0.046919
15 -2.160941 -1.131402 0.036501
7 1.070875 1.228360 -0.137058
7 -1.043548 1.237886 -0.188187
6 0.010176 0.379853 -0.191425
6 2.339160 0.715513 0.019608
6 3.344701 1.619387 0.158000
1 4.363146 1.276564 0.310180
6 3.078908 3.040624 0.134852
6 1.790278 3.499638 0.015091
1 1.584300 4.565517 0.026115
6 0.710703 2.583853 -0.091994
6 -0.678436 2.590817 -0.136933
6 -1.745318 3.519754 -0.142905
1 -1.528114 4.583438 -0.135413
6 -3.044557 3.076030 -0.148715
6 -3.328463 1.658627 -0.110755
1 -4.362768 1.334182 -0.072202
6 -2.326096 0.740312 -0.107379
1 0.012583 -1.159605 1.454428
6 -3.186550 -1.549310 1.535937
|   |   |   |   |
|---|---|---|---|
| 1 | -3.01557 | -2.630493 | 1.627936 |
| 6 | -3.187715 | -1.692938 | -1.411821 |
| 1 | -4.164271 | -1.192916 | -1.377568 |
| 6 | 3.269202 | -1.636118 | 1.453642 |
| 1 | 4.253078 | -1.180190 | 1.278246 |
| 6 | 3.098483 | -1.660217 | -1.411821 |
| 1 | -3.967777 | -3.513290 | -0.476768 |
| 6 | -2.462791 | -1.282947 | -2.691615 |
| 1 | -1.472013 | -1.750458 | -2.737120 |
| 1 | -3.026287 | -1.606280 | -3.573944 |
| 1 | -2.327611 | -0.198597 | -2.753230 |
| 6 | -4.682742 | -1.281745 | 1.416621 |
| 1 | -5.195952 | -1.645272 | 2.314087 |
| 1 | -4.883967 | -0.208328 | 1.345381 |
| 1 | -5.138982 | -1.775311 | 0.554107 |
| 6 | -2.603422 | -0.870660 | 2.772569 |
| 1 | -3.128935 | -1.212580 | 3.671081 |
| 1 | -1.538988 | -1.093916 | 2.875174 |
| 1 | -2.719096 | 0.217448 | 2.708972 |
| 6 | 3.404757 | -3.157081 | 1.478351 |
| 1 | 3.913652 | -3.542537 | 0.589223 |
| 1 | 3.983727 | -3.469459 | 2.354454 |
| 1 | 2.415109 | -3.622969 | 1.530357 |
| 6 | 2.702759 | -1.107508 | 2.767940 |
| 1 | 3.356168 | -1.394091 | 3.599672 |
| 1 | 2.616207 | -0.016635 | 2.761919 |
| 1 | 1.705411 | -1.520915 | 2.943497 |
| 6 | 2.299645 | -1.196415 | -2.701622 |
| 1 | 2.266271 | -0.102357 | -2.756052 |
| 1 | 2.756410 | -1.563878 | -3.627172 |
| 1 | 1.267596 | -1.561910 | -2.663856 |
| 6 | 4.554476 | -1.221736 | -1.565643 |
| 1 | 5.145578 | -1.583786 | -0.719166 |
| 1 | 5.016804 | -1.611064 | -2.480059 |
| 1 | 4.632451 | -0.129919 | -1.598295 |
| 6 | 4.237163 | 3.983496 | 0.267159 |
| 1 | 4.952752 | 3.849468 | -0.552720 |
| 1 | 3.908442 | 5.025677 | 0.260009 |
| 1 | 4.785027 | 3.807809 | 1.200482 |
| 6 | -4.199723 | 4.031933 | -0.162171 |
| 1 | -4.843099 | 3.887059 | 0.713730 |
| 1 | -3.860890 | 5.070757 | -0.163449 |
| 1 | -4.827788 | 3.880697 | -1.048054 |
-----------------------------------------------
Name - R_3B_
Zero-point correction= 0.699124 (Hartree/Particle)
Thermal correction to Energy= 0.740244
Thermal correction to Enthalpy= 0.741188
Thermal correction to Gibbs Free Energy= 0.626560
Sum of electronic and zero-point Energies= -2122.634331
Sum of electronic and thermal Energies= -2122.593211
Sum of electronic and thermal Enthalpies= -2122.592266
Sum of electronic and thermal Free Energies= -2122.706894

Charge = 0 Multiplicity = 1

0 1
26 -0.020925 -1.014206 0.497957
1 -0.293506 -0.502949 1.866110
1 -0.205414 -1.977094 -0.980180
15 -2.189963 -1.094081 0.354767
15 1.994733 -0.238520 0.875766
7 -1.448599 1.292152 -0.480784
7 0.619606 1.693609 -0.275351
6 -0.276714 0.678906 -0.170321
6 -2.636678 0.613599 -0.308684
6 -3.772973 1.321415 -0.544677
1 -4.742041 0.859859 -0.386608
6 -3.722977 2.705971 -0.958290
6 -2.515682 3.351074 -1.059477
1 -2.474722 4.401368 -1.331316
6 -1.315869 2.657168 -0.776626
6 0.047814 2.920855 -0.645220
6 0.934985 4.018256 -0.739464
1 0.558296 4.984985 -1.059082
6 2.255938 3.862397 -0.401598
6 2.735440 2.587393 0.080805
1 3.756924 2.518036 0.438357
6 1.918860 1.501529 0.146063
6 0.727800 -2.031042 -1.595948
6 0.986307 -1.084285 -2.588296
1 0.380354 -0.185131 -2.641051
1 0.171573 -2.397563 1.220398
6 1.482258 -3.201984 -1.534040
6 2.524161 -3.405743 -2.435211
1 3.121781 -4.311184 -2.378126
6 2.807412 -2.442532 -3.402492
1 3.626266 -2.597377 -4.099464
6 2.035228 -1.283887 -3.481937
1 1.259092 -3.927465 -0.758540
1 2.251301 -0.537039 -4.240670
6 -3.273271 -1.168050 1.870462
1 -4.315412 -1.098603 1.530913
6 -3.012305 -2.208427 -0.913927
1 -2.571640 -1.831785 -1.848822
|   |       |          |          |
|---|-------|----------|----------|
| 6 | 3.529153 | -0.965589 | 0.093488 |
| 1 | 3.198292 | -1.142889 | -0.936454 |
| 6 | 2.480968 | 0.144794  | 2.644027 |
| 1 | 3.547276 | 0.409424  | 2.646103 |
| 6 | -2.555915 | -3.658543 | -0.739790 |
| 1 | -2.774941 | -4.230790 | -1.647949 |
| 1 | -1.485530 | -3.729108 | -0.530392 |
| 6 | -3.082515 | -4.142902 | 0.087773 |
| 6 | -4.529179 | -2.120702 | -1.027235 |
| 1 | -4.883098 | -2.773597 | -1.833509 |
| 1 | -5.018316 | -2.452350 | -0.105221 |
| 1 | -4.869337 | -1.107472 | -1.254953 |
| 6 | 3.829406 | -2.324983 | 0.725982 |
| 1 | 2.916054 | -2.902757 | 0.895270 |
| 1 | 4.485154 | -2.902585 | 0.065445 |
| 1 | 4.347036 | -2.206827 | 1.683817 |
| 6 | 4.777333 | -0.092997 | 0.052014 |
| 1 | 5.093795 | 0.222548  | 1.053007 |
| 1 | 5.608530 | -0.660439 | -0.382879 |
| 1 | 4.630645 | 0.796635  | -0.564090 |
| 6 | -3.050040 | -2.495211 | 2.592493 |
| 1 | -1.982147 | -2.641343 | 2.785194 |
| 1 | -3.584901 | -2.495831 | 3.548950 |
| 1 | -3.406612 | -3.349628 | 2.011504 |
| 6 | -2.980470 | 0.006934  | 2.799387 |
| 1 | -1.938703 | -0.023876 | 3.131661 |
| 1 | -3.151600 | 0.969862  | 2.309390 |
| 1 | -3.629986 | -0.048128 | 3.680335 |
| 6 | 2.249054 | -1.092598 | 3.511900 |
| 1 | 2.868420 | -1.940833 | 3.216199 |
| 1 | 2.473498 | -0.856763 | 4.558703 |
| 1 | 1.204289 | -1.406903 | 3.429614 |
| 6 | 1.676724 | 1.317991  | 3.201625 |
| 1 | 1.875567 | 2.251969  | 2.670404 |
| 1 | 0.604515 | 1.105689  | 3.134348 |
| 1 | 1.927975 | 1.466437  | 4.257855 |
| 6 | -5.015630 | 3.412926  | -1.236155 |
| 1 | -5.556271 | 2.938967  | -2.064006 |
| 1 | -5.678613 | 3.382640  | -0.363378 |
| 1 | -4.851100 | 4.460897  | -1.498223 |
| 6 | 3.225600 | 5.003250  | -0.480598 |
| 1 | 3.687818 | 5.197193  | 0.494492 |
| 1 | 4.039840 | 4.782431  | -1.180913 |
| 1 | 2.737122 | 5.923020  | -0.811515 |

Name - R_4B_
Zero-point correction= 0.699689 (Hartree/Particle)
Thermal correction to Energy= 0.740421
Thermal correction to Enthalpy = 0.741365
Thermal correction to Gibbs Free Energy = 0.628956
Sum of electronic and zero-point Energies = -2122.643597
Sum of electronic and thermal Energies = -2122.602865
Sum of electronic and thermal Enthalpies = -2122.601921
Sum of electronic and thermal Free Energies = -2122.714330

Charge = 0 Multiplicity = 1

| Atom | Atomic Number | Atomic Mass | Charge | Multiplicity |
|------|---------------|-------------|--------|--------------|
| 26   | 0.000065      | -0.958964   | 0.692670 |
| 1    | -0.000100     | -0.365806   | 2.133798 |
| 1    | -0.000168     | -2.542075   | 1.068314 |
| 15   | -2.198460     | -0.657635   | 0.619605 |
| 15   | 2.198358      | -0.657713   | 0.619730 |
| 7    | -1.054777     | 1.575447    | -0.156809 |
| 7    | 1.054793      | 1.575381    | -0.156825 |
| 6    | -0.000015     | 0.770451    | 0.099845 |
| 6    | -2.337034     | 1.109681    | 0.025172 |
| 6    | -3.340155     | 1.999382    | -0.199485 |
| 1    | -4.371034     | 1.701555    | -0.041897 |
| 6    | -3.062711     | 3.351392    | -0.624816 |
| 6    | -1.765419     | 3.767550    | -0.792561 |
| 1    | -1.549523     | 4.784664    | -1.104456 |
| 6    | -0.697314     | 2.874762    | -0.548359 |
| 6    | 0.697405      | 2.874716    | -0.548376 |
| 6    | 1.765561      | 3.767434    | -0.792609 |
| 1    | 1.549723      | 4.784559    | -1.104512 |
| 6    | 3.062831      | 3.351197    | -0.624885 |
| 6    | 3.340197      | 1.999181    | -0.199523 |
| 1    | 4.371059      | 1.701292    | -0.041935 |
| 6    | 2.337024      | 1.109548    | 0.025164  |
| 6    | 0.000086      | -1.756294   | -1.158850 |
| 6    | -0.000071     | -0.968151   | -2.333259 |
| 1    | -0.000232     | 0.118387    | -2.249695 |
| 1    | -0.000118     | -2.114108   | 1.795413  |
| 6    | 0.000188      | -3.147950   | -1.410962 |
| 6    | 0.000314      | -3.703296   | -2.689980 |
| 1    | 0.000458      | -4.785463   | -2.806734 |
| 6    | 0.000250      | -2.881705   | -3.813516 |
| 1    | 0.000347      | -3.305660   | -4.814051 |
| 6    | 0.000046      | -1.502884   | -3.622245 |
| 1    | 0.000231      | -3.843230   | -0.570257 |
| 1    | -0.000019     | -0.834802   | -4.481701 |
| 6    | -3.216868     | -0.629087   | 2.189486 |
| 1    | -4.278799     | -0.629741   | 1.909569  |
| 6    | -3.221538     | -1.593174   | -0.630870 |
| 1    | -2.586321     | -1.521565   | -1.522716 |
| 6    | 3.221546      | -1.593384   | -0.630557 |
| 1    | 2.586276      | -1.522100   | -1.522389 |
| 6    | 3.216625      | -0.628988   | 2.189701 |
|   |   |   |   |
|---|---|---|---|
| 1 | 4.278582 | -0.630090 | 1.909883 |
| 6 | -3.300337 | -3.069006 | -0.243590 |
| 1 | -3.649482 | -3.654304 | -1.100662 |
| 1 | -2.322733 | -3.462022 | 0.046451 |
| 1 | -4.007948 | -3.230406 | 0.243590 |
| 6 | -4.601358 | -1.034773 | -0.953662 |
| 1 | -5.102568 | -1.691476 | -1.673913 |
| 1 | -5.244953 | -0.980383 | -0.067761 |
| 1 | -4.543949 | -0.041001 | -1.402699 |
| 6 | 3.300651 | -3.069112 | 0.242940 |
| 1 | 2.323188 | -3.462200 | 0.047466 |
| 1 | 3.649649 | -3.654565 | -1.109966 |
| 1 | 4.008507 | -3.230208 | 0.577122 |
| 6 | 4.601246 | -1.034800 | -0.953551 |
| 1 | 5.244884 | -0.980106 | -0.067699 |
| 1 | 5.102534 | -1.691562 | -1.673693 |
| 1 | 4.543625 | -0.041132 | -1.402791 |
| 6 | -2.900750 | -1.880440 | 3.009476 |
| 1 | -1.848117 | -1.864786 | 3.310024 |
| 1 | -3.514874 | -1.897508 | 3.916850 |
| 1 | -3.081464 | -2.808450 | 2.462810 |
| 6 | -2.908913 | 0.614794 | 3.019732 |
| 1 | -1.831246 | 0.681770 | 3.206171 |
| 1 | -3.227547 | 1.535278 | 2.524914 |
| 1 | -3.419982 | 0.551751 | 3.987076 |
| 6 | 2.899990 | -1.879940 | 3.010106 |
| 1 | 3.080456 | -2.808209 | 2.463805 |
| 1 | 3.514000 | -1.896883 | 3.917561 |
| 1 | 1.847327 | -1.863822 | 3.310526 |
| 6 | 2.909018 | 0.615285 | 3.019486 |
| 1 | 3.227953 | 1.535493 | 2.524345 |
| 1 | 1.831365 | 0.682656 | 3.205860 |
| 1 | 3.420034 | 0.552433 | 3.986870 |
| 6 | 4.220651 | 4.272404 | -0.866897 |
| 1 | 4.878663 | 3.882105 | -1.652086 |
| 1 | 3.885016 | 5.266451 | -1.171856 |
| 1 | 4.832297 | 4.384264 | 0.036041 |
| 6 | -4.220480 | 4.272677 | -0.866771 |
| 1 | -3.884797 | 5.266680 | -1.171821 |
| 1 | -4.878600 | 3.882380 | -1.651871 |
| 1 | -4.832030 | 4.384638 | 0.036220 |

Name - R_TS1B_
Zero-point correction= 0.597289 (Hartree/Particle)
Thermal correction to Energy= 0.632498
Thermal correction to Enthalpy= 0.633442
Thermal correction to Gibbs Free Energy= 0.532683
Sum of electronic and zero-point Energies= -1890.735143
Sum of electronic and thermal Energies= -1890.699934
Sum of electronic and thermal Enthalpies= -1890.698990
Sum of electronic and thermal Free Energies= -1890.799749

1 imaginary frequency.
Charge = 0 Multiplicity = 1

| 0 1 | 26 | -0.002322 | -1.437626 | -0.073428 |
| 1  | -0.025202 | -2.941754 | 0.565808  |
| 15 | -2.167284 | -1.152773 | -0.049494 |
| 15 | 2.171416  | -1.137323 | -0.043402 |
| 7  | -1.067852 | 1.224252  | 0.003571  |
| 7  | 1.046365  | 1.232035  | 0.057778  |
| 6  | -0.007221 | 0.375569  | 0.028635  |
| 6  | -2.342260 | 0.714658  | -0.091248 |
| 6  | -3.351952 | 1.620063  | -0.178239 |
| 1  | -4.377790 | 1.280083  | -0.276804 |
| 6  | -3.081958 | 3.040787  | -0.151486 |
| 6  | -1.789994 | 3.497371  | -0.061593 |
| 1  | -1.584818 | 4.563376  | -0.050651 |
| 6  | -0.713625 | 2.580983  | -0.001598 |
| 6  | 0.681079  | 2.586499  | 0.045021  |
| 6  | 1.749139  | 3.512484  | 0.098471  |
| 1  | 1.533351  | 4.576382  | 0.111160  |
| 6  | 3.047326  | 3.067047  | 0.135712  |
| 6  | 3.332260  | 1.649694  | 0.096192  |
| 1  | 4.366560  | 1.323507  | 0.112435  |
| 6  | 2.329290  | 0.733831  | 0.041293  |
| 1  | -0.016081 | -1.103085 | -1.529626 |
| 6  | 3.255734  | -1.614606 | -1.485039 |
| 1  | 3.106729  | -2.701849 | -1.537521 |
| 6  | 3.140992  | -1.640015 | 1.462932  |
| 1  | 4.119107  | -1.142280 | 1.436552  |
| 6  | -3.338201 | -1.700762 | -1.380854 |
| 1  | -4.315938 | -1.242407 | -1.180852 |
| 6  | -3.030770 | -1.583669 | 1.545871  |
| 1  | -2.939355 | -2.677941 | 1.570360  |
| 6  | 3.321243  | -3.155568 | 1.466573  |
| 1  | 3.806066  | -3.475963 | 2.395440  |
| 1  | 2.344718  | -3.647479 | 1.397693  |
| 1  | 3.937275  | -3.504310 | 0.631683  |
| 6  | 2.372818  | -1.178467 | 2.698484  |
| 1  | 1.378007  | -1.637945 | 2.712846  |
| 1  | 2.901533  | -1.477060 | 3.610594  |
| 1  | 2.248443  | -0.091062 | 2.718837  |
| 6  | 4.743010  | -1.321377 | -1.320890 |
| 1  | 5.295316  | -1.715179 | -2.181629 |
| 1  | 4.925893  | -0.242769 | -1.288278 |
| 1  | 5.170781  | -1.771213 | -0.420819 |
| 6  | 2.712190  | -0.996743 | -2.770827 |
| 1  | 3.270722  | -1.374013 | -3.634577 |
|   | 1    | 2    | 3    |
|---|------|------|------|
| 1 | 1.652636 | -1.228199 | -2.902418 |
| 1 | 2.819851  | 0.093808  | -2.751709  |
| 6 | -3.469790 | -3.221874 | -1.332121  |
| 1 | -3.923513 | -3.569269 | -0.398892  |
| 1 | -4.097095 | -3.572951 | -2.158877  |
| 1 | -2.485808 | -3.694024 | -1.421849  |
| 6 | -2.836342 | -1.226387 | -2.741281  |
| 1 | -3.525575 | -1.549909 | -3.529341  |
| 1 | -2.756006 | -0.135932 | -2.783981  |
| 1 | -1.845554 | -1.641111 | -2.948539  |
| 6 | -2.200886 | -1.021270 | 2.697750   |
| 1 | -2.209823 | 0.074949  | 2.690855   |
| 1 | -2.605340 | -1.353368 | 3.660205   |
| 1 | -1.161012 | -1.356721 | 2.625328   |
| 6 | -4.497210 | -1.188237 | 1.656489   |
| 1 | -5.109773 | -1.620998 | 0.859518   |
| 1 | -4.908541 | -1.533698 | 2.611808   |
| 1 | -4.612314 | -0.099602 | 1.627440   |
| 6 | -4.243174 | 3.986283  | -0.227423  |
| 1 | -4.932587 | 3.834633  | 0.611576   |
| 1 | -3.914079 | 5.028057  | -0.208392  |
| 1 | -4.820139 | 3.830547  | -1.146635  |
| 6 | 4.201768  | 4.021435  | 0.203870   |
| 1 | 4.871005  | 3.894937  | -0.65396   |
| 1 | 3.863165  | 5.060240  | 0.216995   |
| 1 | 4.803188  | 3.850907  | 1.104612   |

Name - R_TS2B_
Zero-point correction= 0.696977 (Hartree/Particle)
Thermal correction to Energy= 0.737334
Thermal correction to Enthalpy= 0.738278
Thermal correction to Gibbs Free Energy= 0.627246
Sum of electronic and zero-point Energies= -2122.623474
Sum of electronic and thermal Energies= -2122.583118
Sum of electronic and thermal Enthalpies= -2122.582174
Sum of electronic and thermal Free Energies= -2122.693205
1 imaginary frequency.
Charge = 0 Multiplicity = 1
0 1
26 0.003825 -1.049506 -0.517370
1 0.039812 -0.625213 -1.968870
1 0.138661 -2.393310 0.148431
15 2.178970 -0.776573 -0.601955
15 -2.145681 -0.586630 -0.700771
7 1.150363 1.472647 0.281709
7 -0.959436 1.564681 0.245832
6 0.063041 0.703236 0.040215
6 2.413578 0.964141 0.063599
|   |       |       |       |
|---|-------|-------|-------|
| 6 | 3.450911 | 1.812871 | 0.287342 |
| 1 | 4.469206 | 1.486194 | 0.106492 |
| 6 | 3.227624 | 3.170003 | 0.732035 |
| 6 | 1.947982 | 3.640888 | 0.891498 |
| 1 | 1.774511 | 4.667426 | 1.199149 |
| 6 | 0.843666 | 2.794175 | 0.640611 |
| 6 | 0.843666 | 2.794175 | 0.640611 |
| 6 | 0.843666 | 2.794175 | 0.640611 |
| 6 | 0.843666 | 2.794175 | 0.640611 |
| 6 | 0.843666 | 2.794175 | 0.640611 |
| 6 | 0.843666 | 2.794175 | 0.640611 |
| 6 | 0.843666 | 2.794175 | 0.640611 |
| 6 | 0.843666 | 2.794175 | 0.640611 |
| 6 | 0.843666 | 2.794175 | 0.640611 |
|   | 1.872486 | -2.228115 | -3.098718 |
|---|----------|-----------|-----------|
| 1 | 3.556841 | -1.850902 | -4.003546 |
| 1 | 3.447803 | -2.765826 | -2.493484 |
| 6 | 2.468264 | 0.522013  | -3.066864 |
| 1 | 1.400892 | 0.360062  | -3.244046 |
| 1 | 2.588566 | 1.485580  | -2.562727 |
| 1 | 2.979450 | 0.578481  | -4.034518 |
| 6 | -2.533152| -1.565008 | -3.283787 |
| 1 | -2.962259| -2.494015 | -2.904484 |
| 1 | -2.913061| -1.407597 | -4.299833 |
| 1 | -1.447402| -1.694200 | -3.326820 |
| 6 | -2.321141| 0.912793  | -3.074314 |
| 1 | -2.623716| 1.822126  | -2.549393 |
| 1 | -1.226676| 0.877626  | -3.099840 |
| 1 | -2.683405| 0.977546  | -4.106368 |
| 6 | -4.008370| 4.426542  | 0.780007  |
| 1 | -4.583449| 4.554651  | -0.144568 |
| 1 | -4.710093| 4.077987  | 1.546883  |
| 1 | -3.636548| 5.407740  | 1.084861  |
| 6 | 4.421321 | 4.041142  | 0.985577  |
| 1 | 5.053992 | 3.624764  | 1.778329  |
| 1 | 5.046923 | 4.126087  | 0.089169  |
| 1 | 4.125065 | 5.048964  | 1.286362  |

Name - R_Ts3b
Zero-point correction= 0.699139 (Hartree/Particle)
Thermal correction to Energy= 0.739238
Thermal correction to Enthalpy= 0.740182
Thermal correction to Gibbs Free Energy= 0.630144
Sum of electronic and zero-point Energies= -2122.643366
Sum of electronic and thermal Energies= -2122.603267
Sum of electronic and thermal Enthalpies= -2122.602323
Sum of electronic and thermal Free Energies= -2122.712361
1 imaginary frequency.
Charge = 0 Multiplicity = 1

0 1
26 0.000112 -0.954802 0.664665
1 -0.001841 -0.404622 2.126994
1 0.419868 -2.388142 1.296750
15 -2.181754 -0.643350 0.617862
15 2.181574 -0.638691 0.619649
1 -1.056705 1.580251 -0.182011
7 1.052294 1.582132 -0.182211
6 -0.001459 0.774438 0.074963
6 -2.337219 1.117249 0.011535
6 -3.342261 2.005368 -0.209840
1 -4.372088 1.709705 -0.042128
6 -3.066658 3.355002 -0.644333
|   |       |       |       |       |
|---|-------|-------|-------|-------|
| 6 | -1.770086 | 3.770652 | -0.818653 | 3.1770657 | -1.374363 |
| 1 | -1.55661 | 4.786668 | -1.134994 | -0.645156 |
| 6 | -0.700519 | 2.879449 | -0.574648 | -0.210246 |
| 6 | 0.693699 | 2.880678 | -0.574828 | -0.574151 |
| 1 | 1.761601 | 3.773765 | -0.819225 | 1.283021 |
| 6 | 0.003262 | -1.779726 | -1.167801 | -1.210246 |
| 6 | 0.001243 | -1.024695 | -2.362323 | -2.362323 |
| 1 | -0.002930 | 0.064304 | -2.305981 | -2.305981 |
| 1 | -0.418071 | -2.394559 | 1.283021 | 1.283021 |
| 6 | 0.008382 | -3.177567 | -1.374363 | -1.374363 |
| 6 | 0.011569 | -3.770191 | -2.636535 | -2.636535 |
| 1 | 0.015599 | -4.855320 | -2.722981 | -2.722981 |
| 6 | 0.009554 | -2.981469 | -3.783865 | -3.783865 |
| 1 | 0.012004 | -3.435479 | -4.771157 | -4.771157 |
| 6 | 0.004243 | -1.597182 | -3.635210 | -3.635210 |
| 1 | 0.010208 | -3.844952 | -0.511644 | -0.511644 |
| 1 | 0.002451 | -0.955979 | -4.514950 | -4.514950 |
| 6 | -3.165029 | -0.611481 | 2.208174 | 2.208174 |
| 1 | -4.231621 | -0.621688 | 1.946994 | 1.946994 |
| 6 | -3.219358 | -1.596264 | -0.606985 | -0.606985 |
| 1 | -2.507360 | -1.532450 | -1.508798 | -1.508798 |
| 6 | 3.223254 | -1.591135 | -0.602068 | -0.602068 |
| 1 | 2.601635 | -1.532014 | -1.504432 | -1.504432 |
| 6 | 3.162929 | -0.601865 | 2.211138 | 2.211138 |
| 1 | 4.229789 | -0.609338 | 1.950933 | 1.950933 |
| 6 | -3.295086 | -3.068749 | -0.205737 | -0.205737 |
| 1 | -3.673040 | -3.656257 | -1.050799 | -1.050799 |
| 1 | -2.311825 | -3.468033 | 0.053227 | 0.053227 |
| 1 | -3.979036 | -3.221475 | 0.633935 | 0.633935 |
| 6 | -4.604052 | -1.039487 | -0.912812 | -0.912812 |
| 1 | -5.116524 | -1.702034 | -1.619534 | -1.619534 |
| 1 | -5.23713 | -0.977367 | -0.017457 | -0.017457 |
| 1 | -4.553229 | -0.049754 | -1.371173 | -1.371173 |
| 6 | 3.303914 | -3.062192 | -0.198367 | -0.198367 |
| 1 | 2.322222 | -3.463637 | 0.064989 | 0.064989 |
| 1 | 3.682586 | -3.651118 | -1.040271 | -1.040271 |
| 1 | 3.989314 | -3.210265 | 0.642801 | 0.642801 |
| 6 | 4.606189 | -1.030420 | -0.908629 | -0.908629 |
| 1 | 5.234929 | -0.963129 | -0.012985 | -0.012985 |
| 1 | 5.121566 | -1.693460 | -1.612775 | -1.612775 |
| 1 | 4.552151 | -0.042392 | -1.370269 | -1.370269 |
| 6 | -2.822096 | -1.853459 | 3.030925 | 3.030925 |
| 1 | -1.758845 | -1.833780 | 3.291837 | 3.291837 |
| 1 | -3.405159 | -1.858907 | 3.958661 | 3.958661 |
| 1 | -3.024461 | -2.787211 | 2.501449 | 2.501449 |
fgdd

Geometries of X-substituted isomers of TS1 (X = F, Me, MeO, Me2N).

Name - TS2_F_m1_
Zero-point correction= 0.693295 (Hartree/Particle)
Thermal correction to Energy= 0.734135
Thermal correction to Enthalpy= 0.735079
Thermal correction to Gibbs Free Energy= 0.622161
Sum of electronic and zero-point Energies= -2221.781209
Sum of electronic and thermal Energies= -2221.740369
Sum of electronic and thermal Enthalpies= -2221.739425
Sum of electronic and thermal Free Energies= -2221.852343
1 imaginary frequency.
Charge =  0  Multiplicity = 1
0 1
26  0.504842  -0.415974  -0.130437
1  0.474315  -0.393101  1.396486
1  1.421712  -1.161140  -1.058842
15 -0.850716  -2.161275  -0.058056
15  1.294867  1.646068  0.022473
7  -2.354061  -0.018356  -0.148476
7  -1.322262  1.818319  -0.062682
6  -1.098580  0.485940  -0.142362
6  -2.544709  -1.380943  -0.151951
|   |   |   |   |
|---|---|---|---|
|6  |-3.831955| -1.814649| -0.190996|
|1  |-4.045598| -2.877916| -0.217611|
|6  |-4.933684| -0.879007| -0.193518|
|6  |-4.691151| 0.471196 | -0.130299|
|1  |-5.516125| 1.176564 | -0.111367|
|6  |-3.363085| 0.954903 | -0.092393|
|6  |-2.680170| 2.169263 | 0.089895 |
|6  |-2.960451| 3.550626 | 0.089895 |
|1  |-3.992788| 3.866092 | 0.105611|
|6  |-1.933981| 4.455739 | 0.199829|
|6  |-0.562482| 4.000888 | 0.197838|
|1  | 0.231159| 4.728418 | 0.329018|
|6  |-0.259007| 2.683859 | 0.055746|
|6  | 2.414284| -1.286420| -0.030264|
|6  | 3.521080| -0.956627| -0.831182|
|1  | 3.388789| -0.383445| -1.746097|
|1  | 0.623274| -0.486617| -1.691383|
|6  | 2.679696| -2.093349| 1.095556 |
|6  | 3.973543| -2.480320| 1.429924 |
|1  | 4.142686| -3.072830| 2.325868 |
|6  | 5.064587| -2.109481| 0.643125 |
|6  | 4.804629| -1.355162| -0.487052|
|1  | 1.863500| -2.370944| 1.752376 |
|6  | 2.267731| 2.418962 | -1.377921|
|1  | 3.137748| 1.753299 | -1.453669|
|6  | 2.171819| 2.265720 | 1.544782 |
|1  | 2.267421| 3.353629 | 1.430174 |
|6  |-0.926586| -3.400681| -1.445553|
|1  |-1.774202| -4.068555| -1.246975|
|6  |-0.973308| -3.221307| 1.481111 |
|1  | 0.061615| -3.567362| 1.610484 |
|6  | 3.563541| 1.641401 | 1.632954 |
|1  | 4.094681| 2.038996 | 2.504896 |
|1  | 3.493942| 0.555208 | 1.741323 |
|1  | 4.173064| 1.847805 | 0.747692 |
|6  | 1.357986| 1.981572 | 2.801785 |
|1  | 1.200979| 0.905539 | 2.916703 |
|1  | 1.890190| 2.359984| 3.681883 |
|1  | 0.375118| 2.461880 | 2.766305 |
|6  | 2.766679| 3.843107 | -1.161230|
|1  | 3.348712| 4.164935 | -2.032236|
|1  | 1.931995| 4.544042 | -1.057512|
|1  | 3.411671| 3.939083 | -0.284073|
|6  | 1.466950| 2.312348 | -2.673109|
|1  | 2.087210| 2.605035 | -3.527232|
|1  | 1.104327| 1.293446 | -2.832620|
|1  | 0.598226| 2.980120 | -2.645299|
|6  | 0.368061| -4.211894| -1.452565|
|1  | 0.520131| -4.762844| -0.518945|
|1  | 0.355598| -4.939206| -2.271583|
1  1.235788  -3.559031  -1.593656
6  -1.160369  -2.707678  -2.792166
1  -1.193238  -3.451578  -3.587788
1  -2.105523  -2.156261  -2.783851
1  -0.357483  -1.997281  -3.000108
6  -1.337419  -2.347338  2.678324
1  -2.377171  -2.008571  2.604768
1  -1.235140  -2.917785  3.607810
1  -0.692800  -1.465167  2.727708
6  -1.888281  -4.437674  1.393241
1  -1.597523  -5.134320  0.602641
1  -1.861213  -4.986964  2.341045
1  -2.928438  -4.139025  1.226406
6  -2.195639  5.925778  0.335108
1  -1.763716  6.320176  1.262389
1  -1.742917  6.485780  -0.491630
1  -3.266377  6.143338  0.342727
6  -6.329652  -1.423149  -0.249205
1  -6.528601  -2.091309  0.596974
1  -7.072672  -0.622325  -0.228183
1  -6.489563  -2.008036  -1.162655
1  6.081261  -2.399748  0.884455
9  5.830178  -0.990229  -1.280115

Name - TS2_F_m2_
Zero-point correction= 0.693074 (Hartree/Particle)
Thermal correction to Energy= 0.733955
Thermal correction to Enthalpy= 0.734899
Thermal correction to Gibbs Free Energy= 0.620955
Sum of electronic and zero-point Energies= -2221.781545
Sum of electronic and thermal Energies= -2221.740663
Sum of electronic and thermal Enthalpies= -2221.739719
Sum of electronic and thermal Free Energies= -2221.853663
1 imaginary frequency.
Charge = 0 Multiplicity = 1

0 1
26  -0.607682  -0.176043  0.297321
1  -0.694255  -0.182993  -1.226727
1  -1.621774  -0.606999  1.320397
15  0.189161  -2.240119  0.191335
15  -0.791669  2.020049  0.114507
7  2.238118  -0.611612  0.073194
7  1.764432  1.441013  -0.009495
6  1.181462  0.229694  0.148856
6  2.035285  -1.971756  0.117921
6  3.145659  -2.753641  0.067750
1  3.051819  -3.832956  0.121856
6  4.462163  -2.171947  -0.063293
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 6 | 4.606328 | -0.810204 | -0.165231 |
| 1 | 5.591277 | -0.369979 | -0.286093 |
| 6 | 3.471435 | 0.031480  | -0.111542 |
| 6 | 3.156440 | 1.388612  | -0.286093 |
| 6 | 3.806360 | 2.629426  | -0.380910 |
| 1 | 4.882530 | 2.655232  | -0.498001 |
| 6 | 3.069057 | 3.787198  | -0.560087 |
| 1 | 1.631002 | 3.742863  | -0.316477 |
| 1 | 1.066012 | 4.662947  | -0.420692 |
| 6 | 0.982736 | 2.570877  | -0.086107 |
| 6 | -2.684817 | -0.473681 | 0.372058  |
| 6 | -3.603925 | 0.168102  | 1.224003  |
| 1 | -0.613306 | -0.179297 | 1.864027  |
| 6 | -3.234457 | -1.213377 | -0.691160 |
| 6 | -4.603054 | -1.229637 | -0.903521 |
| 6 | -5.501172 | -0.560087 | -0.082872 |
| 6 | -4.979241 | 0.136527  | 1.001176  |
| 6 | -1.379636 | 3.070917  | 1.548622  |
| 1 | -2.392624 | 2.684242  | 1.721984  |
| 6 | -1.584087 | 2.828420  | -1.365871 |
| 1 | -1.362752 | 3.901380  | -1.293059 |
| 6 | 0.028465 | -3.417840 | 1.624213  |
| 1 | 0.623235 | -4.310590 | 1.392642  |
| 6 | -0.128048 | -3.322025 | -1.304421 |
| 1 | -1.225321 | -3.375328 | -1.330384 |
| 6 | -3.095846 | 2.616487  | -1.327194 |
| 1 | -3.564114 | 3.116198  | -2.182470 |
| 6 | -3.334865 | 1.550831  | -1.380314 |
| 1 | -3.554531 | 3.012521  | -0.416007 |
| 6 | -0.987453 | 2.300714  | -2.665727 |
| 1 | -1.154846 | 1.223488  | -2.751581 |
| 1 | -1.457651 | 2.802412  | -3.519094 |
| 1 | 0.091327 | 2.477956  | -2.718557 |
| 6 | -1.468457 | 4.573263  | 1.305045  |
| 1 | -1.862427 | 5.069013  | 2.199620  |
| 1 | -0.479515 | 5.001652  | 1.111966  |
| 1 | -2.126946 | 4.831440  | 0.471698  |
| 6 | -0.530842 | 2.765770  | 2.780347  |
| 1 | -0.961602 | 3.244362  | 3.666584  |
| 1 | -0.462645 | 1.689067  | 2.957983  |
| 1 | 0.486914 | 3.152225  | 2.652415  |
| 6 | -1.440206 | -3.811443 | 1.773440  |
| 1 | -1.828239 | -4.322745 | 0.886723  |
| 1 | -1.567465 | -4.483994 | 2.628716  |
| 1 | -2.064608 | -2.927809 | 1.942478  |
| 6 | 0.573331 | -2.792363 | 2.904051  |
| 1 | 0.457887 | -3.491997 | 3.739486  |
| 1 | 1.635649 | -2.546378 | 2.811314  |
| 1 | 0.036786 | -1.870269 | 3.145127  |
| 6 | 0.344412 | -2.604971 | -2.566369 |
|     |        |        |
|-----|--------|--------|
|     | 1.439077 | -2.558089 |
|     | 0.426229  | -4.740758  |
|     | 3.721289  | 5.117612  |
|     | 3.339786  | 5.592368  |
|     | 3.516997  | 5.806155  |
|     | 4.805229  | 5.021243  |
|     | 5.645901  | -3.091237 |
|     | 5.566599  | -3.803620 |
|     | 6.579656  | -2.536689 |
|     | 5.719844  | -3.680738 |
|     | -6.564572 | -0.604038 |
|     | -5.651655 | 0.656147  |
|     | -3.225763 | 0.702598  |
|     | -2.599985 | -1.733723 |
|     | -5.084467 | -1.917820 |

Name - TS2_F_o1_

Zero-point correction= 0.693179 (Hartree/Particle)
Thermal correction to Energy= 0.733980
Thermal correction to Enthalpy= 0.734924
Thermal correction to Gibbs Free Energy= 0.622300

Sum of electronic and zero-point Energies= -2221.785181
Sum of electronic and thermal Energies= -2221.744380
Sum of electronic and thermal Enthalpies= -2221.743436
Sum of electronic and thermal Free Energies= -2221.856060

1 imaginary frequency.
Charge = 0 Multiplicity = 1
|   |       |       |       |
|---|-------|-------|-------|
| 6 | -2.467174 | 2.326014 | 0.081535 |
| 6 | -2.659438 | 3.717386 | 0.245680 |
| 1 | -3.668677 | 4.114696 | 0.289992 |
| 6 | -1.577131 | 4.552993 | 0.368793 |
| 6 | -0.236762 | 4.015426 | 0.323544 |
| 1 | 0.603711  | 4.688492 | 0.455297 |
| 6 | -0.019238 | 2.687787 | 0.131860 |
| 6 | 2.377320  | -1.501825 | 0.002863 |
| 6 | 3.564148  | -1.339706 | -0.713695 |
| 1 | 0.626412  | -0.524218 | 1.672732 |
| 6 | 2.503120  | -2.338627 | 1.130922 |
| 6 | 3.716114  | -2.894797 | 1.525155 |
| 6 | 1.626449  | -2.506813 | 1.744258 |
| 6 | 2.337986  | 2.302177  | -1.504888 |
| 1 | 3.134779  | 1.574025  | -1.691375 |
| 6 | 2.500811  | 2.134336  | 1.422898 |
| 1 | 2.651922  | 3.214581  | 1.296714 |
| 6 | -1.061847 | -3.318571 | -1.480694 |
| 1 | -1.945010 | -3.942695 | -1.295272 |
| 6 | -1.117878 | -3.190036 | 1.446594 |
| 1 | -0.119155 | -3.635446 | 1.552009 |
| 6 | 3.854942  | 1.428193  | 1.398873 |
| 1 | 4.491382  | 1.813949  | 2.203054 |
| 1 | 3.730377  | 0.352404  | 1.550900 |
| 1 | 4.388253  | 1.571027  | 0.453553 |
| 6 | 1.779129  | 1.894647  | 2.743877 |
| 1 | 1.567489  | 0.829573  | 2.872602 |
| 1 | 2.401423  | 2.237072  | 3.576584 |
| 1 | 0.826671  | 2.431775  | 2.788015 |
| 6 | 2.949416  | 3.685810  | -1.319592 |
| 1 | 3.442689  | 3.996070  | -2.247898 |
| 1 | 2.181748  | 4.435366  | -1.100023 |
| 1 | 3.700321  | 3.716504  | -0.525447 |
| 6 | 1.390525  | 2.276749  | -2.702283 |
| 1 | 1.933868  | 2.534315  | -3.617884 |
| 1 | 0.943377  | 1.287120  | -2.827873 |
| 1 | 0.582420  | 3.006774  | -2.575368 |
| 6 | 0.186340  | -4.199372 | -1.498028 |
| 1 | 0.308721  | -4.768591 | -0.570971 |
| 1 | 0.133917  | -4.915478 | -2.325346 |
| 1 | 1.088077  | -3.592915 | -1.633208 |
| 6 | -1.253532 | -2.592265 | -2.807829 |
| 1 | -1.330255 | -3.320248 | -3.623275 |
| 1 | -2.164521 | -1.985903 | -2.806251 |
| 1 | -0.409887 | -1.926995 | -3.011968 |
| 6 | -1.381472 | -2.311042 | 2.666335 |
| 1 | -2.387678 | -1.879012 | 2.617591 |
1   -1.315737    -2.905908    3.583796
1   -0.661675    -1.488730    2.718788
6   -2.138214    -4.318850    1.352189
1   -1.926848    -5.016517    0.537613
1   -2.136266    -4.893947    2.285066
1   -3.152162    -3.927818    1.220593
6   -1.744927    6.030792    0.557771
1   -1.282393    6.364264    1.494145
1   -1.263459    6.589841   -0.253193
1   -2.799759    6.314835    0.582477
6   -6.337688   -1.022410   -0.191850
1   -6.564395   -1.706895    0.634087
1   -7.028948   -0.178530   -0.129352
1   -6.548626   -1.563238   -1.121988
1   5.822329   -3.097289    1.080207
1   5.657102   -1.683543   -0.989458
9   3.540038   -0.592967   -1.849837

Name - TS2_F_o2_
Zero-point correction=                           0.693565 (Hartree/Particle)
Thermal correction to Energy=                    0.734205
Thermal correction to Enthalpy=                  0.735149
Thermal correction to Gibbs Free Energy=         0.623708
Sum of electronic and zero-point Energies=        -2221.786385
Sum of electronic and thermal Energies=           -2221.745745
Sum of electronic and thermal Enthalpies=         -2221.744801
Sum of electronic and thermal Free Energies=      -2221.856242
1 imaginary frequency.
Charge =  0 Multiplicity = 1
0 1

26   -0.617580    -0.364583    0.211813
1   -0.778858    -0.414154   -1.301581
1   -1.443207   -1.049721    1.283389
15   0.707151   -2.134458    0.015662
15   -1.355463    1.714256   -0.006226
7   2.249553   -0.034203    0.187505
7   1.262046    1.820785    0.023415
6   1.004858    0.495978    0.126400
6   2.406639   -1.398244    0.255420
6   3.678685   -1.858985    0.381447
1   3.864319   -2.925496    0.456280
6   4.800490   -0.947384    0.405132
6   4.594612    0.403767    0.273937
1   5.436057    1.089605    0.271700
6   3.280875    0.915039    0.154221
6   2.628608    2.141367    0.029357
6   2.943696    3.513101   -0.105423
1   3.983887    3.823833   -0.104411
|   |        |        |        |
|---|--------|--------|--------|
| 6 | 1.941831 | 4.439971 | -0.252727 |
| 6 | 0.559075  | 4.020268  | -0.251885  |
| 1 | -0.214504 | 4.767701  | -0.388584  |
| 6 | 0.221226  | 2.712846  | -0.096704  |
| 6 | -2.557771 | -1.175391 | 0.429534   |
| 6 | -3.560542 | -0.671557 | 1.280004   |
| 1 | -0.544754 | -0.382993 | 1.780752   |
| 6 | -3.020587 | -2.101491 | -0.506463  |
| 6 | -4.357039 | -2.432916 | -0.681301  |
| 1 | -4.625802 | -3.133872 | -1.465571  |
| 6 | -5.316941 | -1.863888 | 0.150565   |
| 6 | -4.910515 | -0.986863 | 1.150680   |
| 6 | -2.310183 | 2.595276  | 1.344404   |
| 1 | -3.214940 | 1.979660  | 1.426912   |
| 6 | -2.232386 | 2.252130  | -1.559616  |
| 1 | -2.363284 | 3.339733  | -1.490764  |
| 6 | 0.716049  | -3.555231 | 1.215462   |
| 1 | 1.573989  | -4.195438 | 0.972908   |
| 6 | 0.939419  | -2.938721 | -1.660386  |
| 1 | -0.079543 | -3.240973 | -1.920585  |
| 6 | -3.599433 | 1.573513  | -1.621464  |
| 1 | -4.134625 | 1.888855  | -2.524005  |
| 1 | -3.483707 | 0.485913  | -1.653265  |
| 1 | -4.228097 | 1.812967  | -0.758135  |
| 6 | -1.405108 | 1.944918  | -2.802413  |
| 1 | -1.224827 | 0.869162  | -2.880576  |
| 1 | -1.941760 | 2.280412  | -3.697106  |
| 1 | -0.434459 | 2.450307  | -2.778974  |
| 6 | -2.738157 | 4.032765  | 1.072529   |
| 1 | -3.329067 | 4.405389  | 1.917134   |
| 1 | -1.872650 | 4.695097  | 0.972461   |
| 1 | -3.355502 | 4.129204  | 0.175555   |
| 6 | -1.536330 | 2.490403  | 2.656049   |
| 1 | -2.149361 | 2.849359  | 3.490120   |
| 1 | -1.231661 | 1.459444  | 2.858110   |
| 1 | -0.629208 | 3.104658  | 2.618978   |
| 6 | -0.574224 | -4.356312 | 1.051217   |
| 1 | -0.718636 | -4.714413 | 0.027837   |
| 1 | -0.566707 | -5.225388 | 1.718128   |
| 1 | -1.442094 | -3.741123 | 1.309031   |
| 6 | 0.875571  | -3.048265 | 2.645557   |
| 1 | 0.870935  | -3.892037 | 3.344773   |
| 1 | 1.812890  | -2.499754 | 2.778105   |
| 1 | 0.057019  | -2.373791 | 2.913587   |
| 6 | 1.393670  | -1.886608 | -2.669792  |
| 1 | 2.428001  | -1.579418 | -2.476048  |
| 1 | 1.352933  | -2.299569 | -3.683475  |
| 1 | 0.750893  | -1.003190 | -2.624789  |
| 6 | 1.856790  | -4.154648 | -1.689544  |
| 1 | 1.501534  | -4.970613 | -1.054256  |
1 1.921344 -4.541438 -2.712902
1 2.874555 -3.892067 -1.365117
6 2.241838 5.899684 -0.417790
1 1.842234 6.280494 -1.365117
1 1.783314 6.491520 0.383207
1 3.317465 6.091426 -0.405070
6 6.178397 -1.518621 0.556550
1 6.402591 -2.230356 -0.246690
1 6.941081 -0.736410 0.536689
1 6.277818 -2.063353 1.502842
1 -6.364712 -2.119903 0.024780
1 -5.637733 -0.555242 1.832785
1 -3.251173 -0.010486 2.087224
9 -2.154456 -2.715848 -1.341455

Name - TS2_F_p_
Zero-point correction= 0.692825 (Hartree/Particle)
Thermal correction to Energy= 0.733620
Thermal correction to Enthalpy= 0.734564
Thermal correction to Gibbs Free Energy= 0.621091
Sum of electronic and zero-point Energies= -2221.779973
Sum of electronic and thermal Energies= -2221.739179
Sum of electronic and thermal Enthalpies= -2221.738235
Sum of electronic and thermal Free Energies= -2221.851708
1 imaginary frequency.
Charge = 0 Multiplicity = 1

0 1
26 -0.555466 -0.249240 0.213915
1 -0.632588 -0.230133 -1.308828
1 -1.549555 -0.747515 1.239594
15 0.392806 -2.249442 0.083154
15 -0.890632 1.931538 0.057129
7 2.320659 -0.475742 0.102848
7 1.702787 1.539643 0.028231
6 1.202775 0.285477 0.136661
6 2.215985 -1.847849 0.126219
6 3.381504 -2.546416 0.126981
1 3.365107 -3.630785 0.163851
6 4.656244 -1.868149 0.074980
6 4.704907 -0.497339 -0.004503
1 5.659265 0.015480 -0.062586
6 3.510573 0.259164 -0.000948
6 3.100798 1.591638 -0.063098
6 3.669444 2.881079 -0.201600
1 4.747734 2.987407 -0.263188
6 2.856981 3.985652 -0.285801
6 1.421507 3.835323 -0.222360
1 0.795973 4.715741 -0.329086
|   | 6  | 0.845617 | 2.613362 | -0.055505 |
|---|----|----------|----------|-----------|
| 6 | -2.615956 | -0.719241 | 0.266687 |
| 6 | -3.592141 | -0.138258 | 1.094789 |
| 1 | -0.600775 | -0.284497 | 1.787217 |
| 6 | -3.106025 | -1.502272 | -0.795638 |
| 6 | -4.463083 | -1.636084 | -1.059826 |
| 1 | -4.823535 | -2.217935 | -1.903875 |
| 6 | -5.377039 | -1.005197 | -0.225554 |
| 6 | -4.963823 | -0.261849 | 0.860806 |
| 1 | -2.399129 | -1.979112 | -1.471775 |
| 6 | -1.616238 | 2.906292 | 1.483391 |
| 1 | -2.595223 | 2.431514 | 1.615326 |
| 6 | -1.678527 | 2.699662 | -1.445581 |
| 1 | -1.590047 | 3.786912 | -1.330491 |
| 6 | 0.240882 | -3.511124 | 1.443278 |
| 1 | 0.925801 | -4.337497 | 1.212165 |
| 6 | 0.249039 | -3.270935 | -1.483162 |
| 1 | -0.834050 | -3.393583 | -1.586835 |
| 6 | -3.155885 | 2.310692 | -1.494162 |
| 1 | -3.635205 | 2.776398 | -2.361986 |
| 1 | -3.259500 | 1.226757 | -1.578309 |
| 1 | -3.703280 | 2.625159 | -0.596705 |
| 6 | -0.954589 | 2.286012 | -2.718445 |
| 1 | -0.978294 | 1.199034 | -2.832607 |
| 1 | -1.446672 | 2.743671 | -3.589257 |
| 1 | 0.093546 | 2.601027 | -2.713514 |
| 6 | -1.831446 | 4.399068 | 1.256928 |
| 1 | -2.282557 | 4.843725 | 2.153870 |
| 1 | -0.883721 | 4.920567 | 1.087749 |
| 1 | -2.499062 | 4.606618 | 0.417849 |
| 6 | -0.781684 | 2.654221 | 2.735814 |
| 1 | -1.290203 | 3.059024 | 3.621050 |
| 6 | -0.606769 | 1.584924 | 2.889098 |
| 1 | 0.191028 | 3.153574 | 2.659283 |
| 6 | -1.194106 | -4.036062 | 1.469267 |
| 1 | -1.474924 | -4.525157 | 0.525955 |
| 1 | -1.318652 | -4.768141 | 2.273502 |
| 1 | -1.903005 | -3.218065 | 1.635672 |
| 6 | 0.638616 | -2.906443 | 2.789552 |
| 1 | 0.528581 | -3.657989 | 3.579626 |
| 1 | 1.674121 | -2.564132 | 2.781879 |
| 1 | 0.004501 | -2.050266 | 3.032448 |
| 6 | 0.753021 | -2.458350 | -2.673200 |
| 1 | 1.842630 | -2.346672 | -2.630827 |
| 1 | 0.503227 | -2.963829 | -3.607546 |
| 1 | 0.308044 | -1.456856 | -2.679478 |
| 6 | 0.897404 | -4.647962 | -1.447392 |
| 1 | 0.494884 | -5.293226 | -0.659381 |
| 1 | 0.727369 | -5.158338 | -2.406175 |
| 1 | 1.984487 | -4.572654 | -1.311443 |
|   | 3.421400 | 5.360499 | -0.444793 |
|---|----------|----------|------------|
| 1 | 3.048801 | 5.834180 | -1.365976  |
| 1 | 3.126136 | 6.008953 | 0.385850   |
| 1 | 4.512469 | 5.343113 | -0.495300  |
| 6 | 5.904475 | -2.698676 | 0.089368   |
| 1 | 5.919194 | -3.405698 | -0.751948  |
| 1 | 6.799264 | -2.075669 | 0.017882   |
| 1 | 5.975645 | -3.292407 | 1.005961   |
| 1 | -5.697658 | 0.204727 | 1.511243   |
| 9 | -6.94587 | -1.136271 | -0.478408  |

Name - TS2_Me_m1_  
Zero-point correction= 0.728893 (Hartree/Particle)  
Thermal correction to Energy= 0.770769  
Thermal correction to Enthalpy= 0.771713  
Thermal correction to Gibbs Free Energy= 0.656187  
Sum of electronic and zero-point Energies= -2161.873152  
Sum of electronic and thermal Energies= -2161.831276  
Sum of electronic and thermal Enthalpies= -2161.830332  
Sum of electronic and thermal Free Energies= -2161.945858  
1 imaginary frequency.  
Charge = 0  Multiplicity = 1
|   |    |    |    |
|---|----|----|----|
| 1 | 0.637503 | -0.531508 | -1.696663 |
| 6 | 2.603270 | -2.156102 | 1.132717 |
| 6 | 3.886617 | -2.560127 | 1.485712 |
| 1 | 4.033691 | -3.161184 | 2.380465 |
| 6 | 4.988002 | -2.195598 | 0.712458 |
| 6 | 4.804013 | -1.430584 | -0.437881 |
| 1 | 1.770851 | -2.426751 | 1.773031 |
| 6 | 2.300585 | -2.560127 | -1.132717 |
| 1 | 3.153161 | 1.668991 | -1.485712 |
| 6 | 2.231575 | 2.205173 | 1.530312 |
| 1 | 2.336493 | 3.292863 | 1.420055 |
| 1 | 1.770851 | -2.426751 | 1.773031 |
| 6 | 2.300585 | -2.560127 | -1.132717 |
| 1 | 3.153161 | 1.668991 | -1.485712 |
| 6 | 2.231575 | 2.205173 | 1.530312 |
| 1 | 2.336493 | 3.292863 | 1.420055 |
| 1 | 1.770851 | -2.426751 | 1.773031 |
| 6 | 2.300585 | -2.560127 | -1.132717 |
| 1 | 3.153161 | 1.668991 | -1.485712 |
| 6 | 2.231575 | 2.205173 | 1.530312 |
| 1 | 2.336493 | 3.292863 | 1.420055 |
1  -3.124383  6.208694  0.388689
6   -6.372861 -1.276589 -0.238324
1  -6.581541 -1.942617  0.607221
1   -7.096191 -0.458157 -0.209183
1  -6.553689 -1.854532 -1.152329
1   3.363271 -0.462743 -1.688136
1  5.987950 -2.514527  0.997750
6   5.971931 -1.002207 -1.282018
1  6.344119 -0.017959 -0.970544
1   6.806455 -1.704925 -1.201066
1  5.694211 -0.924386 -2.337668

Name - TS2_Me_m2_
Zero-point correction=          0.728898 (Hartree/Particle)
Thermal correction to Energy=          0.770779
Thermal correction to Enthalpy=          0.771723
Thermal correction to Gibbs Free Energy=   0.655544
Sum of electronic and zero-point Energies= -2161.873124
Sum of electronic and thermal Energies= -2161.831243
Sum of electronic and thermal Enthalpies= -2161.830299
Sum of electronic and thermal Free Energies= -2161.946478
1 imaginary frequency.
Charge =  0  Multiplicity = 1
| 1  | -0.610293 | -0.158734 | 1.887552 |
| 6  | -3.274943 | -1.096744 | -0.662252 |
| 6  | -4.647695 | -1.099864 | -0.909480 |
| 6  | -5.494226 | -0.396713 | -0.043134 |
| 6  | -4.960550 | 0.274910  | 1.047635  |
| 1  | -2.629498 | -1.618846 | -1.362166 |
| 6  | -1.279794 | 3.119144  | 1.556013  |
| 1  | -2.301005 | 2.758971  | 1.737988  |
| 6  | -1.509763 | 2.866624  | -1.353833 |
| 1  | -1.259618 | 3.933644  | -1.286705 |
| 6  | -0.046710 | -3.402950 | 1.655816  |
| 1  | 0.521523  | -4.312835 | 1.424223  |
| 1  | -0.237710 | -3.320424 | 1.278785  |
| 6  | -3.026388 | 2.694270  | -1.304980 |
| 1  | -3.486611 | 3.207660  | -2.156716 |
| 1  | -3.294140 | 1.635275  | -1.356137 |
| 6  | -3.468605 | 3.101113  | -0.390432 |
| 6  | -0.935514 | 2.318076  | -2.655055 |
| 1  | -1.126551 | 1.244056  | -2.731535 |
| 1  | -1.401971 | 2.824179  | -3.508001 |
| 1  | 0.146342  | 2.471850  | -2.717993 |
| 1  | -1.331762 | 4.621717  | 1.303524  |
| 1  | -1.705915 | 5.133122  | 2.197838  |
| 1  | -0.333725 | 5.023498  | 1.099840  |
| 1  | -1.990012 | 4.891350  | 0.473617  |
| 6  | -0.431776 | 2.799967  | 2.784687  |
| 1  | -0.843413 | 3.297357  | 3.669732  |
| 1  | -0.393271 | 1.723299  | 2.970867  |
| 1  | 0.595741  | 3.156543  | 2.647802  |
| 6  | -1.523992 | -3.755151 | 1.822759  |
| 1  | -1.933209 | -4.265323 | 0.944952  |
| 1  | -1.661309 | -4.414996 | 2.686432  |
| 1  | -2.123295 | -2.853313 | 1.986471  |
| 6  | 0.528302  | 2.784995  | 2.926180  |
| 1  | 0.406493  | 3.478049  | 3.766249  |
| 1  | 1.594937  | 2.564574  | 2.819393  |
| 1  | 0.016536  | 1.849574  | 3.169487  |
| 6  | 0.238286  | -2.626641 | -2.542634 |
| 1  | 1.333410  | -2.608469 | -2.585214 |
| 1  | 1.023209  | -3.163410 | -3.424625 |
| 1  | -0.121000 | -1.594004 | -2.582077 |
| 6  | 0.274307  | -4.754638 | -1.203010 |
| 1  | -0.123559 | -5.311526 | -0.350650 |
| 1  | -0.019255 | -5.292773 | -2.111442 |
| 1  | 1.367781  | -4.782375 | -1.154226 |
| 6  | 3.861313  | 5.009795  | -0.733813 |
| 1  | 3.483176  | 5.489116  | -1.644490 |
| 1  | 3.685667  | 5.709395  | 0.091829  |
| 1  | 4.940995  | 4.882351  | -0.843339 |
Name - TS2_Me_o1_
Zero-point correction= 0.729578 (Hartree/Particle)
Thermal correction to Energy= 0.771060
Thermal correction to Enthalpy= 0.772004
Thermal correction to Gibbs Free Energy= 0.658326
Sum of electronic and zero-point Energies= -2161.867743
Sum of electronic and thermal Energies= -2161.826262
Sum of electronic and thermal Enthalpies= -2161.825317
Sum of electronic and thermal Free Energies= -2161.938995
1 imaginary frequency.
Charge = 0  Multiplicity = 1
0 1

|   |         |         |         |
|---|---------|---------|---------|
| 6 | 5.557358| -3.248322| -0.147480|
| 1 | 5.447028| -3.959866| -0.974332|
| 1 | 6.505164| -2.721237| -0.280891|
| 1 | 5.626127| -3.837981| 0.774308 |
| 1 | -3.189061| 0.786965 | 2.142735 |
| 1 | -6.567098| -0.388929| -0.222585|
| 1 | -5.617240| 0.805803 | 1.733085 |
| 6 | -5.212269| -1.839069| -2.091274|
| 1 | -5.914866| -2.618772| -1.775369|
| 1 | -5.759673| -1.165991| -2.760714|
| 1 | -4.419987| -2.317364| -2.673965|

S122
|   |       |       |       |       |       |       |
|---|-------|-------|-------|-------|-------|-------|
|   | 1     | -0.761864 | -0.532874 | 1.716156 |
| 6 | -2.579846 | -1.948305 | -1.327980 |
| 6 | -3.768511 | -2.460637 | -1.832200 |
| 6 | -4.941019 | -2.361093 | -1.085823 |
| 6 | -4.885017 | -1.749493 | 0.155927 |
|   | -1.691024 | -2.013478 | -1.943661 |
| 6 | -2.062793 | 2.559286 | 1.568854 |
| 6 | -2.567903 | 1.970780 | 1.759377 |
| 6 | -2.358773 | 2.356925 | -1.338851 |
| 6 | -2.339780 | 3.452951 | -1.271560 |
|   | 0.758338 | -3.377629 | 1.505663 |
| 1 | 1.581868 | -4.075640 | 1.308445 |
| 6 | 0.795302 | -2.341996 | -1.421539 |
| 6 | 0.795941 | -3.553243 | -1.536640 |
| 6 | -3.798794 | 1.866959 | -1.192771 |
| 1 | -4.409642 | 2.260141 | -2.012926 |
| 1 | -3.842042 | 0.774776 | -1.228481 |
| 1 | -4.258143 | 2.190845 | -0.253303 |
| 6 | -1.771689 | 1.941916 | -2.683047 |
| 1 | -1.773151 | 0.853083 | -2.779405 |
| 6 | -2.369136 | 2.370928 | -3.495776 |
| 1 | -0.738987 | 2.285043 | -2.798994 |
| 6 | -2.455445 | 4.022278 | 1.399428 |
| 6 | -2.915247 | 4.390929 | 2.323591 |
| 6 | -1.576549 | 4.646453 | 1.207500 |
| 6 | -3.174782 | 4.178852 | 0.591045 |
| 6 | -1.122107 | 2.381200 | 2.758227 |
| 6 | -1.609159 | 2.713542 | 3.681452 |
| 6 | -0.821330 | 1.336034 | 2.874000 |
| 6 | -0.214195 | 2.981021 | 2.625234 |
| 6 | -0.562840 | 4.144860 | 1.530576 |
| 6 | -0.734293 | 4.708249 | 0.608228 |
| 6 | -0.573525 | 4.854908 | 2.364048 |
| 6 | -1.408197 | 3.460009 | 1.656302 |
| 6 | 1.026490 | -2.678110 | 2.834013 |
| 6 | 1.046748 | -3.414412 | 3.645398 |
| 6 | 1.986977 | -2.153663 | 2.826851 |
| 6 | 0.245923 | -1.943420 | 3.050921 |
| 6 | 1.176362 | -2.393000 | -2.631958 |
| 6 | 2.229705 | -2.095382 | -2.576063 |
| 6 | 1.037053 | -2.965713 | -3.555194 |
| 6 | 0.570930 | -1.482886 | -2.680996 |
| 6 | 1.669327 | -4.486849 | -1.328053 |
| 6 | 1.364906 | -5.162691 | -0.524568 |
| 6 | 1.610290 | -5.047694 | -2.267689 |
| 6 | 2.721461 | -4.223170 | -1.178797 |
| 6 | 2.267751 | 5.837653 | -0.746756 |
| 6 | 1.816959 | 6.163952 | -1.691332 |
| 6 | 1.856625 | 6.479026 | 0.041720 |
| 6 | 3.343112 | 6.022509 | -0.804548 |
6  6.214861  -1.578836   0.116573
1  6.356160  -2.278794   -0.715410
1  6.979467  -0.802263    0.037387
1  6.398415  -2.139732   1.040584
1 -5.879382  -2.756906  -1.464650
1 -5.788675  -1.672253    0.758786
1 -3.779488  -2.929750  -2.813323
6  6.356160  -2.278794   -0.715410
1  6.979467  -0.802263   0.037387
1  6.398415  -2.139732   1.040584
1 -5.879382  -2.756906  -1.464650
1 -5.788675  -1.672253    0.758786
1 -3.779488  -2.929750  -2.813323

Name - TS2_Me_o2_
Zero-point correction=                           0.730117 (Hartree/Particle)
Thermal correction to Energy=                    0.771492
Thermal correction to Enthalpy=                  0.772437
Thermal correction to Gibbs Free Energy=        0.659300
Sum of electronic and zero-point Energies=       -2161.868365
Sum of electronic and thermal Energies=          -2161.826989
Sum of electronic and thermal Enthalpies=        -2161.826045
Sum of electronic and thermal Free Energies=     -2161.939181
1 imaginary frequency.
Charge =   0  Multiplicity = 1                  

0 1
26   0.544630  -0.488217  -0.138031
  0.670454  -0.495776   1.382726
  1.233968  -1.277084  -1.228189
 15  -1.030159  -2.055284   0.015739
 15   1.565018   1.478069   0.024907
  7   -2.250691   0.248158  -0.177967
  7   -1.013837   1.941572   0.027496
  6  -0.945324   0.593445  -0.080487
  6  -2.598398  -1.078609  -0.266998
  6  -3.918540  -1.351430  -0.437530
  1  -4.252387  -2.379235  -0.534371
  6  -4.898443  -0.289173  -0.479475
  6  -4.506323   1.017195  -0.322064
  1  -5.241212   1.816115  -0.333059
  6  -3.137218   1.334535  -0.160117
  6  -2.320054   2.454036  -0.006275
  6  -2.440247   3.856026   0.132688
  1  -3.425716   4.310756   0.112048
  6  -1.320377   4.630750   0.306155
  6  -0.011067   4.019604   0.321773
  1  0.860097    4.650053   0.463271
  6  0.140210   2.678227   0.162969
  6  2.426755  -1.496292  -0.394540
  6  3.314988  -1.111326  -1.417382
|   | 0.498061 | -0.535366 | -1.707284 |
|---|---|---|---|
| 6 | 2.955043 | -2.363367 | 0.595048 |
| 6 | 4.312255 | -2.706868 | 0.566455 |
| 6 | 5.172990 | -2.259477 | -0.430941 |
| 6 | 4.661341 | -1.463769 | -1.447252 |
| 6 | 2.531999 | 2.210597 | -1.403359 |
| 1 | 3.318638 | 1.461876 | -1.559232 |
| 6 | 2.592727 | 1.932419 | 1.508272 |
| 1 | 8.215444 | 3.002115 | 1.413547 |
| 6 | -1.221978 | -3.449289 | -1.201599 |
| 1 | -2.196987 | -3.920003 | -1.020118 |
| 6 | -1.458208 | -2.832464 | 1.669761 |
| 6 | -0.527068 | -3.329495 | 1.961556 |
| 6 | 3.892830 | 1.130574 | 1.492446 |
| 1 | 4.510468 | 1.404100 | 2.355123 |
| 1 | 3.685702 | 0.057735 | 1.543185 |
| 1 | 4.483728 | 1.304789 | 0.587950 |
| 6 | 1.821635 | 1.720361 | 2.805811 |
| 1 | 1.538765 | 0.669699 | 2.913226 |
| 1 | 2.445793 | 2.009136 | 3.659080 |
| 1 | 0.905602 | 2.318971 | 2.835104 |
| 6 | 3.194033 | 3.562971 | -1.167834 |
| 1 | 3.750532 | 3.859460 | -2.064422 |
| 1 | 2.451574 | 4.345135 | -0.979908 |
| 1 | 3.902248 | 3.548373 | -0.335295 |
| 6 | 1.645951 | 2.242274 | -2.646353 |
| 1 | 2.240219 | 2.497283 | -3.50587 |
| 1 | 1.161485 | 1.276222 | -2.815335 |
| 1 | 0.859627 | 2.998812 | -2.541769 |
| 6 | -0.114941 | -4.476827 | -0.973316 |
| 1 | -0.171535 | -4.933607 | 0.020046 |
| 1 | -0.187025 | -5.281648 | -1.712897 |
| 1 | 0.872061 | -4.012387 | -1.075508 |
| 6 | -1.197759 | -2.919232 | -2.632072 |
| 1 | -1.345055 | -3.744759 | -3.337439 |
| 1 | -1.984438 | -2.178262 | -2.803095 |
| 1 | -0.239482 | -2.442821 | -2.856378 |
| 6 | -1.739032 | -1.728297 | 2.686578 |
| 1 | -2.694703 | -1.236057 | 2.472507 |
| 1 | -1.801102 | -2.152553 | 3.694438 |
| 1 | -0.947708 | -0.973465 | 2.667559 |
| 6 | -2.582418 | -3.861163 | 1.652125 |
| 1 | -2.372103 | -4.712462 | 0.998618 |
| 1 | -2.734766 | -4.254976 | 2.663445 |
| 1 | -3.528645 | -3.408638 | 1.338240 |
| 6 | -1.413677 | 6.117813 | 0.473144 |
| 1 | -0.985607 | 6.435521 | 1.431144 |
| 1 | -0.857113 | 6.639808 | -0.314157 |
| 1 | -2.450462 | 6.460814 | 0.436843 |
| 6 | -6.338221 | -0.657300 | -0.677982 |
Name - TS2_MeO_m1_D_
Zero-point correction=          0.734521 (Hartree/Particle)
Thermal correction to Energy=       0.777066
Thermal correction to Enthalpy=      0.778010
Thermal correction to Gibbs Free Energy=  0.661024
Sum of electronic and zero-point Energies= -2236.997544
Sum of electronic and thermal Energies=  -2236.954999
Sum of electronic and thermal Enthalpies=  -2236.954054
Sum of electronic and thermal Free Energies=  -2237.071040

1 imaginary frequency.
Charge =  0  Multiplicity = 1

|   |   |   |   |
|---|---|---|---|
| 1 | -6.684453 | -1.339852 | 0.107101 |
| 1 | -6.982791 | 0.224899  | -0.666118 |
| 1 | -6.486094 | -1.170739 | -1.635403 |
| 1 | 6.221132  | -2.545518 | -0.419010 |
| 1 | 5.298108  | -1.122123 | -2.259616 |
| 1 | 4.702921  | -3.345168 | 1.356791  |
| 1 | 2.919512  | -0.506884 | -1.635403 |
| 6 | 2.121103  | -2.918253 | 1.709278  |
| 1 | 1.534054  | -2.121350 | 2.174698  |
| 1 | 1.410007  | -3.656757 | 1.322294  |
| 1 | 2.738791  | -3.417072 | 2.462424  |

S126
|   |        |          |          |
|---|--------|----------|----------|
| 1 | 0.521212 | -0.419659 | -1.651509 |
| 6 | 2.625477 | -1.837358 | 1.194273  |
| 6 | 3.936160 | -2.106167 | 1.560272  |
| 6 | 5.018398 | -1.638431 | 0.808792  |
| 6 | 4.750106 | -0.898787 | -0.339668 |
| 6 | 1.881774 | 2.621245  | -1.323268 |
| 1 | 2.806266 | 2.032219  | -1.383699 |
| 6 | 1.746888 | 2.465882  | 1.599486  |
| 1 | 1.758675 | 3.557300  | 1.479708  |
| 6 | -0.763356 | -3.469094 | -1.414350 |
| 1 | -1.559299 | -4.204128 | -1.238994 |
| 6 | -0.928198 | -3.262582 | 1.505140  |
| 1 | 0.126077 | -3.523540 | 1.670304  |
| 6 | 3.180569 | 1.951846  | 1.722432  |
| 1 | 3.657323 | 2.390495  | 2.606282  |
| 1 | 3.192102 | 0.863370  | 1.830443  |
| 1 | 3.793531 | 2.202986  | 0.851124  |
| 6 | 0.930195 | 2.124377  | 2.840392  |
| 1 | 0.857608 | 1.039739  | 2.959767  |
| 1 | 1.410551 | 2.549188  | 3.729172  |
| 1 | -0.087018 | 2.523870  | 2.779232  |
| 6 | 2.251955 | 4.083229  | -1.101918 |
| 1 | 2.815621 | 4.454550 | -1.965361 |
| 1 | 1.358587 | 4.709618  | -1.009572 |
| 1 | 2.874166 | 4.234042  | -0.216023 |
| 6 | 1.113999 | 2.443216  | -2.630598 |
| 1 | 1.719813 | 2.788536  | -3.475479 |
| 1 | 0.846844 | 1.395618  | -2.793267 |
| 1 | 0.188883 | 3.031243  | -2.618915 |
| 6 | 0.594893 | -4.167104 | -1.360952 |
| 1 | 0.748756 | -4.708016 | -0.421767 |
| 1 | 0.683068 | -4.888820 | -2.180413 |
| 1 | 1.409561 | -3.441881 | -1.458783 |
| 6 | -1.001066 | -2.810608 | -2.769191 |
| 1 | -0.941309 | -3.561848 | -3.564788 |
| 1 | -1.987161 | -2.338774 | -2.820506 |
| 1 | -0.251267 | -2.038273 | -2.962321 |
| 6 | -1.398025 | -2.406860 | 2.678335  |
| 1 | -2.458268 | -2.151689 | 2.567760  |
| 1 | -1.281180 | -2.956683 | 3.618501  |
| 1 | -0.826121 | -1.476360 | 2.734289  |
| 6 | -1.741265 | -4.548344 | 1.406058  |
| 1 | -1.371321 | -5.230278 | 0.635871  |
| 1 | -1.702821 | -5.082050 | 2.362405  |
| 1 | -2.795313 | -4.334038 | 1.201222  |
| 6 | -2.907719 | 5.724212  | 0.288819  |
| 1 | -2.542999 | 6.151158  | 1.230526  |
| 1 | -2.479578 | 6.325787  | -0.521620 |
| 1 | -3.993229 | 5.846198  | 0.261599  |
| 6 | -6.356511 | -1.961997 | -0.402410 |
Name - TS2_MeO_m1_U_
Zero-point correction= 0.734571 (Hartree/Particle)
Thermal correction to Energy= 0.777053
Thermal correction to Enthalpy= 0.777997
Thermal correction to Gibbs Free Energy= 0.661611
Sum of electronic and zero-point Energies= -2236.997734
Sum of electronic and thermal Energies= -2236.955253
Sum of electronic and thermal Enthalpies= -2236.954308
Sum of electronic and thermal Free Energies= -2237.070694
1 imaginary frequency.
Charge = 0 Multiplicity = 1

1  -6.516983  -2.648731  0.437087
1  -7.168607  -1.230928 -0.399433
1  -6.440075  -2.555083 -1.320788
1   3.272807  -0.066144 -1.622624
1   1.816911  -2.184953  1.826733
1   4.134332  -2.683821  2.460491
1   6.032560  -1.860589  1.120211
8   5.702633  -0.388407 -1.169479
6   7.048888  -0.643233 -0.842935
1   7.646327  -0.165705 -1.618411
1   7.314858  -0.217690  0.133141
1   7.264043  -1.719482 -0.830688

---------------------------------------------------------------
0 1
26  0.365638  -0.404095 -0.058083
  0.239771  -0.362370  1.462220
  1.348075  -1.131187 -0.935445
15  -0.970013  -2.166336 -0.054816
15   1.125523  1.663089  0.130041
  -2.492985  -0.040028 -0.219453
  -1.486926  1.808389 -0.083700
  -1.244285  0.478679 -0.160019
  -2.667410  -1.404868 -0.224472
  -3.947095  -1.853392 -0.314085
  -4.147607  -2.919072 -0.344334
  -5.058467  -0.930586 -0.363609
  -4.834661  0.422335 -0.291494
  -5.668077  1.117868 -0.304626
  -3.514763  0.921390 -0.199923
  -2.849573  2.143213 -0.098841
  -3.150359  3.520568  0.010705
  -4.186135  3.844560 -0.017322
  -2.140395  4.436302  0.173108
  -0.765228  3.996503  0.233647
  -0.012807  4.731241  0.410730
  -0.440368  2.684114  0.095168
  2.272084  -1.268111  0.173217
|   | 3.423908 | -0.923423 | -0.560701 |
|---|----------|-----------|-----------|
| 1 | 0.599018 | -0.491107 | -1.608421 |
| 6 | 2.463088 | -2.073598 | 1.308171  |
| 6 | 3.741353 | -2.452279 | 1.715674  |
| 6 | 4.868793 | -2.070245 | 0.999349  |
| 6 | 4.704591 | -1.304811 | -0.155211 |
| 6 | 2.141530 | 2.446095  | -1.234684 |
| 6 | 1.935142 | 2.297677  | 1.683221  |
| 1 | 2.012716 | 3.387783  | 1.574842  |
| 6 | -0.970668| -3.398424 | -1.450663 |
| 1 | -1.822252| -4.073201 | -1.296748 |
| 6 | -1.147658| -3.238090 | 1.470126  |
| 1 | -0.115196| -3.573980 | 1.639472  |
| 6 | 3.334841 | 1.701297  | 1.824690  |
| 1 | 3.818456 | 2.100155  | 2.723332  |
| 1 | 3.285590 | 0.612521  | 1.916383  |
| 1 | 3.978074 | 1.932213  | 0.969671  |
| 6 | 1.080522 | 1.992364  | 2.907974  |
| 1 | 0.947046 | 0.912598  | 3.017228  |
| 1 | 1.568785 | 2.383913  | 3.807590  |
| 1 | 0.087511 | 2.446725  | 2.833983  |
| 6 | 2.614546 | 3.876441  | -1.003578 |
| 1 | 3.224184 | 4.205692  | -1.852936 |
| 1 | 1.767209 | 4.566149  | -0.932303 |
| 1 | 3.224012 | 3.982115  | -0.102421 |
| 6 | 1.393878 | 2.324737  | -2.559717 |
| 1 | 2.042098 | 2.624590  | -3.390585 |
| 1 | 1.051827 | 1.300237  | -2.729194 |
| 1 | 0.515332 | 2.980072  | -2.567795 |
| 6 | 0.329660 | -4.199246 | -1.401721 |
| 1 | 0.437330 | -4.764567 | -0.470582 |
| 1 | 0.367293 | -4.912663 | -2.232202 |
| 1 | 1.197449 | -3.536575 | -1.484209 |
| 6 | -1.145580| -2.698011 | -2.794053 |
| 1 | -1.132193| -3.436228 | -3.603862 |
| 1 | -2.094418| -2.155169 | -2.845029 |
| 1 | -0.339728| -1.978608 | -2.965195 |
| 6 | -1.570056| -2.377636 | 2.657708  |
| 1 | -2.610285| -2.051019 | 2.545752  |
| 1 | -1.496971| -2.953418 | 3.586664  |
| 1 | -0.939182| -1.487964 | 2.737991  |
| 6 | -2.044283| -4.464088 | 1.336363  |
| 1 | -1.715052| -5.151026 | 0.552326  |
| 1 | -2.047582| -5.021239 | 2.280034  |
| 1 | -3.080841| -4.176800 | 1.131594  |
| 6 | -2.425140| 5.902367  | 0.305043  |
| 1 | -2.042303| 6.295574  | 1.254178  |
| 1 | -1.940574| 6.473187  | -0.495895 |
| 1 | -3.497546| 6.107562  | 0.263269  |
|   | X    | Y    | Z    |
|---|------|------|------|
| 6 | -6.444665 | -1.491174 | -0.474267 |
| 1 | -6.668005 | -2.163571 | 0.362431  |
| 1 | -7.197605 | -0.699373 | -0.480571 |
| 1 | -6.562323 | -2.075972 | -1.394200 |
| 1 | 3.296147  | -0.344628 | -1.471609 |
| 1 | 1.608963  | -2.356603 | 1.912030  |
| 1 | 3.863318  | -3.047906 | 2.617593  |
| 1 | 5.870166  | -2.355715 | 1.304710  |
| 8 | 5.849093  | -0.974173 | -0.816926 |
| 6 | 5.725261  | -0.190012 | -1.975108 |
| 1 | 6.738664  | -0.031830 | -2.348259 |
| 1 | 5.131505  | -0.692975 | -2.750140 |
| 1 | 5.266772  | 0.785672  | -1.760925 |

Name - TS2_MeO_m2_D_
Zero-point correction= 0.734625 (Hartree/Particle)
Thermal correction to Energy= 0.777095
Thermal correction to Enthalpy= 0.778039
Thermal correction to Gibbs Free Energy= 0.661294
Sum of electronic and zero-point Energies= -2236.998427
Sum of electronic and thermal Energies= -2236.955957
Sum of electronic and thermal Enthalpies= -2236.955013
Sum of electronic and thermal Free Energies= -2237.071758
1 imaginary frequency.
Charge = 0 Multiplicity = 1
0 1
26 0.480767 0.042716 -0.427656
1 0.621070 0.013443 1.094209
1 1.518592 -0.060890 -1.514349
15 0.258639 -2.156905 -0.382178
15 0.106984 2.203871 -0.168382
7 -2.127779 -1.128363 0.044859
7 -2.200897 0.975977 0.078214
6 -1.337519 -0.036895 -0.170443
6 -1.578092 -2.386999 -0.139252
6 -2.435620 -3.434492 -0.019189
1 -2.066821 -4.450677 -0.107764
6 -3.842999 -3.221685 0.231314
6 -4.330963 -1.946832 0.380552
1 -5.382983 -1.783133 0.592708
6 -3.465513 -0.835106 0.261781
6 -3.511330 0.555960 0.352769
6 -4.440726 1.579038 0.651649
1 -5.476312 1.318582 0.847181
6 -4.029033 2.887198 0.716484
6 -2.642682 3.223169 0.485591
1 -2.327220 4.255174 0.596203
6 -1.732993 2.267820 0.158969
|   | 2.565630 | 0.292503 | -0.587197 |
|---|----------|----------|-----------|
| 6 | 3.261875 | 1.154770 | -1.448210 |
| 6 | 0.426862 | 0.081983 | -1.993650 |
| 6 | 3.310403 | -0.309525 | 0.446849 |
| 6 | 4.656531 | -0.006691 | 0.644761 |
| 6 | 5.317234 | 0.885844 | -0.207928 |
| 6 | 4.613248 | 1.451630 | -1.257583 |
| 6 | 3.396336 | -1.597086 |
| 1 | 3.278157 | -1.852972 |
| 6 | 3.158324 | 1.288410 |
| 1 | 4.139115 | 1.273230 |
| 6 | -3.190453 | -1.899318 |
| 1 | -4.215811 | -1.678994 |
| 6 | -3.183175 | 0.993904 |
| 1 | -2.960229 | 0.886909 |
| 6 | 3.344730 | 1.144113 |
| 1 | 3.933818 | 1.984658 |
| 1 | 2.376864 | 1.140931 |
| 1 | 3.862523 | 0.219868 |
| 6 | 2.465727 | 2.602043 |
| 1 | 1.471158 | 2.636105 |
| 1 | 3.057962 | 3.442854 |
| 1 | 2.346336 | 2.728480 |
| 6 | 4.867580 | -1.303624 |
| 1 | 5.462992 | -2.205444 |
| 1 | 5.030036 | -1.020879 |
| 1 | 5.267630 | 0.512427 |
| 6 | 2.910904 | -2.778221 |
| 1 | 3.492958 | -3.675837 |
| 1 | 1.853002 | -2.984523 |
| 1 | 3.035290 | -2.569430 |
| 6 | -3.180832 | -2.191206 |
| 1 | -2.674383 | -3.086633 |
| 1 | -3.285745 | -3.972121 |
| 1 | -2.714583 | -2.890399 |
| 1 | -1.636196 | -3.310738 |
| 6 | -2.654994 | 2.347966 |
| 1 | -2.884185 | 2.506559 |
| 1 | -3.127888 | 3.155460 |
| 1 | -1.569616 | 2.407812 |
| 6 | -4.693131 | 0.902140 |
| 1 | -5.117917 | -0.024920 |
| 1 | -5.180551 | 1.733528 |
| 1 | -4.964840 | 0.986187 |
| 6 | 3.995184 | 1.041509 |
| 1 | 4.542222 | 1.936650 |
| 1 | 4.723782 | 0.224001 |
|   |        |        |        |
|---|--------|--------|--------|
| 1 | -5.994050 | 3.614827 | 1.219719 |
| 6 | -4.735784 | -4.421165 | 0.341789 |
| 1 | -4.401554 | -5.091653 | 1.142348 |
| 1 | -5.768597 | -4.133499 | 0.552764 |
| 1 | -4.731248 | -5.004814 | -0.586369 |
| 1 | 6.365611  | 1.103037  | -0.030955 |
| 1 | 5.120485  | 2.132067  | -1.937379 |
| 1 | 2.737430  | 1.598502  | -2.292949 |
| 1 | 2.799931  | -0.969810  | 1.133561 |
| 8 | 5.413047  | -0.524468  | 1.652637 |
| 6 | 4.785156  | -1.412008  | 2.542499 |
| 1 | 4.417947  | -2.312444  | 2.030530 |
| 1 | 5.543595  | -1.701578  | 3.272010 |
| 1 | 3.942574  | -0.939452  | 3.065063 |

Name - TS2\textunderscore MeO\textunderscore m2\textunderscore U\textunderscore _
Zero point correction= 0.734162 (Hartree/Particle)
Thermal correction to Energy= 0.776815
Thermal correction to Enthalpy= 0.777759
Thermal correction to Gibbs Free Energy= 0.658943
Sum of electronic and zero-point Energies= -2236.997375
Sum of electronic and thermal Energies= -2236.954722
Sum of electronic and thermal Enthalpies= -2236.953778
Sum of electronic and thermal Free Energies= -2237.072594
1 imaginary frequency.
Charge = 0 Multiplicity = 1
|   |       |       |       |       |       |
|---|-------|-------|-------|-------|-------|
| 6 | 1.610156 | -2.366187 | 0.143570 |
| 6 | -2.523868 | -0.059000 | -0.582508 |
| 6 | -3.254078 | -0.875572 | -1.470759 |
| 1 | -0.349715 | 0.024037 | -1.956033 |
| 6 | -3.260496 | 0.577485 | 0.424411 |
| 6 | -3.260496 | -0.875572 | -1.470759 |
| 1 | -0.349715 | 0.024037 | -1.956033 |
| 6 | -0.942382 | -3.078874 | 1.277915 |
| 1 | -0.536187 | -4.097998 | 1.231395 |
| 6 | -0.325913 | 3.324386 | -1.748393 |
| 1 | 0.086194 | 4.310978 | -1.500836 |
| 6 | -0.649037 | 3.225532 | 1.163534 |
| 1 | -1.735564 | 3.069208 | 1.120263 |
| 6 | -2.464010 | -3.130723 | 1.151954 |
| 1 | -2.885704 | -3.713669 | 1.978540 |
| 1 | -2.882571 | -2.123177 | 1.190049 |
| 1 | -2.793118 | -3.590107 | 0.214852 |
| 6 | -0.520513 | -2.451019 | 2.601324 |
| 1 | -0.873414 | -1.417822 | 2.661437 |
| 6 | -0.947913 | -3.020867 | 3.434251 |
| 1 | 0.567680 | -2.441641 | 2.718398 |
| 6 | -0.364427 | -4.799404 | -1.343935 |
| 1 | -0.590502 | -5.363908 | -2.255909 |
| 6 | 0.663414 | -5.049160 | -1.060435 |
| 1 | -1.036865 | -5.159901 | -0.561163 |
| 6 | 0.352485 | -2.869742 | -2.789896 |
| 1 | 0.064109 | -3.410173 | -3.698134 |
| 6 | 0.259003 | -1.795455 | -2.972405 |
| 1 | 1.407661 | -3.088971 | -2.590147 |
| 1 | 0.703771 | 4.928724 | 1.126172 |
| 6 | 4.383152 | -4.886562 | 1.844368 |
|   |     |     |         |     |     |     |
|---|-----|-----|---------|-----|-----|-----|
| 1 | 4.713920 | -5.073948 | 0.123948 |
| 1 | 5.768219 | -4.056552 | 1.117769 |
| 6 | 5.134705 | 4.064639 | 0.325690 |
| 1 | 4.871923 | 4.753709 | 1.136984 |
| 1 | 6.145857 | 3.694791 | 0.512064 |
| 1 | 5.155900 | 4.653255 | -0.599105 |
| 1 | -6.389337 | -0.661591 | -0.172564 |
| 1 | -5.148578 | -1.733515 | -2.015663 |
| 1 | -2.734125 | -1.343018 | -2.304899 |
| 1 | -2.771875 | 1.212826 | 1.153180 |
| 8 | -5.207488 | 1.021202 | 1.631957 |
| 6 | -6.577279 | 0.807890 | 1.857101 |
| 1 | -6.797464 | -0.249160 | 2.059282 |
| 1 | -6.840447 | 1.400726 | 2.734886 |
| 1 | -7.188560 | 1.138257 | 1.006182 |

Name - TS2_MeO_o1_D_
Zero-point correction= 0.733847 (Hartree/Particle)
Thermal correction to Energy= 0.776548
Thermal correction to Enthalpy= 0.777492
Thermal correction to Gibbs Free Energy= 0.660135
Sum of electronic and zero-point Energies= -2236.998317
Sum of electronic and thermal Energies= -2236.955616
Sum of electronic and thermal Enthalpies= -2236.954672
Sum of electronic and thermal Free Energies= -2237.072029
1 imaginary frequency.
Charge = 0 Multiplicity = 1

|   |     |     |         |     |     |     |
|---|-----|-----|---------|-----|-----|-----|
| 0 |     |     |         |     |     |     |
| 26 | -0.459704 | -0.386228 | 0.024954 |
| 1 | -0.306831 | -0.306486 | -1.500106 |
| 1 | -1.494825 | -1.106077 | 0.861816 |
| 15 | 0.877540 | -2.155220 | 0.063038 |
| 15 | -1.223043 | 1.684308 | -0.104122 |
| 7 | 2.398969 | -0.026464 | 0.178818 |
| 7 | 1.394715 | 1.820639 | 0.019228 |
| 6 | 1.149773 | 0.492511 | 0.126049 |
| 6 | 2.573999 | -1.391149 | 0.199388 |
| 6 | 3.854949 | -1.838906 | 0.274418 |
| 1 | 4.055551 | -2.903916 | 0.317870 |
| 6 | 4.967723 | -0.916923 | 0.289780 |
| 6 | 4.743124 | 0.434406 | 0.195955 |
| 1 | 5.576766 | 1.129676 | 0.179911 |
| 6 | 3.422216 | 0.932537 | 0.118472 |
| 6 | 2.757654 | 2.152559 | -0.000010 |
| 6 | 3.059692 | 3.525331 | -0.155563 |
| 1 | 4.096637 | 3.846669 | -0.156514 |
| 6 | 2.048974 | 4.438051 | -0.329355 |
| 6 | 0.672021 | 4.000494 | -0.349260 |
|   |   |   |   |
|---|---|---|---|
| 1 | -0.108997 | 4.731443 | -0.529848 |
| 6 | 0.347847 | 2.693634 | -0.164526 |
| 6 | -2.356762 | -1.320699 | -0.246552 |
| 6 | -3.583018 | -1.125039 | 0.425502 |
| 1 | -0.679349 | -0.490796 | 1.562360 |
| 6 | -2.431152 | -2.092162 | -1.417344 |
| 6 | -3.631149 | -2.590429 | -1.923514 |
| 6 | -4.817933 | -2.353355 | -1.242328 |
| 6 | -4.794742 | -1.624215 | -0.056995 |
| 6 | -2.118535 | 2.473361 | 1.337699 |
| 1 | -2.993990 | 1.822348 | 1.440760 |
| 6 | -2.138868 | 2.336236 | -1.589011 |
| 1 | -2.200648 | 3.426296 | -1.471851 |
| 6 | 0.873244 | -3.330794 | 1.508010 |
| 1 | 1.713931 | -4.023636 | 1.375069 |
| 6 | 1.047774 | -3.291344 | -1.416296 |
| 1 | 0.019231 | -3.653871 | -1.550085 |
| 6 | -3.549051 | 1.749860 | -1.623502 |
| 1 | -4.106571 | 2.166800 | -2.469663 |
| 1 | -3.510651 | 0.663381 | -1.741958 |
| 1 | -4.115668 | 1.965802 | -0.711872 |
| 6 | -1.383870 | 2.026754 | -2.876459 |
| 1 | -1.265582 | 0.946389 | -2.996568 |
| 1 | -1.936167 | 2.423438 | -3.736155 |
| 1 | -0.384501 | 2.472848 | -2.876751 |
| 6 | -2.570770 | 3.916683 | 1.153271 |
| 1 | -3.107076 | 4.252220 | 2.048653 |
| 1 | -1.715249 | 4.588056 | 1.023920 |
| 1 | -3.244319 | 4.046744 | 0.301757 |
| 6 | -1.272444 | 2.318827 | 2.598660 |
| 1 | -1.849980 | 2.617456 | 3.480898 |
| 1 | -0.945634 | 1.283223 | 2.724241 |
| 1 | -0.382396 | 2.957576 | 2.551865 |
| 6 | -0.437872 | -4.114783 | 1.499612 |
| 1 | -0.564018 | -4.707438 | 0.587912 |
| 1 | -0.475244 | -4.801080 | 2.352773 |
| 1 | -1.294754 | -3.436865 | 1.572055 |
| 6 | 1.068080 | -2.580704 | 2.821383 |
| 1 | 1.053398 | -3.286375 | 3.659763 |
| 1 | 2.023844 | -2.047919 | 2.842239 |
| 6 | 0.271672 | -1.845553 | 2.968078 |
| 1 | 1.429005 | -2.471323 | -2.646003 |
| 1 | 2.464344 | -2.120042 | -2.567418 |
| 1 | 1.349698 | -3.084253 | -3.550448 |
| 1 | 0.782999 | -1.594151 | -2.747855 |
| 6 | 1.965924 | -4.497582 | -1.254243 |
| 1 | 1.670556 | -5.150492 | -0.428677 |
| 1 | 1.946422 | -5.099096 | -2.170197 |
| 1 | 3.004478 | -4.188712 | -1.097702 |
| 6 | 2.334523 | 5.898332 | -0.513583 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 1 | 1.936756 | 6.261130 | -1.468686 |
| 1 | 1.863956 | 6.496133 | 0.275937  |
| 1 | 3.407877 | 6.102329 | -0.495972 |
| 6 | 6.355192 | -1.476891 | 0.386902  |
| 1 | 6.563748 | -2.165091 | -0.440792 |
| 1 | 7.108666 | -0.685801 | 0.365256  |
| 1 | 6.488763 | -2.044436 | 1.315486  |
| 1 | -1.521224 | -2.262620 | -1.979563 |
| 1 | -3.633155 | -3.154709 | -2.852219 |
| 1 | -5.762628 | -2.733144 | -1.621206 |
| 1 | -5.721094 | -1.447561 | 0.478250  |
| 8 | -3.508102 | -0.408282 | 1.592319  |
| 6 | -4.672210 | -0.270012 | 2.363592  |
| 1 | -4.378875 | 0.279420  | 3.260304  |
| 1 | -5.450880 | 0.298073  | 1.835555  |
| 1 | -5.085134 | -1.244291 | 2.657049  |

Name - TS2_MeO_o2_U_
Zero-point correction=          0.734920 (Hartree/Particle)
Thermal correction to Energy=       0.777188
Thermal correction to Enthalpy=      0.778132
Thermal correction to Gibbs Free Energy= 0.663055
Sum of electronic and zero-point Energies=  -2236.997633
Sum of electronic and thermal Energies=    -2236.955364
Sum of electronic and thermal Enthalpies=   -2236.954420
Sum of electronic and thermal Free Energies= -2237.069497

1 imaginary frequency.
Charge =  0 Multiplicity = 1

26  0.599170  -0.044261  -0.292316
  1  0.801771  -0.061055   1.215837
  1  1.581257  -0.347487  -1.409307
 15  0.065400  -2.186738  -0.141523
 15  0.488167   2.153968  -0.015871
  7  -2.173137  -0.843241  -0.201489
  7  -1.968619   1.242747   0.022956
  6  -1.225380   0.123483  -0.148064
  6  -1.795496  -2.160212  -0.316421
  6  -2.796639  -3.073026  -0.421330
  1  -2.561330  -4.126693  -0.530542
  6  -4.182869  -2.664823  -0.375711
  6  -4.507463  -1.342933  -0.195847
  1  -5.547144  -1.035806  -0.138979
  6  -3.487775  -0.367359  -0.093962
  6  -3.352357   1.010720   0.070469
  6  -4.164512   2.148742   0.282338
  1  -5.243206   2.033581   0.323743
  6  -3.590366   3.383903   0.452674
Name - TS2_MeO_p_D_

Zero-point correction=          0.733893 (Hartree/Particle)
Thermal correction to Energy=     0.775665
Thermal correction to Enthalpy=   0.776609
Thermal correction to Gibbs Free Energy=  0.662692
Sum of electronic and zero-point Energies=   -2236.996444 (Hartree)
Sum of electronic and thermal Energies=  -2236.954673 (Hartree)
Sum of electronic and thermal Enthalpies=     -2236.953728 (Hartree)
Sum of electronic and thermal Free Energies=   -2237.067645 (Hartree)

2 imaginary frequency.
Charge =  0 Multiplicity = 1

----------------------------------------
  0  1
  26 -0.372087  -0.167671    0.284043
  1 -0.488678  -0.158662   -1.237696
  1 -1.368661  -0.553319    1.350033
 15  0.351306  -2.253891    0.142485
 15 -0.486212   2.032241    0.117144
  7  2.455882  -0.696085    0.054088
  7  2.049394   1.371927   -0.019349
  6  1.425942   0.178986    0.131543
  6  2.207665  -2.048999    0.090178
  6  3.291710  -2.867013    0.041403
  1  3.161987  -3.943079    0.087617
  6  4.627445  -2.327756   -0.079351
  6  4.817045  -0.971056   -0.174240
  1  5.816769  -0.563360   -0.287807
  6  3.710231  -0.092293   -0.122279
  6  3.439788   1.274688   -0.182481
  6  4.127857   2.495328   -0.373719
  1  5.207505   2.487034   -0.486842

----------------------------------------
| 6 | 3.431827 | 3.677081 | -0.436046 |
| 6 | 1.992666 | 3.679618 | -0.304816 |
| 1 | 1.458905 | 4.619135 | -0.399984 |
| 6 | 1.305275 | 2.527712 | -0.086464 |
| 6 | -2.465626 | -0.403592 | 0.401043 |
| 6 | -3.347868 | 0.270304 | 1.267521 |
| 1 | -0.378263 | -0.200365 | 1.856741 |
| 6 | -3.080409 | -1.104901 | -0.648692 |
| 6 | -4.458087 | -1.082429 | -0.868692 |
| 6 | -5.290493 | -0.367688 | -0.005391 |
| 6 | -4.723722 | 0.303083 | 1.078494 |
| 6 | -1.032023 | 3.088068 | 1.564261 |
| 1 | -2.051157 | 2.722648 | 1.747182 |
| 6 | -1.267267 | 2.874698 | -1.349069 |
| 1 | -1.032283 | 3.943654 | -1.261798 |
| 6 | 0.135528 | -3.472162 | 1.533869 |
| 1 | 0.716522 | -4.370104 | 1.287471 |
| 6 | 0.021772 | -3.280624 | -1.389869 |
| 6 | -1.076007 | -3.289886 | -1.435153 |
| 6 | -2.781923 | 2.680149 | -1.305770 |
| 6 | -3.248415 | 3.200967 | -2.149532 |
| 1 | -3.035625 | 1.618193 | -1.372914 |
| 6 | -3.230182 | 3.066325 | -0.385199 |
| 6 | -0.681629 | 2.357558 | -2.657948 |
| 6 | -0.856425 | 1.282268 | -2.752808 |
| 6 | -1.153663 | 2.870667 | -3.503567 |
| 6 | 0.397907 | 2.528850 | -2.715263 |
| 6 | -1.091250 | 4.593739 | 1.333720 |
| 6 | -1.454734 | 5.091143 | 2.240262 |
| 6 | -0.097747 | 5.002417 | 1.121682 |
| 6 | -1.762350 | 4.872016 | 0.517006 |
| 6 | -0.176228 | 2.753738 | 2.783541 |
| 6 | -0.589878 | 3.228578 | 3.679957 |
| 6 | -0.125380 | 1.673857 | 2.947796 |
| 6 | 0.846628 | 3.124418 | 2.649883 |
| 6 | -1.344613 | -3.836657 | 1.639033 |
| 1 | -1.721729 | -4.312825 | 0.728309 |
| 1 | -1.506493 | -4.531037 | 2.470776 |
| 6 | -1.953346 | -2.944087 | 1.817540 |
| 6 | 0.664846 | -2.897609 | 2.843690 |
| 6 | 0.521423 | -3.621386 | 3.653911 |
| 6 | 1.732475 | -2.666042 | 2.779432 |
| 6 | 0.138591 | -1.975034 | 3.104572 |
| 6 | 0.543571 | -2.546436 | -2.622139 |
| 6 | 1.639605 | -2.544842 | -2.633979 |
| 6 | 0.199097 | -3.046286 | -3.539797 |
| 6 | 0.199489 | -1.508452 | -2.631333 |
| 6 | 0.521219 | -4.720816 | -1.360676 |
| 6 | 0.095127 | -5.304408 | -0.540430 |
| 6 | 0.249638 | -5.223099 | -2.296094 |
|     | 1      | 26     | 1      | 15     | 7      | 7      | 6      | 6      | 6      | 6      |
|-----|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|     | 1.612729 | -4.759405 | -1.282686 | 5.208815 | 4.854631 | 0.751807 | 2.937943 | 0.788500 | 2.134009 | 6.643795 |
| 6   | 4.128859  | 4.986987  | -0.651116 | 6.732667  | 2.761389  | -0.231734 | 5.868960  | -0.571130 | -2.177207 | 7.237681 |
| 1   | 3.763202  | 5.485122  | -1.556763 | 5.831172  | 3.880116  | 0.802260  | 5.681538  | 0.752947  | -1.142011 | 6.309659 |
| 1   | 3.949083  | 5.672784  | 0.185223  | 5.378507  | 0.838265  | 1.760058  | -2.462727 | -1.646499 | -1.357068 | -4.866256 |
|     | -1.282686 | -4.759405 | -0.651116 | -0.231734 | 0.802260  | -2.134009 | -0.571130 | -2.177207 | 2.134009  | -1.212455 |
| 8   | -6.643795 | -0.275139 | -0.130574 | 0.752947  | -1.142011 | 0.802260  | -4.866256 | -0.571130 | -2.177207 | -6.309659 |
| 6   | -7.237681 | -0.945476 | -1.212455 | -1.142011 | 0.802260  | -2.134009 | -4.866256 | -0.571130 | -2.177207 | -6.309659 |
| 1   | -8.309659 | -0.752947 | -1.142011 | 0.802260  | -2.134009 | -4.866256 | -4.866256 | -0.571130 | -2.177207 | -6.309659 |
| 1   | -8.686960 | -0.571130 | -1.142011 | 0.802260  | -2.134009 | -4.866256 | -4.866256 | -0.571130 | -2.177207 | -6.309659 |
| 1   | -7.064705 | -2.029369 | -1.166566 | 0.802260  | -2.134009 | -4.866256 | -4.866256 | -0.571130 | -2.177207 | -6.309659 |

Name - TS2_MeO_p_U_
Zero-point correction= 0.734078 (Hartree/Particle)
Thermal correction to Energy= 0.776729
Thermal correction to Enthalpy= 0.777673
Thermal correction to Gibbs Free Energy= 0.659728
Sum of electronic and zero-point Energies= -2236.996595
Sum of electronic and thermal Energies= -2236.953944
Sum of electronic and thermal Enthalpies= -2236.953000
Sum of electronic and thermal Free Energies= -2237.070945

1 imaginary frequency.
Charge = 0 Multiplicity = 1

0 1
0 1
26 -0.353725 -0.239463 0.228375
1 -0.384198 -0.215375 -1.297560
1 -1.370177 -0.731549 1.229617
15 0.560721 -2.251291 0.112890
15 -0.660690 1.942014 0.083900
7 2.517235 -0.507861 0.099081
7 1.927664 1.516038 0.035491
6 1.410701 0.269887 0.156623
6 2.391217 -1.878174 0.105952
6 3.545759 -2.594285 0.072909
1 3.512843 -3.678252 0.098289
6 4.829960 -1.935328 -0.003395
6 4.898655 -0.565657 -0.072606
1 5.859922 -0.067822 -0.154374
6 3.715961 0.208751 -0.037880
6 3.324878 1.546452 -0.091129
6 3.904744 2.826096 -0.252990

S140
|   |        |        |        |
|---|--------|--------|--------|
| 1 | 4.983459 | 2.916388 | -0.335081 |
| 6 | 3.106583 | 3.940684 | -0.327758 |
| 6 | 1.669834 | 3.811159 | -0.242039 |
| 1 | 1.055586 | 4.698687 | -0.350620 |
| 6 | 1.083980 | 2.599780 | -0.051625 |
| 6 | -2.418397 | -0.662189 | 0.220803 |
| 6 | -3.402610 | -0.103141 | 1.047023 |
| 1 | -0.445572 | -0.295603 | 1.797988 |
| 6 | -2.906714 | -1.386582 | -0.888075 |
| 6 | -4.259316 | -1.478245 | -1.178285 |
| 6 | -5.207413 | -0.871924 | -0.346341 |
| 6 | -4.773368 | -0.187625 | 0.785033 |
| 6 | -1.343019 | 2.915910 | 1.530711 |
| 1 | -2.326518 | 2.450706 | 1.680722 |
| 6 | -1.465511 | 2.742491 | -1.393069 |
| 1 | -1.316736 | 3.824999 | -1.284437 |
| 6 | 0.424539 | -3.469791 | 1.514836 |
| 1 | 1.085192 | -4.316365 | 1.288469 |
| 6 | 0.354084 | -3.320691 | -1.410856 |
| 1 | -0.737017 | -3.436365 | -1.467781 |
| 6 | -2.961555 | 2.432699 | -1.400710 |
| 1 | -3.441015 | 2.937175 | -2.247127 |
| 1 | -3.132490 | 1.357041 | -1.500226 |
| 6 | -3.464639 | 2.761694 | -0.486161 |
| 6 | -0.803788 | 2.291815 | -2.690313 |
| 1 | -0.892682 | 1.208000 | -2.804966 |
| 1 | -1.286730 | 2.780495 | -3.543077 |
| 1 | 0.260719 | 2.545290 | -2.712406 |
| 6 | -1.538899 | 4.412746 | 1.319191 |
| 1 | -1.969217 | 4.860117 | 2.222594 |
| 1 | -0.583233 | 4.915679 | 1.137805 |
| 1 | -2.212490 | 4.639626 | 0.488743 |
| 6 | -0.490427 | 2.644796 | 2.767800 |
| 1 | -0.971697 | 3.060508 | 3.659871 |
| 1 | -0.338526 | 1.572124 | 2.916107 |
| 1 | 0.494035 | 3.116319 | 2.668088 |
| 6 | -1.020288 | -3.959517 | 1.597743 |
| 1 | -1.338798 | -4.473478 | 0.685237 |
| 1 | -1.137190 | -4.658508 | 2.433171 |
| 1 | -1.706387 | -3.121115 | 1.757876 |
| 6 | 0.878877 | -2.839946 | 2.827316 |
| 1 | 0.783524 | -3.565943 | 3.642642 |
| 1 | 1.923837 | -2.518436 | 2.778798 |
| 1 | 0.270611 | -1.963693 | 3.068637 |
| 6 | 0.817974 | -2.552671 | -2.645519 |
| 1 | 1.908332 | -2.440270 | -2.641566 |
| 1 | 0.539698 | -3.095809 | -3.55168 |
| 1 | 0.372765 | -1.554249 | -2.674171 |
| 6 | 0.987725 | -4.706468 | -1.359621 |
| 1 | 0.611761 | -5.318123 | -0.535315 |
Name - TS2_Me_p_
Zero-point correction= 0.728506 (Hartree/Particle)
Thermal correction to Energy= 0.770566
Thermal correction to Enthalpy= 0.771510
Thermal correction to Gibbs Free Energy= 0.653767
Sum of electronic and zero-point Energies= -2161.873039
Sum of electronic and thermal Energies= -2161.830980
Sum of electronic and thermal Enthalpies= -2161.830036
Sum of electronic and thermal Free Energies= -2161.947779
1 imaginary frequency.
Charge = 0 Multiplicity = 1
|   |        |        |            |            |
|---|--------|--------|-----------|-----------|
|   | 3.628301 | 2.929780 | -0.262255 |           |
| 1 | 4.703571 | 3.052555 | -0.347225 |           |
| 6 | 2.797044 | 4.020424 | -0.328895 |           |
| 6 | 1.365177 | 3.848019 | -0.237833 |           |
| 1 | 0.724645 | 4.717650 | -0.338646 |           |
| 6 | 0.816175 | 2.618883 | -0.051366 |           |
| 6 | -2.584570 | -0.745072 | 0.250673 |           |
| 6 | -3.576392 | -0.209981 | 1.088547 |           |
| 1 | -0.598252 | -0.309526 | 1.804576  |           |
| 6 | -3.060179 | -1.490692 | -0.847191 |           |
| 6 | -4.416964 | -1.622396 | -1.117038 |           |
| 1 | -4.733488 | -2.177930 | -1.998811 |           |
| 6 | -5.388161 | -1.046947 | -0.288172 |           |
| 6 | -4.939964 | -0.345888 | 0.828361  |           |
| 1 | -2.348010 | -1.928177 | -1.538757 |           |
| 6 | -1.622029 | 2.866920 | 1.529518  |           |
| 1 | -2.590693 | 2.371873 | 1.679503  |           |
| 6 | -1.734396 | 2.677925 | -1.393752 |           |
| 1 | -1.623426 | 3.765115 | -1.287227 |           |
| 6 | 0.349252  | -3.467847 | 1.517985  |           |
| 1 | 1.034947  | -4.293192 | 1.287654  |           |
| 6 | 0.254945  | -3.320479 | -1.492667 |           |
| 1 | -0.832718 | 3.467104  | -1.459245 |           |
| 6 | -3.218543 | 2.315771  | -1.404312 |           |
| 1 | -3.712980 | 2.799584  | -2.254203 |           |
| 6 | -3.350999 | 1.234227  | -1.499282 |           |
| 1 | -3.735672 | 2.630476  | -0.492667 |           |
| 6 | -1.053333 | 2.247781  | -2.687946 |           |
| 1 | -1.102266 | 1.161036  | -2.799289 |           |
| 1 | -1.553704 | 2.715796  | -3.543361 |           |
| 1 | 0.001175  | 2.540281  | -2.708509 |           |
| 6 | -1.865123 | 4.355944  | 1.311641  |           |
| 1 | -2.311856 | 4.792143  | 2.212491  |           |
| 1 | -0.925990 | 4.889173  | 1.130591  |           |
| 1 | -2.544126 | 4.557910  | 0.479196  |           |
| 6 | -0.764221 | 2.627553  | 2.769514  |           |
| 1 | -1.260011 | 3.032866  | 3.658374  |           |
| 1 | -0.580639 | 1.560705  | 2.923645  |           |
| 1 | 0.205952  | 3.127826  | 2.669762  |           |
| 6 | -1.078760 | -4.003103 | 1.609851  |           |
| 1 | -1.386935 | -4.526355 | 0.699068  |           |
| 1 | -1.167876 | -4.705856 | 2.445533  |           |
| 1 | -1.789990 | -3.187090 | 1.775562  |           |
| 6 | 0.791181  | -2.823361 | 2.827593  |           |
| 1 | 0.723999  | -3.551775 | 3.643552  |           |
| 1 | 1.824980  | -2.468567 | 2.772647  |           |
| 1 | 0.156787  | -1.966832 | 3.072367  |           |
| 6 | 0.690321  | -2.539187 | -2.644498 |           |
| 1 | 1.777001  | -2.395468 | -2.646064 |           |
| 1 | 0.423231  | -3.089994 | -3.552902 |           |
Name - TS2_NMe2_m1
Zero-point correction=  0.775009 (Hartree/Particle)
Thermal correction to Energy=  0.819316
Thermal correction to Enthalpy=  0.820260
Thermal correction to Gibbs Free Energy=  0.699683
Sum of electronic and zero-point Energies=  -2256.375536
Sum of electronic and thermal Energies=  -2256.331229
Sum of electronic and thermal Enthalpies=  -2256.330285
Sum of electronic and thermal Free Energies=  -2256.450862
1 imaginary frequency.
Charge =  0  Multiplicity = 1

0 1
26 0.217997 -0.351754 -0.020659
1 0.079930 -0.312227  1.498309
1 1.263117 -0.996414 -0.888128
15 -0.971204 -2.214376 -0.018127
15 0.801135  1.768477  0.172665
7 -2.654676 -0.222692 -0.266728
7 -1.807709  1.701544 -0.100424
6 -1.454846  0.395626 -0.164846
6 -2.716192 -1.597343 -0.276803
6 -3.950674 -2.148670 -0.414430
1 -4.062581 -3.227228 -0.449242
6 -5.131091 -1.319372 -0.507125
6 -5.021892  0.047063 -0.426268
1 -5.908520  0.671996 -0.470623
6 -3.751443  0.652429 -0.286435
6 -3.191936  1.924283 -0.163909
|   |       |       |         |         |
|---|-------|-------|---------|---------|
| 6 | -3.606771 | 3.272629 | -0.065231 |
| 1 | -4.664014 | 3.511244 | -0.126601 |
| 6 | -2.680287 | 4.267079 | 0.128571  |
| 6 | -1.275865 | 3.941646 | 0.229781  |
| 1 | -0.565552 | 4.737991 | 0.425143  |
| 6 | -0.841324 | 2.660017 | 0.104162  |
| 6 | 2.185210  | -1.043251| 0.240708  |
| 6 | 3.305461  | -0.606496| 0.126601  |
| 1 | 3.126320  | -0.053157| -1.398686 |
| 1 | 0.475807  | -0.427480| -1.566808 |
| 6 | 2.430208  | -1.828723| 1.382122  |
| 6 | 3.733015  | -2.096077| 1.785624  |
| 1 | 3.906527  | -2.686668| 2.682917  |
| 6 | 4.832722  | -1.620205| 1.077421  |
| 6 | 4.639796  | -0.850409| -0.080235 |
| 1 | 1.599970  | -2.182919| 1.981942  |
| 6 | 1.774857  | 2.633264 | -1.174115 |
| 1 | 2.705174  | 2.050371 | -1.193350 |
| 6 | 1.532416  | 2.464522 | 1.738459  |
| 1 | 1.535083  | 3.556852 | 1.625341  |
| 6 | -0.801423 | -3.490925| -1.362702 |
| 1 | -1.595921 | -4.235127| -1.222563 |
| 6 | -1.138337 | -3.242216| 1.539214  |
| 1 | -0.092914 | -3.490352| 1.768672  |
| 6 | 2.966543  | 1.965873 | 1.909355  |
| 1 | 3.403368  | 2.399379 | 2.816100  |
| 1 | 2.987829  | 0.876514 | 2.004182  |
| 1 | 3.610781  | 2.234916 | 1.066424  |
| 6 | 0.677897  | 2.106537 | 2.949078  |
| 1 | 0.620037  | 1.020680 | 3.064512  |
| 1 | 1.119932  | 2.537490 | 3.854672  |
| 1 | -0.343350 | 2.488611 | 2.853213  |
| 6 | 2.122939  | 4.097861 | -0.936135 |
| 1 | 2.717144  | 4.477378 | -1.775445 |
| 1 | 1.220248  | 4.714887 | -0.878689 |
| 1 | 2.707008  | 4.252319 | -0.025307 |
| 6 | 1.064759  | 2.449253 | -2.512572 |
| 1 | 1.698738  | 2.806868 | -3.331592 |
| 1 | 0.818560  | 1.398612 | -2.688646 |
| 1 | 0.131756  | 3.024180 | -2.536247 |
| 6 | 0.560775  | -4.168134| -1.220132 |
| 1 | 0.669871  | -4.684918| -0.261371 |
| 1 | 0.702882  | -4.906848| -2.016666 |
| 1 | 1.370107  | -3.433681| -1.288282 |
| 6 | -0.971494 | -2.854835| -2.738233 |
| 1 | -0.859576 | -3.615920| -3.518716 |
| 1 | -1.958812 | -2.395909| -2.849276 |
| 1 | -0.221547 | -2.075729| -2.901440 |
| 6 | -1.680985 | -2.373681| 2.670891  |
| 1 | -2.735329 | -2.128708| 2.497771  |
### Calculation Details

#### Energy Contributions
- **Zero-point correction to Energy**: 0.774467 (Hartree/Particle)
- **Thermal correction to Energy**: 0.818943
- **Thermal correction to Enthalpy**: 0.819887
- **Thermal correction to Gibbs Free Energy**: 0.816978
- **Sum of electronic and zero-point Energies**: -2256.376223
- **Sum of electronic and thermal Energies**: -2256.331747
- **Sum of electronic and thermal Enthalpies**: -2256.330803
- **Sum of electronic and thermal Free Energies**: -2256.452847

1 imaginary frequency.

Charge = 0 Multiplicity = 1

#### Atomic Coordinates

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| 1    | -1.613197 | -2.909353 | 3.623964 |
| 1    | -1.119287 | -1.438365 | 2.745787 |
| 6    | -1.934803 | -4.535694 | 1.412552 |
| 1    | -1.513895 | -5.226886 | 0.677611 |
| 1    | -1.950864 | -5.054002 | 2.378010 |
| 1    | -2.975993 | -4.333127 | 1.140708 |
| 6    | -3.087891 | 5.704656 | 0.252481 |
| 1    | -2.771465 | 6.123317 | 1.215122 |
| 1    | -2.623600 | 6.316480 | -0.529964 |
| 1    | -4.171344 | 5.822428 | 0.173474 |
| 6    | -6.461638 | -1.991082 | -0.670108 |
| 1    | -6.659502 | -2.684273 | 0.155990 |
| 1    | -7.276359 | -1.263610 | -0.701901 |
| 1    | -6.497595 | -2.578311 | -1.595353 |
| 1    | 5.830834 | -1.857246 | 1.426094 |
| 7    | 5.707324 | -0.330557 | -0.797482 |
| 6    | 7.024031 | -0.855143 | -0.531354 |
| 1    | 7.105571 | -1.939421 | -0.714206 |
| 1    | 7.748953 | -0.343961 | -1.168074 |
| 1    | 7.314949 | -0.667000 | 0.507604 |
| 6    | 5.463952 | 0.188221 | -2.120798 |
| 1    | 6.405416 | 0.546787 | -2.541773 |
| 1    | 5.037088 | -0.558240 | -2.810949 |
| 1    | 4.777527 | 1.041588 | -2.087590 |

Name: TS2_NMe2_m2
Zero-point correction= 0.774467 (Hartree/Particle)
Thermal correction to Energy= 0.818943
Thermal correction to Enthalpy= 0.819887
Thermal correction to Gibbs Free Energy= 0.697843
Sum of electronic and zero-point Energies= -2256.376223
Sum of electronic and thermal Energies= -2256.331747
Sum of electronic and thermal Enthalpies= -2256.330803
Sum of electronic and thermal Free Energies= -2256.452847

1 imaginary frequency.
Charge = 0 Multiplicity = 1
|   |       |       |       |
|---|-------|-------|-------|
| 6 | -3.801646 | 3.436684 | -0.331408 |
| 6 | -4.359755 | 2.194804 | -0.509740 |
| 1 | -5.409799 | 2.096837 | -0.767452 |
| 6 | -3.569269 | 1.031780 | -0.362134 |
| 6 | -3.695425 | -0.353352 | -0.465376 |
| 6 | -4.670984 | -1.316723 | -0.812044 |
| 1 | -5.679596 | -0.993165 | -1.049825 |
| 6 | -4.336156 | -2.646932 | -0.869973 |
| 6 | -2.983873 | -3.067792 | -0.582857 |
| 1 | -2.726839 | -4.116292 | -0.689680 |
| 6 | -2.033162 | -2.171036 | -0.210060 |
| 6 | 2.343808 | -0.464980 | 0.720979 |
| 6 | 2.945798 | -1.376756 | 1.605001 |
| 1 | 0.175910 | -0.139101 | 2.048792 |
| 6 | 3.165086 | 0.099331 | -0.267077 |
| 6 | 4.512948 | -0.265341 | -0.439731 |
| 6 | 5.069818 | -1.198507 | 0.457530 |
| 6 | 4.283980 | -1.735249 | 1.467103 |
| 6 | -0.140433 | -3.427858 | 1.619832 |
| 1 | 0.913344 | -3.368933 | 1.923469 |
| 6 | 0.449440 | -3.206387 | -1.244470 |
| 1 | -0.101688 | -4.156204 | -1.250664 |
| 6 | 0.511691 | 3.126096 | 1.980172 |
| 1 | 0.256092 | 4.169523 | 1.755749 |
| 6 | 1.067729 | 3.105873 | -0.891659 |
| 1 | 2.117999 | 2.821209 | -0.738236 |
| 6 | 1.939220 | -3.482283 | -1.049217 |
| 1 | 2.313579 | -4.098474 | -1.874519 |
| 1 | 2.505539 | -2.546765 | -1.033435 |
| 1 | 2.151316 | -4.009258 | -0.114043 |
| 6 | 0.193001 | -2.490596 | -2.565747 |
| 1 | 0.694664 | -1.519017 | -2.573687 |
| 1 | 0.576757 | -3.095703 | -3.395101 |
| 1 | -0.874594 | -2.318422 | -2.734834 |
| 6 | -0.478342 | -4.880200 | 1.303247 |
| 1 | -0.373656 | -5.489176 | 2.208567 |
| 1 | -1.515980 | -4.981679 | 0.968107 |
| 1 | 0.175557 | -5.311860 | 0.541080 |
| 6 | -1.000750 | -2.902921 | 2.766555 |
| 1 | -0.838073 | -3.502727 | 3.668766 |
| 1 | -0.766415 | -1.858584 | 2.990149 |
| 1 | -2.064742 | -2.965182 | 2.510333 |
| 6 | 1.994265 | 3.029481 | 2.335978 |
| 1 | 2.638826 | 3.435327 | 1.549812 |
| 1 | 2.200481 | 3.584911 | 3.257516 |
| 1 | 2.288584 | 1.986754 | 2.495267 |
| 6 | -0.371941 | 2.648576 | 3.127746 |
| 1 | -0.169858 | 3.241897 | 4.026671 |
| 1 | -1.434589 | 2.749359 | 2.885979 |
| 1 | -0.178409 | 1.596058 | 3.353264 |
|   |   |   |   |
|---|---|---|---|
| 6 | 0.635274 | 2.609134 | -2.268150 |
| 1 | -0.402547 | 2.896673 | -2.472948 |
| 1 | 1.266189 | 3.052845 | -3.046436 |
| 1 | 0.699608 | 1.518926 | -2.329042 |
| 6 | 0.960578 | 4.624006 | -0.800029 |
| 1 | 1.339622 | 5.022699 | 0.144603 |
| 1 | 1.544051 | 5.082719 | -1.606504 |
| 1 | -0.074695 | 4.956803 | -0.926235 |
| 6 | -5.342429 | -3.692865 | -1.245976 |
| 1 | -5.019003 | -4.251925 | -2.131919 |
| 1 | -5.474836 | -4.422777 | -0.438624 |
| 1 | -6.317824 | -3.250950 | -1.463493 |
| 6 | -4.614125 | 4.689128 | -0.470794 |
| 1 | -4.206245 | 5.341181 | -1.252238 |
| 1 | -5.652896 | 4.466285 | -0.726311 |
| 1 | -4.612587 | 5.267501 | 0.460693 |
| 1 | 6.109085 | -1.495027 | 0.379430 |
| 1 | 4.730732 | -2.441733 | 2.163213 |
| 1 | 2.361419 | -1.795877 | 2.422459 |
| 1 | 2.716783 | 0.795992 | -0.960434 |
| 7 | 5.266501 | 0.267755 | -1.481139 |
| 6 | 6.698322 | 0.101852 | -1.447471 |
| 1 | 7.133690 | 0.568375 | -2.33514 |
| 1 | 7.168479 | 0.547961 | -0.55327 |
| 1 | 6.968334 | -0.959314 | -1.474209 |
| 6 | 4.755821 | 1.424851 | -2.173545 |
| 1 | 4.596618 | 2.292241 | -1.509930 |
| 1 | 5.462994 | 1.715758 | -2.953019 |
| 1 | 3.802354 | 1.200185 | -2.663321 |

Name - TS2_NMe2_o1_
Zero-point correction=               0.775627 (Hartree/Particle)
Thermal correction to Energy=                   0.819383
Thermal correction to Enthalpy=                  0.820327
Thermal correction to Gibbs Free Energy=        0.702483
Sum of electronic and zero-point Energies=   -2256.371391
Sum of electronic and thermal Energies=        -2256.327634
Sum of electronic and thermal Enthalpies=      -2256.326690
Sum of electronic and thermal Free Energies=   -2256.444534
1 imaginary frequency.
Charge =  0 Multiplicity = 1

|   |   |   |   |
|---|---|---|---|
| 0 | 1 |   |   |
| 26 | 0.387936 | -0.340915 | 0.057052 |
| 1 | 0.192569 | -0.252930 | 1.574016 |
| 1 | 1.468608 | -0.939489 | -0.800308 |
| 15 | -0.872799 | -2.166266 | 0.000466 |
| 15 | 1.057244 | 1.755836 | 0.180309 |
| 7 | -2.478245 | -0.102848 | -0.185027 |
|   | 7   | 6   | 5   | 4   | 3   | 2   | 1   |
|---|------|------|------|------|------|------|------|
|   | -1.557809 | 1.785567 | -0.006242 |
|   | -1.255057 | 0.468192  | -0.092748  |
|   | -2.593844 | -1.473820 | -0.209455  |
|   | -3.850829 | -1.975024 | -0.335890  |
|   | -4.005158 | -3.047644 | -0.384423  |
|   | -4.999746 | -1.100360 | -0.398869  |
|   | -4.836393 | 0.259466  | -0.300309  |
|   | -5.698643 | 0.918807  | -0.321075  |
|   | -3.541792 | 0.813439  | -0.172618  |
|   | -2.932631 | 2.061286  | -0.041663  |
|   | -3.293863 | 3.422995  | 0.083135   |
|   | -4.342170 | 3.702560  | 0.046006   |
|   | -2.326491 | 4.378732  | 0.272562   |
|   | -0.933889 | 3.999295  | 0.340085   |
|   | -0.187925 | 4.765275  | 0.524598   |
|   | -0.552556 | 2.703337  | 0.192249   |
|   | 2.327480  | -1.211546 | 0.371417   |
|   | 3.587561  | -1.014431 | -0.246975  |
|   | 0.661593  | -0.429685 | -1.473410  |
|   | 2.348331  | -1.943677 | 1.574535   |
|   | 3.522269  | -2.388860 | 2.176829   |
|   | 3.474980  | -2.907332 | 3.131304   |
|   | 4.746377  | -2.149716 | 1.564075   |
|   | 4.767834  | -1.480247 | 0.347615   |
|   | 1.413285  | -2.106768 | 2.095881   |
|   | 1.937707  | 2.532022  | -1.272981  |
|   | 2.797813  | 1.860313  | -1.380731  |
|   | 1.920740  | 2.467001  | 1.666781   |
|   | 1.948500  | 3.556427  | 1.531170   |
|   | -0.781051 | -3.373965 | -1.414254  |
|   | -1.618542 | -4.075599 | -1.309068  |
|   | -1.055347 | -3.274531 | 1.499080   |
|   | -0.019727 | -3.593571 | 1.681447   |
|   | 3.348594  | 1.928299  | 1.739954   |
|   | 3.871789  | 2.371056  | 2.594819   |
|   | 3.345647  | 0.841694  | 1.864479   |
|   | 3.926853  | 2.158018  | 0.839343   |
|   | 1.150695  | 2.151207  | 2.943986   |
|   | 1.070808  | 1.069123  | 3.079867   |
|   | 1.670526  | 2.581322  | 3.807714   |
|   | 0.135859  | 2.559946  | 2.917573   |
|   | 2.402025  | 3.972027  | -1.097382  |
|   | 2.926790  | 4.304076  | -2.000844  |
|   | 1.553147  | 4.649856  | -0.953878  |
|   | 3.088729  | 4.098458  | -0.256070  |
|   | 1.079197  | 2.381356  | -2.526659  |
|   | 1.654088  | 2.672947  | -3.412975  |
|   | 0.745549  | 1.347596  | -2.651293  |
|   | 0.193283  | 3.025617  | -2.477105  |
|   | 0.536897  | -4.141600 | -1.323350  |

S149
|   |       |         |         |         |         |
|---|-------|---------|---------|---------|---------|
| 1 | 0.604445 | -4.744946 | -0.412634 |
| 1 | 0.649408 | -4.815914 | -2.180006 |
| 1 | 1.390097 | -3.455482 | -1.320525 |
| 6 | -0.924475 | -2.653770 | -2.750817 |
| 1 | -0.853177 | -3.373709 | -3.573920 |
| 1 | -1.888765 | -2.142078 | -2.829020 |
| 1 | -0.140494 | -1.901188 | -2.875207 |
| 6 | -1.517759 | -2.443606 | 2.693123 |
| 1 | -2.564459 | -2.143091 | 2.568617 |
| 1 | -1.444041 | -3.030604 | 3.614975 |
| 1 | -0.915957 | -1.535589 | 2.795411 |
| 1 | -1.923380 | -4.516049 | 1.327860 |
| 1 | -1.574059 | -5.176294 | 0.529561 |
| 1 | -1.920907 | -5.097012 | 2.257169 |
| 1 | -2.964430 | -4.246347 | 1.123116 |
| 6 | -2.677183 | 5.828472 | 0.425083 |
| 1 | -2.330341 | 6.219185 | 1.389009 |
| 1 | -2.201732 | 6.434706 | -0.354960 |
| 1 | -3.756447 | 5.988250 | 0.365266 |
| 6 | -6.357522 | -1.718017 | -0.550942 |
| 1 | -6.569303 | -2.416626 | 0.267101 |
| 1 | -7.143917 | -0.959368 | -0.558037 |
| 1 | -6.430772 | -2.287945 | -1.484780 |
| 1 | 5.674129 | -2.488105 | 2.017372 |
| 1 | 5.719495 | -1.316387 | -0.148641 |
| 7 | 3.661739 | -0.305830 | -1.491278 |
| 6 | 4.900291 | 0.393312 | -1.752007 |
| 1 | 5.740609 | -0.266902 | -2.034530 |
| 1 | 4.745172 | 1.091145 | -2.583563 |
| 1 | 5.198624 | 0.967749 | -0.870806 |
| 6 | 3.274838 | -1.094348 | -2.647678 |
| 1 | 3.145660 | -0.434678 | -3.513242 |
| 1 | 4.029170 | -1.860460 | -2.902749 |
| 1 | 2.323257 | -1.597582 | -2.471798 |

Name - TS2_NMe2_o2_
Zero-point correction= 0.775147 (Hartree/Particle)
Thermal correction to Energy= 0.818939
Thermal correction to Enthalpy= 0.819883
Thermal correction to Gibbs Free Energy= 0.702508
Sum of electronic and zero-point Energies= -2256.371402
Sum of electronic and thermal Energies= -2256.327609
Sum of electronic and thermal Enthalpies= -2256.326665
Sum of electronic and thermal Free Energies= -2256.444040
1 imaginary frequency.
Charge = 0 Multiplicity = 1

0 1
26 -0.497465 -0.136621 -0.302288
|   |      |      |      |
|---|------|------|------|
| 1 | -0.604924 | -0.159245 | 1.215963 |
| 1 | -1.533587 | -0.071551 | -1.406876 |
| 15 | -0.504111 | 2.085692 | -0.214852 |
| 15 | 0.149844 | -2.248431 | -0.039592 |
| 7 | 1.999571 | 1.316348 | -0.201550 |
| 7 | 2.305831 | -0.759001 | 0.028297 |
| 6 | 1.316516 | 0.144970 | -0.165223 |
| 6 | 1.316272 | 2.500413 | -0.323836 |
| 6 | 2.069099 | 3.629074 | -0.404622 |
| 1 | 1.587555 | 4.594295 | -0.521055 |
| 6 | 3.511028 | 3.571234 | -0.322934 |
| 6 | 4.142444 | 2.366922 | -0.134214 |
| 1 | 5.223651 | 2.320583 | -0.048587 |
| 6 | 3.387580 | 1.173168 | -0.057569 |
| 6 | 3.589332 | -0.196042 | 0.109821 |
| 6 | 4.650131 | -1.099831 | 0.348600 |
| 1 | 5.666558 | -0.723902 | 0.412224 |
| 6 | 4.391877 | -2.437308 | 0.518121 |
| 6 | 3.035682 | -2.929406 | 0.438097 |
| 1 | 2.851647 | -3.985577 | 0.601389 |
| 6 | 1.997540 | -2.091438 | 0.177943 |
| 6 | -2.568789 | -0.657888 | -0.594678 |
| 6 | -2.901907 | -1.674326 | -1.512634 |
| 1 | -0.438997 | -0.129437 | -1.868693 |
| 6 | -3.637015 | -0.194812 | 0.209367 |
| 6 | -4.895249 | -0.809235 | 0.139358 |
| 1 | -5.687151 | -0.466156 | 0.799720 |
| 6 | -5.163599 | -1.845301 | -0.747265 |
| 6 | -4.153355 | -2.274647 | -1.597803 |
| 6 | 0.039597 | -3.521431 | -1.413488 |
| 1 | -1.041583 | -3.589539 | -1.584605 |
| 6 | -0.328641 | -3.224792 | 1.473415 |
| 1 | 0.208456 | -4.180303 | 1.421986 |
| 6 | -1.204773 | 3.144999 | -1.575499 |
| 1 | -0.887656 | 4.178670 | -1.385380 |
| 6 | -0.961068 | 2.994061 | 1.352757 |
| 1 | -1.987563 | 2.642365 | 1.498757 |
| 6 | -1.833210 | -3.486914 | 1.438912 |
| 1 | -2.134660 | -4.066413 | 2.318561 |
| 1 | -2.388700 | -2.544747 | 1.437657 |
| 1 | -2.139863 | -4.053538 | 0.547821 |
| 6 | 0.091395 | -2.514663 | 2.755308 |
| 1 | -0.365023 | -1.523078 | 2.814668 |
| 1 | -0.224161 | -3.101361 | 3.625442 |
| 1 | 1.176883 | -2.385281 | 2.806130 |
| 6 | 0.560509 | -4.921415 | -1.110259 |
| 1 | 0.400314 | -5.567726 | -1.980968 |
| 1 | 1.636895 | -4.913128 | -0.912746 |
| 1 | 0.054065 | -5.389125 | -0.261819 |
| 6 | 0.694619 | -2.953358 | -2.670087 |
|   |    |             |             |             |
|---|----|-------------|-------------|-------------|
| 1 | 0.491475 | -3.598312   | -3.531964   |             |
| 1 | 0.330297 | -1.945258   | -2.888833   |             |
| 1 | 1.782076 | -2.895853   | -2.543926   |             |
| 6 | -2.729142 | 3.070053    | -1.539408   |             |
| 1 | -3.137302 | 3.457119    | -0.601604   |             |
| 1 | -3.156221 | 3.654484    | -2.361987   |             |
| 1 | -3.067918 | 2.033911    | -1.643019   |             |
| 6 | -0.656969 | 2.715125    | -2.932846   |             |
| 1 | -1.060547 | 3.363205    | -3.719030   |             |
| 1 | 0.434952 | 2.777379    | -2.966298   |             |
| 1 | -0.937155 | 1.682613    | -3.158938   |             |
| 6 | -0.098730 | 2.484194    | 2.504446    |             |
| 1 | 0.931708 | 2.846279    | 2.408847    |             |
| 1 | -0.491821 | 2.847335    | 3.460669    |             |
| 1 | -0.080252 | 1.390879    | 2.522599    |             |
| 6 | -0.940638 | 4.515826    | 1.288170    |             |
| 1 | -1.610774 | 4.920222    | 0.524618    |             |
| 1 | -1.259983 | 4.926410    | 2.253157    |             |
| 1 | 0.069256 | 4.895638    | 1.099817    |             |
| 6 | 5.490395 | -3.420502   | 0.791222    |             |
| 1 | 5.330200 | -3.937334   | 1.744823    |             |
| 1 | 5.533691 | -4.191955   | 0.013341    |             |
| 1 | 6.465875 | -2.929976   | 0.833712    |             |
| 6 | 4.282263 | 4.852782    | -0.425558   |             |
| 1 | 3.975342 | 5.562603    | 0.351650    |             |
| 1 | 5.356757 | 4.683312    | -0.322049   |             |
| 1 | 4.109092 | 5.342172    | -1.391291   |             |
| 1 | -6.152626 | -2.294066   | -0.780237   |             |
| 1 | -4.337704 | -3.054752   | -2.332078   |             |
| 1 | -2.135585 | -1.977153   | -2.223508   |             |
| 7 | -3.461940 | 0.882990    | 1.140952    |             |
| 6 | -3.050027 | 0.402373    | 2.448870    |             |
| 1 | -3.844220 | -0.185594   | 2.944245    |             |
| 1 | -2.155877 | -0.211706   | 2.330123    |             |
| 1 | -2.799995 | 1.251648    | 3.095733    |             |
| 6 | -4.597645 | 1.774864    | 1.261385    |             |
| 1 | -4.274246 | 2.694100    | 1.766971    |             |
| 1 | -4.971706 | 2.040400    | 0.269685    |             |
| 1 | -5.438188 | 1.365524    | 1.850237    |             |

Name - TS2_NMe2_p_
Zero-point correction= 0.775302 (Hartree/Particle)
Thermal correction to Energy= 0.819504
Thermal correction to Enthalpy= 0.820448
Thermal correction to Gibbs Free Energy= 0.699571
Sum of electronic and zero-point Energies= -2256.373352
Sum of electronic and thermal Energies= -2256.329150
Sum of electronic and thermal Enthalpies= -2256.328206
Sum of electronic and thermal Free Energies= -2256.449083
1 imaginary frequency.
Charge = 0 Multiplicity = 1

|   |   |   |   |   |
|---|---|---|---|---|
| 0 | 1 | 26 | -0.186038 | -0.167370 | 0.250959 |
| 1 | 1 | -0.279780 | -0.161820 | -1.270981 |
| 1 | 1 | -1.192135 | -0.546225 | 1.309025 |
| 15 | 15 | 0.533838 | -2.252003 | 0.118656 |
| 15 | 15 | -0.291001 | 2.031612 | 0.073558 |
| 7 | 7 | 2.645836 | -0.703231 | 0.095672 |
| 7 | 7 | 2.246206 | 1.365120 | -0.001378 |
| 6 | 6 | 1.615754 | 0.174358 | 0.137247 |
| 6 | 6 | 2.392807 | -2.055060 | 0.136429 |
| 6 | 6 | 3.475966 | -2.875677 | 0.131424 |
| 1 | 1 | 3.342162 | -3.951055 | 0.183372 |
| 6 | 6 | 4.816243 | -2.339826 | 0.048768 |
| 6 | 6 | 5.012136 | -0.984609 | -0.053847 |
| 1 | 1 | 6.016112 | -0.580259 | -0.138261 |
| 6 | 6 | 3.906292 | -0.103009 | -0.045133 |
| 6 | 6 | 3.640770 | 1.264019 | -0.122375 |
| 6 | 6 | 4.336698 | 2.482290 | -0.301128 |
| 1 | 1 | 5.419045 | 2.471115 | -0.384470 |
| 6 | 6 | 3.645220 | 3.665073 | -0.389060 |
| 6 | 6 | 2.202997 | 3.671724 | -0.295033 |
| 1 | 1 | 1.674486 | 4.612431 | -0.406479 |
| 6 | 6 | 1.507061 | 2.522403 | -0.090615 |
| 6 | 6 | -2.275140 | -0.386733 | 0.328208 |
| 6 | 6 | -3.172456 | 0.274644 | 1.181360 |
| 1 | 1 | -2.781433 | 0.782591 | 2.063657 |
| 1 | 1 | -0.218639 | -0.199326 | 1.823576 |
| 6 | 6 | -2.886814 | -1.080378 | -0.732347 |
| 6 | 6 | -4.256271 | -1.053678 | -0.964787 |
| 1 | 1 | -4.644658 | -1.595701 | -1.820450 |
| 6 | 6 | -5.128890 | -0.336299 | -0.123647 |
| 6 | 6 | -4.549904 | 0.310254 | 0.979361 |
| 1 | 1 | -2.266952 | -1.626308 | -1.436534 |
| 1 | 1 | -5.167709 | 0.841883 | 1.694759 |
| 6 | 6 | -0.868646 | 3.098465 | 1.500427 |
| 1 | 1 | -1.896316 | 2.743181 | 1.653020 |
| 6 | 6 | -1.033683 | 2.872462 | -1.413705 |
| 1 | 1 | -0.785175 | 3.938562 | -1.328985 |
| 6 | 6 | 0.256004 | -3.488631 | 1.482665 |
| 1 | 1 | 0.842707 | -4.386927 | 1.251320 |
| 6 | 6 | 0.267151 | -3.253844 | -1.442703 |
| 1 | 1 | -0.826976 | -3.247869 | -1.542989 |
| 6 | 6 | -2.551099 | 2.698738 | -1.399950 |
| 1 | 1 | -2.992984 | 3.216482 | -2.258752 |
| 1 | 1 | -2.817326 | 1.639876 | -1.461326 |
| 1 | 1 | -3.013713 | 3.100283 | -0.493149 |
| 6 | 6 | -0.429041 | 2.339096 | -2.707389 |
|    |     |     |     |     |     |     |     |     |
|----|-----|-----|-----|-----|-----|-----|-----|-----|
|    | -0.619597 | 1.266439 | -2.801449 |
| 1  | -0.874433  | 2.856019  | -3.565122 |
| 1  | 0.654203   | 2.492531  | -2.742296 |
| 6  | -0.905325  | 4.603738  | 1.262071  |
|    | -1.296766  | 5.108862  | 2.152666  |
|    | 0.099456   | 5.001438  | 1.085131  |
| 1  | -1.542805  | 4.885588  | 3.626556  |
| 1  | -0.053328  | 2.761781  | 2.746337  |
| 6  | -0.484201  | 3.251507  | 2.921744  |
|    | -0.024248  | 1.682959  | 2.638753  |
| 1  | 0.979047   | 3.114360  | 2.636565  |
| 1  | -1.229199  | -3.846454 | 1.519147  |
| 1  | -1.567117  | -4.312945 | 0.588189  |
| 1  | -1.430671  | -4.547497 | 2.33617  |
| 1  | -1.841724  | -2.952501 | 1.677258  |
| 6  | 0.731679   | -2.932764 | 2.820891  |
| 1  | 0.551843   | -3.665966 | 3.615279  |
| 1  | 1.801887   | -2.704563 | 2.804162  |
| 1  | 0.198514   | -2.011357 | 3.071701  |
| 6  | 0.859379   | -2.509608 | 2.636565  |
| 1  | 1.954661   | -2.528777 | 2.597285  |
| 1  | 0.549114   | -2.988288 | 3.571718  |
| 1  | 0.533262   | -1.465820 | 2.644736  |
| 6  | 0.750316   | -4.698812 | 1.407093  |
| 1  | 0.271569   | -5.290049 | 0.622259  |
| 1  | 0.530257   | -5.185144 | 2.364304  |
| 1  | 1.834981   | -4.748831 | 1.265055  |
| 6  | 4.350167   | 4.972327  | 0.594648  |
| 1  | 4.013061   | 4.561819  | -1.515976 |
| 1  | 4.145073   | 5.666316  | 0.229000  |
| 1  | 5.432618   | 4.838398  | -0.660688 |
| 6  | 5.968095   | -3.299621 | 0.059100  |
| 1  | 5.895068   | -4.015714 | -0.767984 |
| 1  | 6.924454   | -2.778586 | -0.029818 |
| 1  | 5.987430   | -3.640660 | 0.986613  |
| 7  | -6.496628  | -0.271533 | -0.378198 |
| 6  | -7.064825  | -1.231883 | -1.292160 |
| 1  | -6.912701  | -2.277486 | -0.976270 |
| 1  | -8.138513  | -1.051790 | -1.377303 |
| 1  | -6.637264  | -1.117681 | -2.293771 |
| 6  | -7.358009  | 0.215378  | 0.670083  |
| 1  | -7.099863  | 1.246046  | 0.935469  |
| 1  | -8.389511  | 0.221430  | 0.311650  |
| 1  | -7.313884  | -0.391750 | 1.590025  |

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