Supplementary Information

B-H Activation and H-H Formation: Two consecutive Heterolytic Processes on an

Osmium-Hydrogensulfide Bond

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Experimental Section

General Methods and Instrumentation. All manipulations were performed with rigorous exclusion of air at an argon/vacuum manifold using standard Schlenk-tube techniques or in a drybox (MB-UNILAB). Solvents were dried by the usual procedures and distilled under argon prior to use or obtained oxygen- and water-free from an MBraun solvent purification apparatus. Pentane was stored over P_2O_5 in the drybox. Pinacolborane (HBpin = 4,4,5,5-tetramethyl-1,3,2-dioxaborolane) and 9borabicyclo[3.3.1]nonane dimmer ((HBbn)₂) were purchased from commercial sources and used without further purification. Catecholborane (HBcat = 1,3,2-benzodioxaborolane) was purchased from commercial sources and distilled in a Kugelrohr distillation oven. The starting materials $OsDCl(CO)(P^{i}Pr_{3})_{2}^{1}$ and $OsH(CO)(SH)(P^{i}Pr_{3})_{2}$ (1)² were prepared according to published methods. OsD(CO)(SH)(PⁱPr₃)₂ (1-d) was prepared by addition of NaSH·xH₂O (200 mg, 3.6 mmol) to a THF/CH₃OH (15 mL in a 4:1 ratio) suspension of OsDCl(CO)(PⁱPr₃)₂ (470 mg, 0.82 mmol). The mixture was stirred at room temperature for 5 min, and the solvent was removed in vacuo to give an orange oil. Toluene (15 mL) was added, and the resulting suspension was filtered through Celite. The filtrate was concentrated to dryness, and addition of pentane $(2 \times 3 \text{ mL})$ caused the precipitation of an orange solid which was separated by decantation, dried in vacuo, and characterized by ¹H, ²H, and ${}^{31}P{}^{1}H$ NMR spectroscopy as a 0.7:0.3 mixture of 1-d and 1. Spectroscopic data for 1-d: ${}^{2}H$ NMR $(46.07 \text{ MHz}, C_6H_6, 298 \text{ K}) \delta -23.1 (\text{Os}-\text{D}); {}^{31}\text{P} \{ {}^{1}\text{H} \} \text{ NMR} (121.49 \text{ MHz}, C_6D_6, 298 \text{ K}) \delta 44.1.$

NMR spectra were recorded on Varian Gemini 2000, Bruker ARX 300, Bruker Avance 300 MHz, and Bruker Avance 400 MHz instruments. Chemical shifts (expressed in parts per million) are referenced to residual solvent peaks (¹H, ¹³C{¹H}), external H₃PO₄ (³¹P{¹H}), or BF₃·OEt₂ (¹¹B). Coupling constants, *J*, and *N* ($N = J_{H-P} + J_{H-P'}$ or $J_{C-P} + J_{C-P'}$) are given in hertz. Infrared spectra were recorded on a Perkin-Elmer 1730 spectrometer as CH₂Cl₂ solutions. C, H, and S analyses were carried out in a Perkin-Elmer 2400 CHNS/O analyzer.

Preparation of OsH(η^2 -H₂)(CO)(SBpin)(PⁱPr₃)₂ (2). Pinacolborane (25.3 µL, 0.174 mmol) was added to a solution of 1 (100 mg, 0.174 mmol) in 3 mL of toluene. The solution was stirred for 5 min at room temperature. During this time the solution changed from orange to light yellow. After that, the solvent was removed in vacuo to give an orange oil, which was extracted with pentane. The pentane solution was passed through Celite and cooled at 243 K to give red crystals suitable for X-ray diffraction. Yield 30 mg (25 %). Anal. Calcd for C₂₅H₅₇BO₃OsP₂S: C, 42.85; H, 8.20; S, 4.58. Found: C, 43.01; H, 8.51; S, 4.74. IR (CH₂Cl₂, cm⁻¹): v(CO) 1911 (s). ¹H NMR (300 MHz, C₆D₆, 298 K): δ 2.6 (m, 6H, PCHCH₃), 1.26 (dvt, N = 13.5, $J_{H-H} = 7.2$, 18H, PCHCH₃), 1.22 (dvt, N = 13.7, $J_{H-H} = 7.1$,

18H, PCHC*H*₃), 1.16 (s, 12H, Bpin), -3.08 (br, 2H, OsH₂), -7.19 (t, 1H, $J_{H-P} = 20.2$, OsH). T_1 (OsH₂, C₇D₈, 300 MHz, 193 K): 8 ± 1 ms. ³¹P{¹H} NMR (121.49 MHz, C₆D₆, 298 K): δ 30.2 (s). ¹¹B NMR (96.29 MHz, C₆D₆, 298 K): δ 35 (br).

Determination of the $J_{\text{H-D}}$ Value for OsH(η^2 -HD)(CO)(SBpin)(PⁱPr₃)₂ (2-*d*). Pinacolborane (3.8 μ L, 0.026 mmol) was added to an NMR tube containing a solution of 1-*d* and 1 in a 0.7:0.3 ratio (15 mg, 0.026 mmol) in 0.5 mL of C₆D₆. After 5 min, the ¹H{³¹P} and ³¹P NMR spectra showed the presence of a 0.30:0.46:0.23 mixture of **3**, **3**-*d* and OsD(η^2 -H₂)(CO)(SBpin)(PⁱPr₃)₂. Selected data for 2-*d* are as follows. ¹H NMR (300 MHz, C₆D₆, 298 K): δ –3.09 (t (1:1:1), $J_{\text{H-D}} = 27$). $d_{\text{H-H}}(\text{calcd}) = 0.97$ Å.³

Reaction of 1 with Catecholborane: Formation of $OsH(\eta^2-H_2)(CO)(SBcat)(P^iPr_3)_2$ (3) and $Os(Bcat)(CO)(SH)(P^iPr_3)_2$ (6). Catecholborane (18.6 µL, 0.174 mmol) was added to a solution of 1 (100 mg, 0.174 mmol) in 3 mL of toluene. The solution was stirred for 5 min at room temperature. During this time the solution changed from orange to light yellow. The NMR spectra of the solution showed a 1:0.5 mixture of complexes **3** and **6** (*vide infra*). The solvent was removed in vacuo to give an orange oil which was washed with pentane (6 × 2 mL) to afford a yellow solid. It was separated by decantation, dried in vacuo, and characterized as a 1:0.2 mixture of complexes **3** and **6**. Yield 45 mg (37 %). Spectroscopic data for **3** are as follows. IR (CH₂Cl₂, cm⁻¹): v(CO) 1919 (s). ¹H NMR (300 MHz, C₆D₆, 298 K): δ 7.07 (m, 2H, Bcat), 6.78 (m, 2H, Bcat), 2.5 (m, 6H, PCHCH₃), 1.17 (dvt, *N* = 13.0, *J*_{H-H} = 6.6, 18H, PCHCH₃), 1.13 (dvt, *N* = 13.0, *J*_{H-H} = 6.6, 18H, PCHCH₃), 1.13 (dvt, *N* = 13.0, *J*_{H-H} = 6.6, 18H, PCHCH₃), -2.75 (br, 2H, OsH₂), -7.04 (t, 1H, *J*_{H-P} = 19.4, OsH). *T*₁ (OsH₂, C₇D₈, 300 MHz, 183 K): 43 ± 1 ms. ³¹P{¹H} NMR (121.49 MHz, C₆D₆, 298 K): δ 30.5 (s). ¹¹B NMR (96.29 MHz, C₆D₆, 298 K): δ 36 (br).

Determination of the J_{H-D} **Value for OsH**(η^2 -H-D)(CO)(SBcat)(PⁱPr₃)₂ (3-*d*). Catecholborane (2.8 μ L, 0.026 mmol) was added to an NMR tube containing a solution of 1-*d* and 1 in a 0.7:0.3 ratio (15 mg, 0.026 mmol) in 0.5 mL of C₆D₆. After 5 min, the ¹H{³¹P} and ³¹P NMR spectra showed the presence of a mixture of 3, 3-*d*, OsD(η^2 -H₂)(CO)(SBcat)(PⁱPr₃)₂ and 6. Selected data for 3-*d* are as follows. ¹H NMR (300 MHz, C₆D₆, 298 K): δ -2.76 (t (1:1:1), J_{H-D} = 27). d_{H-H} (calcd) = 0.97 Å.³

Preparation of OsH(η^2 -H₂)(CO)(SBbn)(PⁱPr₃)₂ (4). 9-borabicyclo[3.3.1]nonane dimer (25.4 mg, 0.104 mmol) was added to a solution of 1 (100 mg, 0.174 mmol) in 3 mL of toluene. The solution was stirred for 2 h at room temperature. During this time the solution changed from orange to light orange. After that, the solvent was removed in vacuo to give an orange oil. Yield 117 mg (97 %). Pentane (2 mL) was added and the resulting solution was passed through Celite and cooled at 243 K to give orange

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crystals suitable for X-ray diffraction. Anal. Calcd for $C_{27}H_{59}BOOsP_2S$: C, 46.67; H, 8.56; S, 4.61. Found: C, 46.95; H, 8.73; S, 4.62. IR (CH₂Cl₂, cm⁻¹): v(CO) 1915 (s). ¹H NMR (300 MHz, C₆D₆, 298 K): δ 2.48 (m, 6H, PCHCH₃), 2.02-1.86 (m, 12H, Bbn), 1.55-1.45 (m, 2H, Bbn), 1.2 (dvt, N = 13.8, $J_{H-H} = 6.9$, 18H, PCHCH₃), 1.18 (dvt, N = 13.7, $J_{H-H} = 6.8$, 18H, PCHCH₃), -3.67 (br, 2H, OsH₂), -6.35 (t, 1H, $J_{H-P} = 20.4$, OsH). $T_{1(min)}$ (OsH₂, C₇D₈, 300 MHz, 203 K): 13 ± 1 ms. ³¹P{¹H} NMR (121.49 MHz, C₆D₆, 298 K): δ 31.4 (s). ¹¹B NMR (96.29 MHz, C₆D₆, 298 K): δ 76 (br).

Determination of the J_{H-D} Value for OsH(η^2 -H-D)(CO)(SBbn)(PⁱPr₃)₂ (4-*d*). (HBbn)₂ (3.2 mg, 0.016 mmol) was added to an NMR tube containing a solution of 1-*d* and 1 in a 0.7:0.3 ratio (15 mg, 0.026 mmol) in 0.5 mL of C₆D₆. After 5 min, the ¹H{³¹P} and ³¹P NMR spectra showed the presence of a 0.30:0.46:0.23 mixture of 4, 4-*d* and OsD(η^2 -H₂)(CO)(SBbn)(PⁱPr₃)₂. Selected data for 4-*d* are as follows. ¹H NMR (300 MHz, C₆D₆, 298 K): δ -3.69 (t (1:1:1), J_{H-D} = 26). d_{H-H} (calcd) = 0.99 Å.³

Reaction of 1 with excess of Pinacolborane: Formation of OsH₂(η²-H–Bpin)(CO)(PⁱPr₃)₂ (5). Pinacolborane (30.2 μL, 0.208 mmol) was added to an NMR tube containing a solution of 1 (15 mg, 0.026 mmol) in 0.5 mL of toluene-*d*₈. The solution changed from orange to pale yellow. After 17 h the NMR spectra showed the quantitative formation of **5**. ¹H{¹¹B} NMR (400 MHz, C₇D₈, 298 K): δ 2.30 (m, 6H, PCHCH₃), 1.23 (dvt, N = 14, *J*_{H–H} = 7.2, 18H, PCHCH₃), 1.21 (dvt, N = 14.2, *J*_{H–H} = 7.0, 18H, PCHCH₃), 1.1 (s, 12H, Bpin), –9.8 (br, 1H, BH), –10.5 (br, 2H, OsH). ¹H{¹¹B} NMR (400 MHz, C₇D₈, 298 K): δ 2.30 (m, 6H, PCHCH₃), 1.1 (s, 12H, Bpin), –9.8 (br, 1H, BH), –10.5 (br, 2H, OsH). ¹H{¹¹B} NMR (400 MHz, C₇D₈, 283 K): δ –9.5 (br, 1H, BH), –9.8 (br, 1H, OsH), –11.2 (dt, 1H, *J*_{H–P} = 20.1, *J*_{H–H} = 5.2, OsH). ³¹P{¹H} NMR (162 MHz, C₇D₈, 298 K): δ 38.0 (s). ¹¹B NMR (128 MHz, C₇D₈, 298 K): δ 34 (br).

Preparation of Os(Bcat)(CO)(SH)(PⁱPr3)² (6). *Method A.* Catecholborane (18.6 μ L, 0.174 mmol) was added to a solution of **1** (100 mg, 0.174 mmol) in 3 mL of toluene. The solution was stirred for 5 min at room temperature. During this time the solution changed from orange to light yellow. The solvent was removed in vacuo to give an orange oil which was treated with pentane (3 mL) to afford a yellow solid. The solvent was removed under vacuum and the product was kept under dynamic vacuum for 10 h to yield a yellow solid. Yield 117 mg (97 %).

Method B. Catecholborane (18.6 μ L, 0.174 mmol) was added to a solution of **1** (100 mg, 0.174 mmol) in 3 mL of toluene. The solution was stirred for 5 min at room temperature. During this time the solution changed from orange to light yellow. The solvent was removed in vacuo to give an orange oil which was washed with pentane (6 × 2 mL) to afford a yellow solid. The pentane solution was passed through Celite and cooled at 243 K to give **6** as orange crystals suitable for X-ray diffraction. Yield 50 mg (42 %). Anal. Calcd for C₂₅H₄₇BO₃OsP₂S: C, 43.47; H, 6.86; S, 4.64. Found: C, 43.73; H, 7.32; S,

4.63. IR (CH₂Cl₂, cm⁻¹): v(CO) 1900 (s). ¹H NMR (300 MHz, C₆D₆, 298 K): δ 7.18 (m, 2H, Bcat), 6.8 (m, 2H, Bcat), 2.91 (t, 1H, $J_{\text{H-P}}$ = 19.5, SH), 2.61 (m, 6H, PCHCH₃), 1.24 (dvt, N = 13.9, $J_{\text{H-H}}$ = 7.1, 18H, PCHCH₃), 1.04 (dvt, N = 13.1, $J_{\text{H-H}}$ = 7.1, 18H, PCHCH₃). ³¹P{¹H} NMR (121.49 MHz, C₆D₆, 298 K): δ 34.5 (s). ¹¹B NMR (96.29 MHz, C₆D₆, 298 K): δ 35 (br).

Structural Analysis of Complexes 2, 4, and 6. X-ray data were collected for all complexes on a Bruker Smart APEX CCD diffractometer equipped with a normal focus, 2.4 kW sealed tube source (Mo radiation, $\lambda = 0.71073$ Å) operating at 50 kV and 30 mA. Data were collected over the complete sphere. Each frame exposure time was 20 s or 10 s (4 and 6) covering 0.3° in ω . Data were corrected for absorption by using a multiscan method applied with the SADABS program.⁴ The structures of all compounds was solved by direct methods. Refinement, by full-matrix least squares on F^2 with SHELXL97,⁵ was similar for all complexes, including isotropic and subsequently anisotropic displacement parameters. The C-H hydrogen atoms were calculated and refined using a restricted riding model. The SH hydrogen atom of 6 was located in the difference Fourier map and refined freely. All hydride ligands of 2 and 4 were located in the Fourier difference maps. The ability to find hydrides of heavy metals depends strongly of the quality of the data.⁶ In Fig. S2 we can see these maps (*left*, without hydrides; *right* with hydrides for reference purposes) in the plane P-Os-P for 2 (top) and 4 (botom) visualized with the Platon program.⁷ Firstly, these H atoms were refined in the same way as heavier isotropic atoms. However, their positions and atomic displacement factors are affected by the big residuals close to osmium atoms, especially in 2, as we can see in Fig. S2. Finally a restrained model was used. In 2 the osmium-hydride distances were fixed to 1.59(1) Å [DFIX utility, 3 restrains], whereas the angles and displacement factors were free to refine. On the contrary, in 4 the hydrides refined to acceptable geometrical positions, but the displacement parameters were fixed to a multiplicity of the osmium one. The validity of the model used in the refinement of the hydride ligands in 2 and 4 is given by the similarity of the final geometries, and especially by the agreement with the NMR spectroscopic data and the theoretical calculations.



Fig S1 Ortep drawings of 2, 4 and 6. Thermal ellipsoids are shown at 50% level.



Fig S2 Difference Fourier maps for **2** (top) and **4** (bottom) in the P-Os-P plane without hydrides (left) and with hydrides (right).

Crystal data for **2** (CCDC 936598): C₂₅H₅₇BO₃OsP₂S, M_W 700.72, red, irregular block (0.16 x 0.12 x 0.08), triclinic, space group Pī, *a*: 9.0107(5) Å, *b*: 11.3802(6) Å, *c*: 16.2396(8) Å, *α*: 96.9060(10) °, β : 96.1840(10) °, γ : 106.0440(10) °, V = 1571.36(14) Å³, Z = 2, D_{calc}: 1.481 g cm⁻³, F(000): 716, T = 100(2) K, μ : 4.248 mm⁻¹. 19347 measured reflections (20: 3-58°, ω scans 0.3°), 7308 unique (R_{int} = 0.0271); min./max. transm. Factors 0.673/0.862. Final agreement factors were R¹ = 0.0239 (6790 observed reflections, I > 2 σ (I)) and wR² = 0.0540; data/restraints/parameters 7308/3/326; GoF = 1.056. Largest peak and hole 1.407 (close to osmium atom) and -0.498 e/ Å³.

Crystal data for **4** (CCDC 936599): C₂₇H₅₉BOOsP₂S, M_W 694.75, orange, irregular block (0.25 x 0.14 x 0.07), orthorhombic, space group Pbca, *a*: 11.5073(5) Å, *b*: 20.3829(9) Å, *c*: 27.0237(12) Å, V = 6338.5(5) Å³, Z = 8, D_{calc}: 1.456 g cm⁻³, F(000): 2848, T = 100(2) K, μ 4.208 mm⁻¹). 74109 measured reflections (20: 3-58°, ω scans 0.3°), 7829 unique (R_{int} = 0.0365); min./max. transm. Factors 0.668/0.862. Final agreement factors were R¹ = 0.0219 (6448 observed reflections, I > 2 σ (I)) and wR² = 0.0533; data/restraints/parameters 7829/0/319; GoF = 1.034. Largest peak and hole 1.258 (close to osmium atom) and -0.489 e/ Å³.

Crystal data for **6** (CCDC 93660): C₂₅H₄₇BO₃OsP₂S, M_W 690.64, orange, irregular block (0.22 x 0.15 x 0.05), monoclinic, space group P2₁/n, *a*: 16.2977(7) Å, *b*: 10.9590(5) Å, *c*: 16.8715(7) Å, *β*: 106.1190(10)°, V = 2894.9(2) Å³, Z = 4, D_{calc}: 1.585 g cm⁻³, F(000): 1392, T = 100(2) K, µ: 4.611 mm⁻¹. 34451 measured reflections (20: 3-58°, ω scans 0.3°), 7005 unique (R_{int} = 0.0322); min./max. transm. Factors 0.673/0.862. Final agreement factors were R¹ = 0.0237 (6132 observed reflections, I > 2 σ (I)) and wR² = 0.0562; data/restraints/parameters 7005/0/313; GoF = 0.988. Largest peak and hole 1.323 (close to osmium atom) and -0.932 e/ Å³.

Computational Details and Cartesian Coordinates of Model Complexes. The theoretical calculations were carried out on the model complexes by optimizing the structures at the M06-DFT levels⁸ with the Gaussian 09 program⁹ in vacuo. The basis sets used were LANL2DZ basis and pseudopotentials for Os, and 6-31G(d,p) for the rest of atoms. All stationary points were confirmed by having only positive vibrational frequencies for intermediates or one negative frequency for transition states. Transition state search was performed in a two-stage process: first, a relaxed PES scan of the key bonds broken or formed was performed, and then the highest energy structure was optimized as transition state by the default Gaussian09 algorithm. The chemical correctness of the transition states found was confirmed by visual inspection of the normal mode having the negative vibrational frequency, followed by calculating intrinsic reaction coordinates routes (IRC, 50 maximum points in each direction with standard stepsize, 0.01 Bohr) towards the corresponding minima, and reoptimizing from the final phase of the IRC paths to reach each minima. In this way we have calculated the complexes **B**₁, **B**₂ and **C**₁, **C**₂ as conformational isomers by rotation about the osmium-phosphorous single bonds. The TS of these rotations were not calculated by their chemical meaningless.

All the Gibbs energies collected in the text are calculated at 298.15 K and 1 atm.



Fig. S3 Energy profile (Δ G, kcal·mol⁻¹) for the formation of OsH(SBpin)(η^2 -H₂)(CO)(PMe₃)₂ (**2t**) from OsH(SH)(CO)(PMe₃)₂ (**1t**) and HBpin. Drawings of **B**₁and **C**₂are omitted for clarity.

1t

Os	-0.00500000	0.06206500	-0.00419000
Н	-0.01147800	0.59377700	1.52059100
P	2.34950800	0.01179000	0.15906300
P	-2.34721000	-0.01457500	0.15609500
S	0.13431900	-2.24676300	-0.61359800
0	-0.02691900	2.97125000	-0.82184900
С	-0.01944400	1.85997100	-0.44930100
С	3.16813900	1.63227300	0.38575800
Н	2.76457700	2.10999200	1.28465700
С	2.94871700	-0.94904800	1.59744100
Н	4.04361300	-0.93774200	1.65778400
С	3.29452200	-0.72947400	-1.22469000
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С	-2.96436600	-1.09709100	1.50052100
Н	-2.60955800	-2.12105900	1.34620700
С	-3.30275700	-0.59643800	-1.29813800
Н	-4.37668100	-0.64320200	-1.08080300
Н	-3.12982700	0.09179900	-2.13180100
Н	-2.94941100	-1.58699500	-1.60285800
Н	-4.06005700	-1.09145600	1.54715500
Н	-2.55518100	-0.73865400	2.45083400
Н	-2.77240400	1.96570800	1.47743000
Н	-4.26053800	1.44658500	0.62901900
Н	4.25428800	1.52152100	0.48572700
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Н	4.37041300	-0.74494500	-1.01295200
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Thermal correction to Gibbs Free Ene	ergy= 0.206536	
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Sum of electronic and thermal Energie	es= -1525.461137	
Sum of electronic and thermal Enthalp	pies= -1525.460193	
Sum of electronic and thermal Free El	nergies= -1525.531136	

HBpin

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В	0.00015300	1.92712600	-0.00019800
C	-0.77780800	-0.18678700	0.05459500
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С	-1.34678900	-1.10409800	1.11623800
Н	-0.98127400	-0.84934700	2.11487100
Н	-1.09008000	-2.14954800	0.90301300
Н	-2.43865100	-1.01948900	1.12542800
C	0.77780400	-0.18689400	-0.05460200
С	1.47414700	-0.43348300	1.27534700
Н	2.53696200	-0.19503900	1.16296300
Н	1.38747500	-1.47915600	1.59185900
Н	1.06646800	0.20686400	2.06568000
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Н	1.08975600	-2.14993800	-0.90249900
Н	2.43861100	-1.02025100	-

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Thermal correction to Gibbs Free Ener	gy= 0.157627
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Sum of electronic and thermal Energie	s= -411.420632
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File Type log Calculation Type FREQ Calculation Method RM00 Basis Set Gen Charge 0 Spin Singlet RMS Gradient Norm 0.0000666 RMS Gradient Norm 0.0000666 Dipole Moment 2.5642 Debye Oct Job cpu time: 0 hours 53 minutus 18.0	File Name	borano	. 141 T. A T
Calculation Type FFEO Calculation Method RM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -411.62045039 RMS Gradient Norm 0.0000866 Jipole Moment 2.5642 Dehyee C1 Job cpu time: 0 hours 53 minut ust.	File Type	.log	
Calculation Method RM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -411.6204503 RMS Gradient Norm 0.0000666 Jipole Moment 2.5642 Point Group C1	Calculation Type	FREQ	
Basis Set Gen Charge 0 Spin Singlet E(RM06) -411.6204503 a.u. RMS Gradient Norm 0.0000066 a.u. Imaginary Freq 0 - Dipole Moment 2.5642 Debye Point Group C1 - Job cpu time: 0 days b hours 53 misus transmostrational seconds.	Calculation Method RM06		
Charge 0 Spin Singlet E(RM06) -411.62045038 a.u. RMS Gradient Norm 0.0000686 a.u. Imaginary Freq 0 Dipole Moment 2.5642 Debye Point Group C1	Basis Set	Gen	
Spin Singlet E(PM06) -411.6204503 a.u. RMS Gradient Norm 0.00000666 a.u. Imaginary Freq 0 0 Dipole Moment 2.5642 Debye Point Group C1 Job cpu time: 0 days 0 hours 53 minutes 18.0	Charge	0	
E(RM06) -411.62045039 a.u. RMS Gradient Norm 0.00000666 a.u. Imaginary Freq 0 0 Dipole Moment 2.5642 Debye Point Group C1 1 Job cpu time: 0 days 0 hours 53 minutes 18.0	Spin	Singlet	
RMS Gradient Norm 0.00000666 a.u. Imaginary Freq 0 0 Dipole Moment 2.5642 Debye Point Group C1 0 Job cpu time: 0 days of hours 53 minutes 18.0 seconds. 1	E(RM06)	-411.62045039	a.u.
Imaginary Freq 0 Dipole Moment 2.5642 Debye Point Group C1 C1 Job cpu time: 0 days 0 hours 53 minutes 18.0 seconds. Seconds. Seconds.	RMS Gradient Norm	0.0000686	a.u.
Dipole Moment 2.5642 Debye Point Group C1 Job cpu time: 0 days 0 hours 53 minutes 18.0 seconds. 18.0	Imaginary Freq 0		
Point Group C1 Job cpu time: 0 days 0 hours 53 minutes 18.0 seconds.	Dipole Moment 2.5642 Debye		
Job cpu time: 0 days 0 hours 53 minutes 18.0 seconds.	Point Group	C1	

1.12500600

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A

05	1 16579700	0 12976100	0 01004300
ц Ц	2 45476900	0.35073300	0.01001000
11	2.43470500	0.33073300	1 10055000
H	-0.33061200	-0.16821500	-1.18255000
P	1./84/4900	-2.153/8600	0.00089200
P	0.72103700	2.44047500	0.25705300
S	-0.11735500	-0.55611500	2.05756200
0	-2.13677700	-1.39613000	-0.79497500
0	-2.18345000	0.83779100	-0.28305800
0	2 86161500	0 86062800	-2 39429300
в	-1 43099800	-0 24372600	-0 64178900
C	2 46036500	1 15704200	0.25700200
	-3.46036300	-1.13764300	-0.23799300
C	-3.49672800	-1./6689500	1.13325500
H	-3.27139100	-2.83603600	1.04886500
Н	-4.48782200	-1.66384900	1.59018500
H	-2.73994300	-1.32108900	1.78738100
С	-4.46604900	-1.86136300	-1.14719700
Н	-4.37516000	-1.55807200	-2.19369600
Н	-5.48908000	-1.65474000	-0.80770900
н	-4 30448100	-2 94291700	-1 09200600
C	-3 56516800	0 10886000	-0.27544500
C	-3.303108000	0.40880000	-0.2/544500
	-4.10224900	0.96406600	-1.54951000
H	-4.04851300	2.05142400	-1.56022400
Н	-5.25495700	0.74893700	-1.61112800
H	-3.69067600	0.55512200	-2.43951500
С	-4.23656100	1.01007100	0.94111400
Н	-3.69426300	0.75716400	1.85771300
Н	-5.27100300	0.65619400	1.03317100
Н	-4.25977900	2.10175300	0.84520200
С	2.19811000	0.55728000	-1.47816100
С	2.88758100	-2.69707700	-1.35729000
Н	3.80562700	-2.10042300	-1.33802300
C	2,71319600	-2.67906800	1,48701600
н	2 94660500	-3 75008400	1 45300900
	0 42692700	-3 38041600	-0.07440300
u u	-0 27297300	-3 10220500	0.74512500
11 C	2 22557500	2 42107500	0.53733700
C II	2.23537500	3.4310/300	0.00122700
H	2.93544900	3.24410100	-0.28422100
C	-0.39351100	3.05221400	1.5/601200
Н	-1.38405000	2.60525600	1.434/0000
С	0.01295900	3.25172800	-1.22795400
H	-0.08049600	4.33536100	-1.08664900
Н	0.66173900	3.05251900	-2.08789400
H	-0.97425500	2.82038700	-1.42249100
Н	-0.47221300	4.14472800	1.52542700
Н	-0.00391500	2.76546900	2.55848600
Н	2.70954800	3.10715500	1.46874900
Н	2.01190500	4.50419500	0.58972800
Н	3.14278800	-3.75873800	-1.25674800
н	2,39419900	-2.53243100	-2.32080800
н	0 81/52000	-4 40351000	0 00200100
11 U	_0 12207000	-3 25006000	-1 01205400
11	-0.1230/000	-3.23090900	-1.01303400
п	2.11440100	-2.43313900	2.3/34/300
н	3.64041300	-2.10015100	1.545/8500
Н	-0.63149500	0.61943600	2.4/248900

Zero-point correction=	0.449847 (Hartree/Particle)
Thermal correction to Energy=	0.480545
Thermal correction to Enthalpy=	0.481490
Thermal correction to Gibbs Free Ener	gy= 0.389695
Sum of electronic and zero-point Energy	gies= -1936.929554
Sum of electronic and thermal Energie	s= -1936.898856
Sum of electronic and thermal Enthalp	ies= -1936.897911
Sum of electronic and thermal Free Er	ergies= -1936.989706

F	rimero		
File Name	m-ts3-a-freq		
File Type	.log		
Calculation Type	FREQ		
Calculation Method	RM06		
Basis Set	Gen		
Charge	0		
Spin	Singlet		
E(RM06)	-1937.37940096	a.u.	
RMS Gradient Norm	0.00000738	a.u.	
Imaginary Freq	0		
Dipole Moment	3.2015	Debye	
Point Group	C1		
Job cpu time: 0 days 13 hours 29 minutes 57.1 seconds.			

TS1

Os	-1.15850000	0.15495200	-0.02850600
н	-2.42312800	0.42122300	-1.02696400
	0 01100000	0.01010500	1 05105000
п	0.31106600	-0.21318300	1.03123600
P	-1.89388300	-2.09539900	0.00298700
P	-0.61882300	2.44464700	-0.28784700
S	0.31239800	-0.65802400	-1.89702400
0	2 04190700	1 46550500	0 61044700
0	2.04189700	-1.46550500	0.01044700
0	2.16210800	0.77649300	0.09936700
0	-2.85898600	0.98486800	2.33468900
В	1.33149500	-0.31961600	0.30814100
C	3 41065000	-1 21504400	0 24761300
C	3.41003000	1.21304400	1 1 0 0 1 0 0 0
C	3.63/28500	-1./4295600	-1.16281800
H	3.33393200	-2.79585500	-1.19021100
Н	4.69456800	-1.68105500	-1.44706700
н	3,03359400	-1.21003400	-1.90301800
c.	4 20217200	-1 07154200	1 21252500
	4.3021/200	-1.9/134200	1.21332300
Н	4.05916600	-1./4500200	2.25525200
H	5.35904500	-1.73343500	1.03664700
Н	4.16966300	-3.04851100	1.06322900
С	3,50963300	0.34324100	0.35783500
0	2.05050000	0.00000000	1.7000400
C	3.85857700	0.82382800	1.76000400
Н	3.73555100	1.91233100	1.80037900
H	4.89472200	0.58926400	2.03078600
Н	3,19118400	0.38006200	2.50782600
C	4 42714500	0 99475500	-0 65690100
	4.42/14500	0.33473300	1 0110100
Н	4.10088500	0./9026/00	-1.68146400
H	5.45914500	0.64063400	-0.53904700
Н	4.42366400	2.08106500	-0.50974200
С	-2.20615600	0.64800500	1,42390800
Ċ	-2 07695100	-2 54620000	1 22526000
	-3.07095100	-2.34029900	1.052020000
Н	-3.96339300	-1.90/32900	1.25395/00
С	-2.78412500	-2.60445500	-1.51167300
Н	-3.07528900	-3.66088900	-1.46808600
С	-0.61282100	-3.39538200	0.16369100
u u	0 12874400	-3 27572700	-0 63425200
	0.120/4400	5.27572700	0.03423200
C	-2.09145800	3.513/2400	-0.491/8800
H	-2.76465600	3.35937200	0.35819500
С	0.44893400	2.99699800	-1.67003500
Н	1,42945300	2.51731100	-1.57646400
Ċ	0 20423200	2 20005200	1 16406100
	0.20425200	3.20003200	1.10490100
Н	0.3/465800	4.2/3/6100	1.01964300
H	-0.42853500	3.04869300	2.04653600
Н	1.15986300	2.68746900	1.32091500
н	0.57163500	4.08601700	-1.63694900
ц	-0.00564400	2 71022500	-2 62602600
п	-0.00504400	2.71032300	-2.02092000
Н	-2.62263100	3.22233200	-1.40314000
Н	-1.81249300	4.57276600	-0.54775800
Н	-3.37933800	-3.59669100	1.23983500
Н	-2.61426100	-2.38075100	2.30366200
	1 05015000	1 20550000	0 10660400
п	-1.02912800	-4.39338800	U.1009400
Н	-0.08924800	-3.27379200	1.11741000
H	-2.13371500	-2.43235300	-2.37541100
Н	-3.67473800	-1.97840100	-1.62452500
Н	0.77355100	0.50267600	-2.40775900
	0.,, <u>000100</u>	0.0020,000	

Zero-point correction=	0.448809 (Hartree/Particle)
Thermal correction to Energy=	0.478570
Thermal correction to Enthalpy=	0.479514
Thermal correction to Gibbs Free Ener	rgy= 0.391081
Sum of electronic and zero-point Energy	gies= -1936.928640
Sum of electronic and thermal Energie	-1936.898879
Sum of electronic and thermal Enthalp	ies= -1936.897934
Sum of electronic and thermal Free Er	nergies= -1936.986368

p	rimeG2:M1:V1	- Gauss		
File Name	m-ts3-freq			
File Type	.log			
Calculation Type	FREQ			
Calculation Method	RM06			
Basis Set	Gen			
Charge 0				
Spin	Singlet			
E(RM06)	-1937.37744880	a.u.		
RMS Gradient Norm	0.00000335	a.u.		
Imaginary Freq	1			
Dipole Moment	1.8865	Debye		
Point Group	C1			
Job cpu time: 0 days 14 hours 32 minutes 47.1 seconds.				
	w File Save Data	J		

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0.s	-1.17036800	0.13857600	-0.04887200
ц Ц	-2 48024900	0 36093100	-1 01649500
11	2.40024900	0.30033100	1.01049500
Н	0.38605900	-0.14665800	0.89201900
P	-1.84075800	-2.13081300	0.01239400
P	-0.70053600	2.44620000	-0.28296800
S	0.38961000	-0.60877100	-1.88044600
0	2.05869400	-1.44674700	0.42135300
0	2 22221000	0 80721900	-0.09482200
0	2.222210000	0.00721900	0.00402200
0	-2.83179900	0.89238800	2.36000300
В	1.34841500	-0.30013200	0.029/5900
С	3.44405600	-1.15722100	0.21029200
С	3.82037800	-1.56524600	-1.20952200
Н	3.49746900	-2.60032300	-1.36820900
н	4,90378100	-1.51358500	-1.37250300
U U	3 32262600	_0 9/178800	-1 95905300
11 C	4 25022000	1 06120000	1 20276400
	4.23923900	-1.90139000	1.203/6400
Н	3.88631500	-1.8339//00	2.22393500
H	5.31630000	-1.66690400	1.17237800
H	4.19846000	-3.02653000	0.95369900
С	3.48895600	0.38498000	0.42970200
С	3,52530500	0.76407200	1,90515400
H	3 37882300	1 84683000	1 99703000
u u	4 49496200	0 51049200	2 27117500
н	4.48488200	0.51048200	2.3/11/300
н	2.72268300	0.26251500	2.45869000
С	4.59676900	1.10101800	-0.31514000
Н	4.51280700	0.96220600	-1.39688300
H	5.58020800	0.73836200	0.01061100
Н	4.54849300	2.17594000	-0.10651100
С	-2.19470500	0.58387400	1,42816200
c	-3 15008600	-2 53663400	1 22519700
U U	4 01005000	1 00600000	1 04207500
п о	-4.01983900	-1.09009000	1.04297300
C	-2.56912300	-2./3326200	-1.55489200
H	-2.84726800	-3.79158500	-1.48310600
С	-0.56881100	-3.40061700	0.36600300
H	0.22938400	-3.34303100	-0.38177600
С	-2.19477200	3.49401600	-0.42298600
Н	-2.84060500	3.31090800	0.44251300
C	0 32989000	3 04008400	-1 67601100
U U	1 32078600	2 57809100	-1 60215000
н а	1.32078000	2.37809100	-1.00213000
C	0.15868200	3.10983600	1.16292100
Н	0.31177900	4.24963000	1.04703400
H	-0.43793900	2.97970500	2.06184600
H	1.12541100	2.66302300	1.26432300
Н	0.43475200	4.13028000	-1.62674800
Н	-0.13490200	2,77093100	-2.63087300
н	-2 74734000	3 21219100	-1 32454800
 Ц	_1 93507900	1 55861000	-0 16125900
11	-1.93307900	JJUU1900	1 14152400
п	-3.44683000	-3.388/2900	1.14153400
Н	-2.78839600	-2.34306600	2.24019100
Н	-1.00568400	-4.40675600	0.36231800
H	-0.11199500	-3.19401200	1.33898300
Н	-1.84249700	-2.59615900	-2.36227700
Н	-3.45338400	-2.13125600	-1.78620800
Н	0.75508600	0.56508800	-2.43660600

Zero-point correction=	0.449283 (Hartree/Particle)
Thermal correction to Energy=	0.479357
Thermal correction to Enthalpy=	0.480301
Thermal correction to Gibbs Free Ener	gy= 0.391685
Sum of electronic and zero-point Energy	gies= -1936.929064
Sum of electronic and thermal Energie	s= -1936.898990
Sum of electronic and thermal Enthalp	ies= -1936.898046
Sum of electronic and thermal Free Er	ergies= -1936.986663

File Name m-ts3 ¹ b-freq File Type .log File Type .log Calculation Type FREO Calculation Method RM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.37834735 RMS Gradient Norm 00000072 Imaginary Freq 0 Dipole Moment 1.3375 Debye C1 Job cpu time: 0 days 14 hours 34 minutus 44.8 seconds.	p	rimero G2:	M1:V1 ·	
File Type log Calculation Type FREO Calculation Method RM06 Basis Set Gen Spin Singlet E(RM06) -1937.37834735 a.u. RMS Gradient Norm Imaginary Freq 0 Dipole Moment 1.3375 Debye C1 Job cpu time: 0 days 14 hours 34 minutust s4.8 asconds.	File Name	m-ts3-b-fred	1	
Calculation Type FREO Calculation Method PM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.37834735 a.u. RMS Gradient Norm 0.00000772 a.u. Imaginary Freq 0 Dipole Moment 1.3375 Debye Point Group C1 Job cpu time: 0 days 14 hours 34 minutes 44.8 seconds.	File Type	ile Type .log		
Calculation Method RM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.37834735 RMS Gradient Norm 0.0000072 Imaginary Freq 0 Dipole Moment 1.3375 Point Group C1 Jobcpu time: 0 descritted	Calculation Type	FREC	1	
Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.37834735 RMS Gradient Norm 0.0000072 Imaginary Freq 0 Dipole Moment 1.3375 Debye C1 Job cpu time: 0 days 14 hours 34 minutust s4.8 seconds.	Calculation Method	RM08	ŝ	
Charge 0 Spin Singlet E(RM06) -1937.37834735 RMS Gradient Norm 0.00000722 RMS Gradient Norm 0.00000722 Jopole Moment 1.3375 Dipole Moment 1.3375 Dipole Moment 0.13375 Debye C1 Job cpu time: 0 days 14 hours 34 minutus 44.8 seconds. seconds.	Basis Set	Ger	1	
Spin Singlet E(RM06) -1937.37834735 a.u. RMS Gradient Norm 0.00000772 au. Imaginary Freq 0 0 Dipole Moment 1.3375 Debye Point Group C1 0 Job cpu time: 0 days 14 hours 34 minutes 44.8 seconds.	Charge 0			
E(RM06) -1937.37834735 a.u. RMS Gradient Norm 0.0000072 a.u. Imaginary Freq 0 Dipole Moment 1.3375 Debye Point Group C1 Job cpu time: 0 days 14 hours 34 minutes 44.8 seconds.	Spin	Single	t	
RMS Gradient Norm 0.00000772 a.u. Imaginary Freq 0	E(RM06) -1937.37834735 a.u.			
Imaginary Freq 0 Dipole Moment 1.3375 Debye Point Group C1 C1 Job cpu time: 0 days 14 hours 34 minutes 44.8 seconds. S2	RMS Gradient Norm 0.00000772 a.u.			
Dipole Moment 1.3375 Debye Point Group C1 C1 Job cpu time: 0 days 14 hours 34 minutes 44.8 seconds.	Imaginary Freq	()	
Point Group C1 Job cpu time: 0 days 14 hours 34 minutes 44.8 seconds.	Dipole Moment	1.3375	Debye	
Job cpu time: 0 days 14 hours 34 minutes 44.8 seconds.	Point Group	C'		

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09	1 18538000	0 07463400	-0 11867700
	2.50120000	0.05100100	1 00045000
н	2.50139900	0.25403500	-1.08845800
Н	-0.36550200	-0.17699700	0.81493200
Р	0.97884800	2.43340300	-0.04479400
- D	1 50757000	-2 26649100	_0 1/172/00
F	1.30/3/900	-2.20040100	-0.141/2400
S	-0.47681200	0.08249900	-2.00425200
0	-2.15516600	0.98315700	0.25339000
0	-2 09025300	-1 32037100	-0 05055200
0	2.09020000	1.02007100	0.00000200
0	2.98618500	0.22861600	2.30407400
В	-1.33704200	-0.12307700	-0.06096800
С	-3.50799800	0.52313800	0.14342500
Ċ	-3 98133400	0 74061700	-1 28920200
	2 01175000	1 70070100	1.55546000
H	-3.811/5200	1./90/8100	-1.55546900
Н	-5.05120000	0.52644200	-1.40035800
Н	-3.42131400	0.12248600	-1.99817700
C	-1 37038600	1 32995300	1 09348900
		1.32995500	1.0053000
н	-3.96294500	1.32946700	2.10853200
H	-5.39377200	0.93407900	1.12332200
Н	-4.42134600	2.36968900	0.75081600
C	-3 36596100	-0 98510600	0 50983300
0	3.30330100	0.90510000	0.00000000
C	-3.28315100	-1.21/65100	2.01434200
H	-2.96857800	-2.25273400	2.19049500
Н	-4.24872000	-1.06647700	2.51165900
н	-2.54221500	-0.55357300	2,47461600
C	-1 12391900	-1 88514600	_0 09509400
	4.42554500	1.0000140000	1 10000500
H	-4.398/5100	-1.82698800	-1.18802500
H	-5.42576800	-1.58945100	0.24259800
H	-4.25352100	-2.92061200	0.22070600
С	2.28977200	0.16642600	1.36480600
Ċ	2 57200000	3 32024300	_0 10926000
	2.57500900	3.32824300	-0.10828000
Н	3.06424800	3.11568500	-1.062/0800
С	-0.02819200	3.28304600	-1.31439500
Н	-0.00550800	4.36725200	-1.15339700
Ċ	0 22922800	3 04271500	1 50928500
	0.77946200	2 61820700	1 60466000
п	-0.77848200	2.01029700	1.36463900
С	3.24941300	-2.79510200	-0.33127500
H	3.84572700	-2.31632500	0.45316500
С	0.63005100	-3.31948300	-1.35757700
н	-0 45068100	-3 19212200	-1 22437300
	1 00140600	3.0000000	1 42007000
C	1.02140600	-3.06080600	1.43607800
H	1.20675800	-4.14162500	1.42387500
Н	1.58521800	-2.60405100	2.25678100
Н	-0.04505300	-2.87067400	1.60143900
ц	0 88761700	-4 37302600	-1 19723000
11	0.00701/00	2.02701000	2.27000200
н	0.90/00600	-3.03/01200	-2.3/890300
H	3.62572600	-2.45017200	-1.29922200
H	3.35427900	-3.88416100	-0.25745800
Н	2,43059500	4.40960800	0.00380500
н	3 21754800	2 95832400	0 69649800
11	0.17(00)00	2.33032400	1 52005400
Н	0.1/683600	4.13802400	1.53095400
H	0.82601700	2.68961400	2.35746600
H	-1.06082100	2.92356000	-1.23780000
Н	0.35196200	3.05049300	-2.31414000
н	-0 56365000	-1 22870300	-2 30851100
	0.0000000		

Zero-point correction=	0.449234 (Hartree/Particle)
Thermal correction to Energy=	0.479432
Thermal correction to Enthalpy=	0.480376
Thermal correction to Gibbs Free Ener	rgy= 0.391336
Sum of electronic and zero-point Energy	gies= -1936.929926
Sum of electronic and thermal Energie	s= -1936.899729
Sum of electronic and thermal Enthalp	ies= -1936.898784
Sum of electronic and thermal Free Er	ergies= -1936.987824

P	rimero		
File Name	m-13-freq		
File Type	.log		
Calculation Type	FREQ		
Calculation Method	RM06		
Basis Set	Gen		
Charge	0		
Spin	Singlet		
E(RM06)	-1937.37916069	a.u.	
RMS Gradient Norm 0.00000961 a.u.			
Imaginary Freq 0			
Dipole Moment	1.4164	Debye	
Point Group C1			
Job cpu time: 0 days 13 hours 44 minutes 22.5 seconds.			

TS2

Os	1.18538000	0.07463400	-0.11867700
н	2 50139900	0 25403500	-1 08845800
11	2.30133300	0.23403300	1.00043000
Н	-0.36550200	-0.1/699/00	0.81493200
P	0.97884800	2.43340300	-0.04479400
P	1.50757900	-2.26648100	-0.14172400
2	0 47601000	0 00240000	2 00425200
5	-0.4/001200	0.08249900	-2.00425200
0	-2.15516600	0.98315700	0.25339000
0	-2.09025300	-1.32037100	-0.05055200
0	2 00610500	0 22961600	2 20407400
-	2.90010300	0.22801000	2.30407400
В	-1.33704200	-0.12307700	-0.06096800
С	-3.50799800	0.52313800	0.14342500
C	-3 98133400	0 74061700	-1 28920200
	2 01175200	1 70070100	1 55520200
H	-3.811/5200	1./90/8100	-1.55546900
H	-5.05120000	0.52644200	-1.40035800
Н	-3.42131400	0.12248600	-1.99817700
C	-4 37038600	1 32995300	1 09348900
0	1.57050000	1.020000	1.05540500
Н	-3.96294500	1.32946700	2.10853200
Н	-5.39377200	0.93407900	1.12332200
н	-4,42134600	2.36968900	0.75081600
C	-3 36596100	-0.09510600	0 50002000
C	-3.30390100	-0.98510800	0.00903300
C	-3.28315100	-1.21765100	2.01434200
Н	-2.96857800	-2.25273400	2.19049500
Н	-4 24872000	-1 06647700	2 51165900
	0.54001500	1.00017700	2.01100500
H	-2.54221500	-0.5535/300	2.4/461600
C	-4.42394900	-1.88514600	-0.09509400
Н	-4.39875100	-1.85698800	-1.18802500
ч	-5 12576800	-1 58945100	0 24259800
11	1.05050100	1.50545100	0.24255000
H	-4.25352100	-2.92061200	0.22070600
С	2.28977200	0.16642600	1.36480600
С	2.57300900	3.32824300	-0.10826000
Ч	3 06424900	2 11569500	-1 06270900
11	5.00424000	5.11500500	1.00270000
C	-0.02819200	3.28304600	-1.31439500
Н	-0.00550800	4.36725200	-1.15339700
C	0 22922800	3 04271500	1 50928500
U U	0.77046200	2 61820700	1 60466000
п	-0.77840200	2.01029700	1.38403900
C	3.24941300	-2.79510200	-0.33127500
Н	3.84572700	-2.31632500	0.45316500
C	0 63005100	-3 31948300	-1 35757700
U U	0.45069100	3 10212200	1 22/27200
H	-0.45068100	-3.19212200	-1.2243/300
C	1.02140600	-3.06080600	1.43607800
Н	1.20675800	-4.14162500	1.42387500
Н	1 58521800	-2 60405100	2 25678100
11	0.0450521000	2.00405100	1 0142000
H	-0.04505300	-2.8/06/400	1.60143900
Н	0.88761700	-4.37302600	-1.19723000
Н	0.90700600	-3.03701200	-2.37890300
ч	3 62572600	-2 45017200	-1 20022200
11	2.02372000	2.45017200	1.29922200
н	3.3542/900	-3.88416100	-0.25/45800
Н	2.43059500	4.40960800	0.00380500
Н	3.21754800	2.95832400	0.69649800
н	0 17683600	4 13802400	1 53005400
	0.17003000		1.00000400
н	0.82601/00	2.68961400	2.35/46600
Н	-1.06082100	2.92356000	-1.23780000
Н	0.35196200	3.05049300	-2.31414000
н	-0.56365000	-1.22870300	-2.30851100

Zero-point correction=	0.445852 (Hartree/Particle)
Thermal correction to Energy=	0.475518
Thermal correction to Enthalpy=	0.476462
Thermal correction to Gibbs Free Ener	gy= 0.388320
Sum of electronic and zero-point Energy	gies= -1936.916164
Sum of electronic and thermal Energie	s= -1936.886498
Sum of electronic and thermal Enthalp	ies= -1936.885553
Sum of electronic and thermal Free Er	ergies= -1936.973696

p	rimero		
File Name	m-ts2-freq-¿		
File Type	.log		
Calculation Type	FREQ		
Calculation Method	RM06		
Basis Set	Gen		
Charge 0			
Spin	Singlet		
E(RM06)	-1937.36201572	a.u.	
RMS Gradient Norm	0.00000873	a.u.	
Imaginary Freq 1			
Dipole Moment	5.4372	Debye	
Point Group C1			
Job cpu time: 0 days 14 hours 29 minutes 5.3 seconds.			

 $\mathbf{C}_{\mathbf{1}}$

05	1 23826800	0 07469200	-0 11137800
	2 42220000	0 24206900	1 22966700
п	2.43339900	0.24300800	-1.32800700
H	-0.14771800	-0.11438500	0.91175300
P	1.00721100	2.41144800	-0.02689400
P	1 49940300	-2 25469900	-0 07687100
1	1.400000	2.23405500	0.07007100
S	-0.42/35200	0.06851800	-2.05541400
0	-2.40527400	1.01697000	-0.28662800
0	-2.47330100	-1.25760600	-0.63529400
0	3 21448300	0 20584000	2 15644000
0	1 00041600	0.20004000	2.13044000
В	-1.82841600	-0.07850000	-0.851/0100
C	-3.63385500	0.55462000	0.32841300
С	-4.75801400	0.94823900	-0.61665800
н	-4.72053800	2.03083100	-0.77612400
ц.	-5 7/1/1300	0 69399500	_0 20492300
11	J. /4141500	0.05555500	0.20452500
н	-4.649//600	0.45942200	-1.5915/000
C	-3.79477700	1.25383700	1.66080100
Н	-2.92027300	1.10342100	2.30057500
н	-4.68464300	0.88511400	2.18628100
11	2 01040700	2 22012000	1 40704500
п ~	-3.91940700	2.33013000	1.49/04500
C	-3.42335200	-0.99584900	0.43190500
C	-2.76808900	-1.44454900	1.72778100
Н	-2.51597300	-2.50785400	1.63554300
н	-3.44748900	-1.32937200	2.58005100
11	1 04001000	0 00000400	1 02424100
п ~	-1.04091000	-0.89328400	1.92434100
C	-4.66885500	-1.81/16/00	0.1/419900
H	-5.08484900	-1.63568200	-0.82051300
Н	-5.43736700	-1.59145200	0.92416300
н	-4.42624900	-2.88223700	0.25145300
C	2 44300700	0 16110400	1 2721/200
	2.44303700	0.10110400	1.27214300
C	2.58300500	3.34060000	0.0/883300
H	3.18431900	3.10921900	-0.80587000
С	0.16259400	3.26694400	-1.41655100
Н	0.19622300	4.35370000	-1.27423600
C	0 07159100	3 06129500	1 /08/2600
	0.07100100	2 (7010500	1 24025500
п	-0.95002500	2.07010500	1.34233300
C	3.17564600	-2.88448700	-0.46818300
Н	3.89000800	-2.41213500	0.21506900
С	0.44472100	-3.31262500	-1.15055800
Н	-0 61384800	-3 09820100	-0 95637500
	1 10020200	3.03020100	1 5000/500
	1.19630300	-3.02095700	1.36234300
H	1.38270800	-4.10207900	1.55030300
Н	1.85027900	-2.54817000	2.30304900
Н	0.15965400	-2.82336700	1.85393600
н	0 64028400	-4 37242100	-0 94848200
ц	0.66636400	-3 12040300	-2 20734000
п	0.00030400	-3.12040300	-2.20734900
н	3.43/91400	-2.58136/00	-1.48651200
H	3.24119500	-3.97518700	-0.37052500
Н	2.41146900	4.42199100	0.14454400
Н	3.13876200	3.00671600	0.96154700
Н	0 05352200	4 15806700	1 42943200
н	0 52670700	2 60005000	2 22072100
11	0.020/9/00	2.00003000	2.320/2100
н	-0.88554600	2.94855800	-1.46184/00
H	0.65279700	3.00681000	-2.36060100
Н	-0.47484300	-1.23296000	-2.41455900

Zero-point correction=	0.446409 (Hartree/Particle)
Thermal correction to Energy=	0.476579
Thermal correction to Enthalpy=	0.477523
Thermal correction to Gibbs Free Ener	gy= 0.388397
Sum of electronic and zero-point Energy	gies= -1936.915919
Sum of electronic and thermal Energie	s= -1936.885749
Sum of electronic and thermal Enthalp	ies= -1936.884805
Sum of electronic and thermal Free Er	ergies= -1936.973931

File Name Im124req File Type Jog Calculation Type FRE0 Calculation Method FRM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937 3623864 RMS Gradient Norm 0.00001010 Rub Gradient Norm 0.00001010 Dipole Moment 5.6456 Debye Point Group Job cpu time: 0 days 14 hours 56 minutes 46.8	pr	imero	G2:M1	.:V1 -	C
File Type Jog Calculation Method R4M6 Calculation Method R4M6 Calculation Method R4M6 Basis Set Gen Charge 0 Spin Singlet E(R4M05) -1937.3622864 a.u Imaginary Freq 0 Dipole Moment 56.85 Debye Point Group C Job cpu time: 0 days 14 hours 56 minutes 46.8	File Name		m-12-freq		1
Calculation Type FRE0 Calculation Method RM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.3622864 a.u. RMS Gradient Norm 0.00001010 a.u. Imaginary Freq 0 0 Dipole Moment 5.6455 Debye Point Group c.t c	File Type		.log		
Calculation Method FMM05 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.36232864 RMS Gradient Norm 0.00001010 Junaginary Freq 0 Dipole Moment 5.6456 Debye Debye Job cpu time: 0 days 14 hours 56 minutes 46.8 another	Calculation Type		FREQ		
Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.08021064 a.u. RMS Gradient Norm 0.00010 a.u. Imaginary Freq 0 0 Dipole Moment 5.6456 Debye Point Group C1	Calculation Method		RM06		
Charge 0 Spin Singlet E(RM06) -1937.38623664 a.u. RMS Gradient Norm 0.00001010 a.u. Imaginary Freq 0 0 Dipole Moment 5.6455 Debye Point Group C.t C	Basis Set		Gen		
Spin Singlet E(RM06) -1937.36232864 a.u. RMS Gradient Norm 0.000010101 a.u. Imaginary Freq 0 0 Dipole Moment 5.6456 Debye Point Group C1	Charge		0		
E(RM06) -1937.36232664 a.u. RMS Gradient Norm 0.00001010 a.u. Imaginary Freq 0 0 Dipole Moment 5.6456 Debye Point Group C1 C1	Spin		Singlet		
RMS Gradient Norm 0.00001010 au Imaginary Freq 0 0 Dipole Moment 5.6455 Debye Point Group C1 1	E(RM06)	-1937	.36232864	a.u.	
Imaginary Freq 0 Dipole Moment 5.6456 Debye Point Group C1 C1	RMS Gradient Norm	(0.00001010	a.u.	
Dipole Moment 5.6456 Debye Point Group C1 Job cpu time: 0 days 14 hours 56 minutes 46.8 accorded	Imaginary Freq		0		
Point Group C1 Job cpu time: 0 days 14 hours 56 minutes 46.8	Dipole Moment		5.6456	Debye	
Job cpu time: 0 days 14 hours 56 minutes 46.8	Point Group		C1		
seconds.					

 $\mathbf{C}_{\mathbf{2}}$

05	-1.24200700	0.08320200	-0.06974400
H	-2 34487100	0 22964500	-1 37731800
Н	0 07953000	-0 12369200	1 02972700
P	-1 69957500	-2 22328300	0.00640500
I D	0.01220000	2.22320300	0.15210700
P	-0.91326900	2.40209000	-0.15510700
5	0.43682800	-0.46610600	-1.92648300
0	2.40166400	-1.40552400	-0.16266900
0	2.70491000	0.78494500	-0.78177300
0	-3.26728400	0.66816400	2.07768500
В	1.94189900	-0.33944300	-0.85786900
С	3.66635800	-1.00294300	0.41697200
С	4.75038900	-1.61561600	-0.45459800
Н	4.59370300	-2.69820500	-0.49975900
Н	5.75055300	-1.42913600	-0.04734100
н	4.70961700	-1.22615900	-1.47817300
С	3,73650900	-1.55983000	1.82255100
H	2.85222600	-1.28313700	2.40431700
H	4 63409600	-1 19920900	2 34047800
н	3 78566500	-2 65312700	1 77986000
C C	3 61003300	2.03312700	1.77500000
C	2 06621000	1 21/16000	1 54590200
	2.96631000	1.21410000	1.22002100
н	2.85264300	2.28529600	1.33802100
H	3.58693200	1.10661900	2.44235300
Н	1.96918700	0.79633500	1.73855100
C	4.93407000	1.22384700	0.02153000
Н	5.35320900	0.87575200	-0.92622800
Н	5.65913100	1.02556200	0.82081200
Н	4.79389300	2.30783400	-0.04550900
С	-2.48026400	0.42190000	1.24181300
С	-2.87550300	-2.74699900	1.30958200
Н	-3.81819300	-2.20386900	1.18890900
С	-2.45575700	-2.95837200	-1.49623300
Н	-2.61935600	-4.03771400	-1.38621400
С	-0.29742500	-3.37080600	0.30716000
H	0.45513500	-3.26242700	-0.48145000
C	-2 41979100	3 35940400	-0 57942600
Н	-3 21100600	3 09853400	0 13212700
C	0 31147600	3 12914000	-1 31688600
e H	1 30763200	2 70672600	-1 13777800
11 C	1.30703200	2.1072000	1 42166000
U U	-0.44013300	3.19/30200	1 22021100
п	-0.37642600	4.20000000	1.33931100
H	-1.1935/300	2.94065800	2.18450800
H	0.52035700	2.79495900	1./6/6/500
Н	0.34906200	4.21836200	-1.19651400
Н	0.01065000	2.91131500	-2.34938600
Н	-2.75570100	3.06093000	-1.57720400
Н	-2.24209600	4.44174300	-0.54866200
Н	-3.06375600	-3.82591100	1.25794800
Н	-2.46121300	-2.49504600	2.29122800
Н	-0.63631000	-4.41363800	0.34486700
Н	0.17924400	-3.09494000	1.25379000
Н	-1.80093100	-2.77482600	-2.35505400
Н	-3.40765600	-2.45319700	-1.68697600
Н	0.61798400	0.73148800	-2.52567700

Zero-point correction=	0.446896 (Hartree/Particle)
Thermal correction to Energy=	0.477015
Thermal correction to Enthalpy=	0.477960
Thermal correction to Gibbs Free Ener	rgy= 0.388735
Sum of electronic and zero-point Energy	gies= -1936.914153
Sum of electronic and thermal Energie	-1936.884034
Sum of electronic and thermal Enthalp	ies= -1936.883089
Sum of electronic and thermal Free Er	nergies= -1936.972314

primero G2:M1:V1 - G				
File Name	m-t	st-a-req		
File Type		.log		
Calculation Type		FREQ		
Calculation Method		RM06		
Basis Set		Gen		
Charge		0		
Spin		Singlet		
E(RM06)	-1937.3	36104896	a.u.	
RMS Gradient Norm	0.1	00002634	a.u.	
Imaginary Freq		0		
Dipole Moment		5.7829	Debye	
Point Group		C1		
Job cpu time: 0 days 16 hours 56 minutes 43.0 seconds.				

TS3

_			
Os	-1.30834100	0.11841000	-0.10684300
H	-2.33106800	0.17346500	-1.49520700
Н	-0.22474900	-0.15970200	1.19305200
P	-1.83705300	-2.17010100	0.14230900
P	-0.65863000	2.39654600	-0.19525700
9	0 48658600	-0 75029100	-1 88625100
5	0.40000000	1 40020200	0 61764600
0	2.73841200	-1.48938300	-0.51/54500
0	2.34966400	0./4932300	-0.23900100
0	-3.61012200	1.01793700	1.61416100
В	1.91593600	-0.42931100	-0.78213100
С	3.93160000	-0.94132200	0.08813500
С	4.93730200	-0.73046100	-1.03330400
Н	5.08119500	-1.68017500	-1.55870700
Н	5 90890300	-0 39907500	-0 64912500
11	4 67772700	0.00760000	1 75014200
п С	4.57772700	1 02020000	-1.75914200
	4.46608400	-1.93939900	1.09222700
Н	3.69936300	-2.23554700	1.81308200
Н	5.32213000	-1.52145900	1.63672400
Н	4.80516600	-2.83927500	0.56817100
С	3.40131000	0.39047200	0.69679200
С	2.75883900	0.19175100	2.06058400
Н	2.24620200	1.11002600	2.36583300
Н	3 51353000	-0 04616400	2 81892600
н	2 00539600	-0 60307700	2 02700200
C C	1 100030000	1 51005500	2.03700200
	4.40000000	1.77664000	0.74525500
н	4.///89300	1.77654900	-0.25321800
н	5.263/1100	1.2442/100	1.3/430300
Н	3.94551500	2.41158100	1.17676600
C	-2.71015200	0.66284100	0.95592100
C	-3.08800800	-2.52635100	1.43020500
Н	-4.01878200	-2.00349000	1.18764300
С	-2.50986000	-3.04833100	-1.31646600
Н	-2.71494000	-4.10261400	-1.09356900
С	-0.44661000	-3.25099400	0.64558700
Н	0.35615900	-3.18072100	-0.09598900
C	-2.08124600	3.54216500	-0.35781500
U U U U U U U U U U U U U U U U U U U	-2 76334200	3 40594900	0 48756500
C	0 /1282000	2 97369300	-1 56871600
Ч	1 20016400	2.97309300	_1 52219400
	1.30010400	2.40404500	1.02210400
	0.21030900	3.07730000	1.20333400
н	0.32594600	4.16572600	1.19440300
Н	-0.35368300	2.82082300	2.16815900
Н	1.19576900	2.60392100	1.32193800
Н	0.56688300	4.05642900	-1.48904200
Н	-0.06720800	2.75009600	-2.52770000
Н	-2.62573400	3.29509500	-1.27486200
Н	-1.75006100	4.58707000	-0.39225900
Н	-3.28247100	-3.60205100	1.51126900
Н	-2.72543200	-2.14648200	2.39131500
н	-0.76802300	-4.29560900	0.73835900
н	-0.05929500	-2.89451000	1.60578000
н	-1 78658300	-2 98322300	-2 13594900
и П	-3 43058300	-2 54838700	_1 63285500
11	0 52650100	2.34030700	1 77000000
п	-0.33020100	0.38509/00	-1.11898000

Zero-point correction=	0.442591 (Hartree/Particle)
Thermal correction to Energy=	0.472946
Thermal correction to Enthalpy=	0.473890
Thermal correction to Gibbs Free Ener	gy= 0.382202
Sum of electronic and zero-point Energy	gies= -1936.900631
Sum of electronic and thermal Energie	s= -1936.870276
Sum of electronic and thermal Enthalp	ies= -1936.869331
Sum of electronic and thermal Free Er	nergies= -1936.961019

File Name File Type Calculation Type Calculation Method Basis Set Charge Spin Fin Fin Charge	m-ts1-freq .log FREQ RM06 Gen 0						
File Type Calculation Type Calculation Method Basis Set Charge Spin Erch460	log. FREQ RM06 Gen 0						
Calculation Type Calculation Method Basis Set Charge Spin Environ	FREQ RM06 Gen 0						
Calculation Method Basis Set Charge Spin	RM06 Gen 0						
Basis Set Charge Spin	Gen 0						
Charge Spin	0	Charge 0					
Spin	Spin Singlet						
E(RM06) -1937.34322158 a.u.							
E(RMUb)	-1937.34322158	a.u.					
RMS Gradient Norm	0.00000218	a.u.					
Imaginary Freq	1						
Dipole Moment	4.3461	Debye					
Point Group	C1						
Job cpu time: 0 days 14 hours 51 minutes 27.3 seconds.							

2ta

Os	-1.42681400	0.05466800	-0.15191000
н	-2.53285100	-0.32211200	-1.56619400
ц	_0 33207900	-0.00690400	1 06561000
п	-0.33297800	-0.00080400	1.00001000
P	-1.419/2600	-2.31576000	0.0921/600
P	-0.92761600	2.38089500	-0.16970400
S	0.43562300	-0.41679500	-1.80940300
0	2.91545300	-1.18205800	-0.77180000
0	2.21641100	0.84376900	0.02120900
0	-3 63207200	0 49303300	1 87703300
в	1 91037300	-0 23569200	-0 79525800
0	1.02404000	0.2000200	0.75525000
C	4.03424300	-0.6091/200	-0.0/435600
C	4.95112900	0.00046100	-1.12546300
H	5.20743800	-0.77346100	-1.85638100
Н	5.88013000	0.38375800	-0.68689000
Н	4.45235700	0.81649100	-1.66045400
С	4.75702600	-1.70988000	0.67374400
н	4.07458500	-2.28011100	1.31143900
н	5 56215500	-1 29819300	1 29573600
11	5.50215500	2 405 64000	1.23373000
H A	5.20581400	-2.40564000	-0.04347400
C	3.34603800	0.45806600	0.82523700
С	2.79841300	-0.12408100	2.12154500
Н	2.12712200	0.60729900	2.58562800
Н	3.59981100	-0.35910300	2.83198000
Н	2.21749600	-1.03505600	1.93454500
С	4.18476800	1.68380600	1.12168400
ц Ц	1 11898700	2 22503700	0 20802200
11	F 10025000	1 40510600	1 64504400
п	5.10855800	1.40519600	1.04304400
Н	3.62/41400	2.36829200	1.//185800
С	-2.79211300	0.32036000	1.08160300
С	-2.70923700	-3.00810500	1.19455500
Н	-3.70001900	-2.75368600	0.80357000
С	-1.61498400	-3.31072300	-1.42911800
Н	-1.51418800	-4.38127800	-1.21498900
C	0 11350000	-2 99681700	0 82167300
U U	0 97282300	-2 71640900	0 20077700
	2 40117600	2./1040500	0.20077700
	-2.40117600	3.4/291/00	-0.20259600
н	-3.04/6/600	3.24003800	0.65032000
С	0.08670400	3.04370400	-1.53475700
H	1.07138600	2.56964800	-1.49916300
C	-0.03782100	2.97073900	1.31211300
Н	0.08763300	4.05977400	1.29042900
Н	-0.59378700	2.67894600	2.20908500
н	0.94078500	2,48006100	1.32014200
н	0 18611600	4 13165100	-1 43780500
и и	-0.37624800	2 70250000	-2 40412000
п	-0.37024800	2.79239000	-2.49413900
H	-2.96849800	3.28983000	-1.12156200
н	-2.11489300	4.53079700	-0.16057200
H	-2.61925400	-4.09780900	1.27539200
Н	-2.61190000	-2.56145900	2.18975300
Н	0.05332500	-4.08948000	0.89398200
Н	0.24308700	-2.57197700	1.82309500
Н	-0.84364300	-2,99862400	-2.14094100
н	-2 60106500	-3 11859300	-1 86569200
11	2.00100000	0 5000000	1 650000000
п	-2.38096400	0.52020400	-I.00092200

Zero-point correction=	0.448617 (Hartree/Particle)
Thermal correction to Energy=	0.478897
Thermal correction to Enthalpy=	0.479841
Thermal correction to Gibbs Free Ener	rgy= 0.390152
Sum of electronic and zero-point Energy	gies= -1936.944713
Sum of electronic and thermal Energie	es= -1936.914432
Sum of electronic and thermal Enthalp	ies= -1936.913488
Sum of electronic and thermal Free Er	nergies= -1937.003177

File Name Interfere File Type Jog Calculation Type FREO Calculation Method FMM6 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.3933219 AMS Gradient Norm 0.00000687 Dipole Moment 1.8279 Debye Debye Point Group C1	pri	mero	G2:M1	L:V1 - 0
File Type Jog Calculation Type FRE0 Calculation Method RM66 Basis Sot Gen Charge 0 Spin Singlet E(RM6b) -1937.3332919 RMS Gradient Norm 0.0000687 Maginary Freq 0 Dipole Moment 18279 Point Group C1	File Name		m-11-freq	
Calculation Type FRE0 Calculation Method RM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937 39332019 a.u. Imaginary Freq 0 0 Dipole Moment 18279 Debye Jobb cpu time: 0 43 3 hours 50 minutes 37.8	File Type		.log	
Calculation Method FM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.333219 RMS Gradient Norm 0.00000687 Jungianary Freq 0 Dipole Moment 1.8279 Point Group C1	Calculation Type		FREQ	
Basis Sot Gen Charge 0 Spin Singlet E(RM06) 1937.3832819 a.u RMS Gradient Norm 0.0000067 a.u Imaginary Freq 0 0 Dipole Moment 18279 Debe Point Group C1 37.8	Calculation Method		RM06	
Charge 0 Spin Singlet E(RM06) -1937.3933291 a.u RMS Gradient Norm 0.00000687 a.u Imaginary Freq 0 0 Dipole Moment 1.8279 Debye Point Group C1	Basis Set		Gen	
Spin Singlet E(RM06) -1937.3933219 a.u. RMS Gradient Norm 0.00000687 a.u. Imaginary Freq 0 Dipole Moment 1.8279 Debie Debie Debie Debie Point Group C1 C1 C1	Charge		0	
E(RM06) -1937.3832819 a.u. RMS Gradient Norm 0.0000687 a.u. Imaginary Freq 0 0 Dipole Moment 18279 Debye Point Group C1 C1	Spin		Singlet	
RMS Gradient Norm 0.00000687 a.u. Imaginary Freq 0 0 0 Dipole Moment 1.8279 Debye 0 Point Group C1 1 0 0 Job cpu time: 0 days 13 hours 50 minutes 37.8 0 0 0	E(RM06)	-1937	39332919	a.u.
Imaginary Freq 0 Dipole Moment 1.8279 Debye Point Group C1 C1 Job cpu time: 0 days 13 hours 50 minutes 37.8	RMS Gradient Norm	0	.00000687	a.u.
Dipole Moment 1.8279 Debye Point Group C1 Job cpu time: 0 days 13 hours 50 minutes 37.8	Imaginary Freq		0	
Point Group C1 Job cpu time: 0 days 13 hours 50 minutes 37.8	Dipole Moment		1.8279	Debye
Job cpu time: 0 days 13 hours 50 minutes 37.8	Point Group		C1	
seconds.				

2t

0.5	-1 31789200	0 19461500	-0 06983100
н	-0 44481700	-0.55000700	-1 50437300
н Н	-2 16564000	0.48383300	1 30883300
n D	-2.26241300	-1 02015600	1.30883300
r D	-2.30241300	-1.93913000	0.01740000
P	-0.37892900	2.33004400	0.3//35100
S	0.38585000	-0.94//5200	1.423/0300
0	3.08/35900	-1.46345800	0.92133400
0	2.2381/300	0.20/04500	-0.39432800
0	-3.53652900	1.42984200	-1./2194100
В	1.963//400	-0.72849100	0.60160800
С	4.07469200	-1.18981200	-0.08281700
C	3.91231200	-2.242/6500	-1.1/153900
H	3.98691200	-3.23366900	-0.71173400
H	4.68811300	-2.15943900	-1.94189000
Н	2.92950300	-2.16576100	-1.65195800
С	5.45405100	-1.29121100	0.53450700
Н	5.54063400	-0.67709400	1.43489000
Н	6.22523700	-0.98134900	-0.18254000
Н	5.65401100	-2.33008300	0.81825200
С	3.67001000	0.23391200	-0.55826100
С	4.20668100	1.33177500	0.35068400
Н	3.72519500	2.28181100	0.08959800
Н	5.29010200	1.45774900	0.24121400
Н	3.98493100	1.11590000	1.40280400
С	3.99835400	0.54668900	-2.00341500
Н	3.49136200	-0.13582600	-2.69115900
Н	5.07994500	0.48121700	-2.17815000
Н	3.68348400	1.56828800	-2.24643700
С	-2.67301300	0.95464600	-1.09258200
С	-3.97007800	-2.08659200	-0.84749600
Н	-3.83622200	-1.87576800	-1.91362000
С	-1.41439400	-3.35236600	-0.65452600
Н	-1.94032300	-4.30022900	-0.48902300
С	-2.77636200	-2.49572800	1.70762100
Н	-1.86189300	-2.51076800	2.30891200
С	-1.64354400	3.62061200	0.67845700
Н	-2.26071400	3.31861000	1.53064600
С	0.63895700	3.08509500	-0.94509900
Н	1.46490000	2.39923300	-1.16438200
С	0.68283200	2.48753800	1.85348800
Н	1.00248700	3.52884600	1.98144800
Н	0.12374300	2.15368300	2.73298600
Н	1.55401800	1.83561900	1.74500300
Н	1.03023300	4.06461500	-0.64383400
Н	0.02516400	3.20027400	-1.84515100
Н	-2.29386000	3.71330100	-0.19761900
Н	-1.17816700	4.59134100	0.88753000
Н	-4.39200000	-3.09128800	-0.72594400
Н	-4.66880800	-1.34846200	-0.43984600
Н	-3.22724900	-3.49501200	1.69048200
Н	-3.47552600	-1.78151600	2.15343200
Н	-0.43904400	-3.37680200	-0.15678600
Н	-1.26012700	-3.20623700	-1.72921200
Н	-0.02311600	0.17919900	-1.36976300

Zero-point correction=	0.447696 (Hartree/Particle)
Thermal correction to Energy=	0.478305
Thermal correction to Enthalpy=	0.479249
Thermal correction to Gibbs Free Ener	gy= 0.387841
Sum of electronic and zero-point Energy	gies= -1936.944982
Sum of electronic and thermal Energie	s= -1936.914373
Sum of electronic and thermal Enthalp	ies= -1936.913429
Sum of electronic and thermal Free Er	ergies= -1937.004838

File Name m-10-freq File Type .log Calculation Type FREC Calculation Method RM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.39267833 a.u. RMS Gradient Norm 0.00000351 a.u. Imaginary Freq 0 Dipole Moment 2.3863 Point Group C1 Job cpu time: 0 days 14 hours 10 minutus 15.6	p	rimero 🤆	52:	M1:V1
File Type log Calculation Type FRE0 Calculation Method RM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.33267833 RMS Gradient Norm 0.0000031 Imaginary Freq 0 Dipole Moment 2.3663 Job cpu time: 0	File Name	m-10-fr	ed	
Calculation Type FFEC0 Calculation Method FRM00 Charge Genometric Charge Genometric Spin Singlet F(RM06) -1937.39267633 RMS Gradient Norm 0.00000351 Imaginary Freq 0.0 Dipole Moment 2.3863 Point Group C1 Jb cpu time: 0.444 hours 10 minutus	File Type		log	
Calculation Method RM06 Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.39267833 RMS Gradient Norm 0.00000361 Imaginary Freq 0 Dipole Moment 2.3863 Point Group C1 Job cpu time: 0 days 14 hours 10 misutus ts.6	Calculation Type	FRI	EQ	
Basis Set Gen Charge 0 Spin Singlet E(RM06) -1937.38267833 a.u. RMS Gradient Norm 0.0000031 a.u. Imaginary Freq 0 0 Dipole Moment 2.3663 Debye Point Group C1	Calculation Method	RM	106	
Charge 0 Spin Singlet E(RM06) -1937.39267833 a.u. RMS Gradient Norm 0.00000351 a.u. Imaginary Freq 0 0 Dipole Moment 2.3863 Debye Point Group C1	Basis Set	G	ien	
Spin Singlet E(RM06) -1937.39267833 a.u. RMS Gradient Norm 0.00000351 a.u. Imaginary Freq 0 0 Dipole Moment 2.3863 Debye Point Group C1 Job cpu time: 0 days 14 hours 10 minutes 16.6	Charge		0	
E(RM06) -1937.39267833 a.u. RMS Gradient Norm 0.0000031 a.u. Imaginary Freq 0 0 Dipole Moment 2.3663 Debye Point Group C1 0 Job cpu time: 0 days 14 hours 10 minutes 16.6 seconds.	Spin	Sing	glet	
RMS Gradient Norm 0.00000351 a.u. Imaginary Freq 0 0 Dipole Moment 2.3863 Debye Point Group C1 0 Job cpu time: 0 days 14 hours 10 minutus 16.6 seconds. 0	E(RM06)	-1937.392678	333	a.u.
Imaginary Freq 0 Dipole Moment 2.3863 Debye Point Group C1 C1 Job cpu time: 0 days 14 hours 10 minutes 16.6 seconds. C1	RMS Gradient Norm	0.000003	351	a.u.
Dipole Moment 2.3863 Debye Point Group C1 C1 Job cpu time: 0 days 14 hours 10 minutes 16.6 seconds.	Imaginary Freq		0	
Point Group C1 Job cpu time: 0 days 14 hours 10 minutes 16.6 seconds.	Dipole Moment	2.38	363	Debye
Job cpu time: 0 days 14 hours 10 minutes 16.6 seconds.	Point Group		C1	
	Job cpu time: 0 days se	: 14 hours 10 mi conds.	inut	tes 16.6

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