Supplementary Information

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

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Contents:

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 9-borabicyclo[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 $OsDCl(CO)(P^iPr_3)_2$[1] and $OsH(CO)(SH)(P^iPr_3)_2$ (**1**)[2] were prepared according to published methods. $OsD(CO)(SH)(P^iPr_3)_2$ (**1-*d***) was prepared by addition of $NaSH{\cdot}xH_2O$ (200 mg, 3.6 mmol) to a THF/CH_3OH (15 mL in a 4:1 ratio) suspension of $OsDCl(CO)(P^iPr_3)_2$ (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 × 3 mL) caused the precipitation of an orange solid which was separated by decantation, dried in vacuo, and characterized by ^1H, ^2H, and $^{31}P\{^1H\}$ NMR spectroscopy as a 0.7:0.3 mixture of **1-*d*** and **1.** Spectroscopic data for **1-*d***: ^2H NMR (46.07 MHz, C_6H_6, 298 K) δ −23.1 (Os−D); $^{31}P\{^1H\}$ NMR (121.49 MHz, C_6D_6, 298 K) δ 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, $^{13}C\{^1H\}$), external H_3PO_4 ($^{31}P\{^1H\}$), or $BF_3{\cdot}OEt_2$ (^{11}B). Coupling constants, J, and N ($N = J_{H\text{-}P} + J_{H\text{-}P'}$ or $J_{C\text{-}P} + J_{C\text{-}P'}$) are given in hertz. Infrared spectra were recorded on a Perkin-Elmer 1730 spectrometer as CH_2Cl_2 solutions. C, H, and S analyses were carried out in a Perkin-Elmer 2400 CHNS/O analyzer.

Preparation of $OsH(\eta^2\text{-}H_2)(CO)(SBpin)(P^iPr_3)_2$ (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 $C_{25}H_{57}BO_3OsP_2S$: C, 42.85; H, 8.20; S, 4.58. Found: C, 43.01; H, 8.51; S, 4.74. IR (CH_2Cl_2, cm^{-1}): ν(CO) 1911 (s). ^1H NMR (300 MHz, C_6D_6, 298 K): δ 2.6 (m, 6H, PC*H*CH_3), 1.26 (dvt, N = 13.5, J_{H-H} = 7.2, 18H, PCHC*H*$_3$), 1.22 (dvt, N = 13.7, J_{H-H} = 7.1,

18H, PCHCH_3), 1.16 (s, 12H, Bpin), −3.08 (br, 2H, OsH_2), −7.19 (t, 1H, J_{H-P} = 20.2, OsH). T_1 (OsH_2, C_7D_8, 300 MHz, 193 K): 8 ± 1 ms. $^{31}P\{^1H\}$ NMR (121.49 MHz, C_6D_6, 298 K): δ 30.2 (s). ^{11}B NMR (96.29 MHz, C_6D_6, 298 K): δ 35 (br).

Determination of the J_{H-D} Value for OsH(η^2-HD)(CO)(SBpin)(P^iPr_3)$_2$ (2-*d*). Pinacolborane (3.8 μL, 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 C_6D_6. After 5 min, the $^1H\{^{31}P\}$ and ^{31}P NMR spectra showed the presence of a 0.30:0.46:0.23 mixture of **3**, **3-*d*** and OsD(η^2-H_2)(CO)(SBpin)(P^iPr_3)$_2$. Selected data for **2-*d*** are as follows. ^1H NMR (300 MHz, C_6D_6, 298 K): δ −3.09 (t (1:1:1), J_{H-D} = 27). d_{H-H}(calcd) = 0.97 Å.[3]

Reaction of 1 with Catecholborane: Formation of OsH(η^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 (CH_2Cl_2, cm^{-1}): ν(CO) 1919 (s). ^1H NMR (300 MHz, C_6D_6, 298 K): δ 7.07 (m, 2H, Bcat), 6.78 (m, 2H, Bcat), 2.5 (m, 6H, PC*H*CH_3), 1.17 (dvt, *N* = 13.0, J_{H-H} = 6.6, 18H, PCHCH_3), 1.13 (dvt, *N* = 13.0, J_{H-H} = 6.6, 18H, PCHCH_3), –2.75 (br, 2H, OsH_2), −7.04 (t, 1H, J_{H-P} = 19.4, OsH). T_1 (OsH_2, C_7D_8, 300 MHz, 183 K): 43 ± 1 ms. $^{31}P\{^1H\}$ NMR (121.49 MHz, C_6D_6, 298 K): δ 30.5 (s). ^{11}B NMR (96.29 MHz, C_6D_6, 298 K): δ 36 (br).

Determination of the J_{H-D} Value for OsH(η^2-H-D)(CO)(SBcat)(P^iPr_3)$_2$ (3-*d*). Catecholborane (2.8 μL, 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 C_6D_6. After 5 min, the $^1H\{^{31}P\}$ and ^{31}P NMR spectra showed the presence of a mixture of **3**, **3-*d***, OsD(η^2-H_2)(CO)(SBcat)(P^iPr_3)$_2$ and **6**. Selected data for **3-*d*** are as follows. ^1H NMR (300 MHz, C_6D_6, 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-H_2)(CO)(SBbn)(P^iPr_3)$_2$ (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

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 (CH_2Cl_2, cm^{-1}): ν(CO) 1915 (s). ^1H NMR (300 MHz, C_6D_6, 298 K): δ 2.48 (m, 6H, PC*H*CH_3), 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, PCHC*H*$_3$), 1.18 (dvt, N = 13.7, J_{H-H} = 6.8, 18H, PCHC*H*$_3$), −3.67 (br, 2H, OsH_2), −6.35 (t, 1H, J_{H-P} = 20.4, OsH). $T_{1(min)}$ (OsH_2, C_7D_8, 300 MHz, 203 K): 13 ± 1 ms. $^{31}P\{^1H\}$ NMR (121.49 MHz, C_6D_6, 298 K): δ 31.4 (s). ^{11}B NMR (96.29 MHz, C_6D_6, 298 K): δ 76 (br).

Determination of the J_{H-D} Value for OsH(η^2-H-D)(CO)(SBbn)(P^iPr_3)$_2$ (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 C_6D_6. After 5 min, the $^1H\{^{31}P\}$ and ^{31}P NMR spectra showed the presence of a 0.30:0.46:0.23 mixture of **4**, **4-*d*** and OsD(η^2-H_2)(CO)(SBbn)(P^iPr_3)$_2$. Selected data for **4-*d*** are as follows. ^1H NMR (300 MHz, C_6D_6, 298 K): δ −3.69 (t (1:1:1), J_{H-D} = 26). d_{H-H}(calcd) = 0.99 Å.[3]

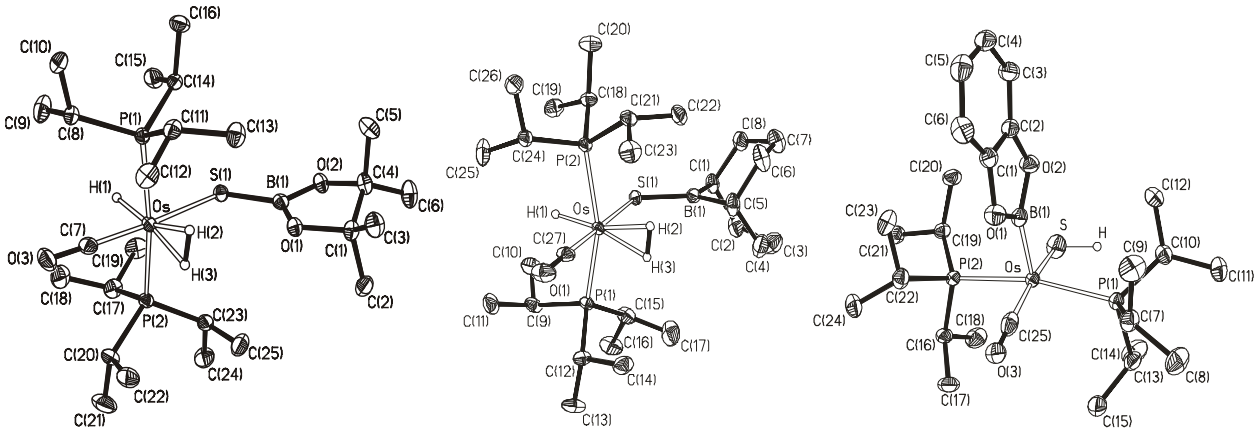
Reaction of 1 with excess of Pinacolborane: Formation of OsH_2(η^2-H–Bpin)(CO)(P^iPr_3)$_2$ (5). Pinacolborane (30.2 μL, 0.208 mmol) was added to an NMR tube containing a solution of **1** (15 mg, 0.026 mmol) in 0.5 mL of toluene-d_8. The solution changed from orange to pale yellow. After 17 h the NMR spectra showed the quantitative formation of **5**. $^1H\{^{11}B\}$ NMR (400 MHz, C_7D_8, 298 K): δ 2.30 (m, 6H, PC*H*CH_3), 1.23 (dvt, N = 14, J_{H-H} = 7.2, 18H, PCHC*H*$_3$), 1.21 (dvt, N = 14.2, J_{H-H} = 7.0, 18H, PCHC*H*$_3$), 1.1 (s, 12H, Bpin), −9.8 (br, 1H, BH), −10.5 (br, 2H, OsH). $^1H\{^{11}B\}$ NMR (400 MHz, C_7D_8, 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). $^{31}P\{^1H\}$ NMR (162 MHz, C_7D_8, 298 K): δ 38.0 (s). ^{11}B NMR (128 MHz, C_7D_8, 298 K): δ 34 (br).

Preparation of Os(Bcat)(CO)(SH)(P^iPr_3)$_2$ (6). *Method A.* 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 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 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 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 $C_{25}H_{47}BO_3OsP_2S$: C, 43.47; H, 6.86; S, 4.64. Found: C, 43.73; H, 7.32; S,

4.63. IR (CH_2Cl_2, cm^{-1}): ν(CO) 1900 (s). ^1H NMR (300 MHz, C_6D_6, 298 K): δ 7.18 (m, 2H, Bcat), 6.8 (m, 2H, Bcat), 2.91 (t, 1H, J_{H-P} = 19.5, SH), 2.61 (m, 6H, PC*H*CH_3), 1.24 (dvt, *N* = 13.9, J_{H-H} = 7.1, 18H, PCHC*H*$_3$), 1.04 (dvt, *N* = 13.1, J_{H-H} = 7.1, 18H, PCHC*H*$_3$). $^{31}P\{^1H\}$ NMR (121.49 MHz, C_6D_6, 298 K): δ 34.5 (s). ^{11}B NMR (96.29 MHz, C_6D_6, 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, λ = 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.



2 **4** **6**

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

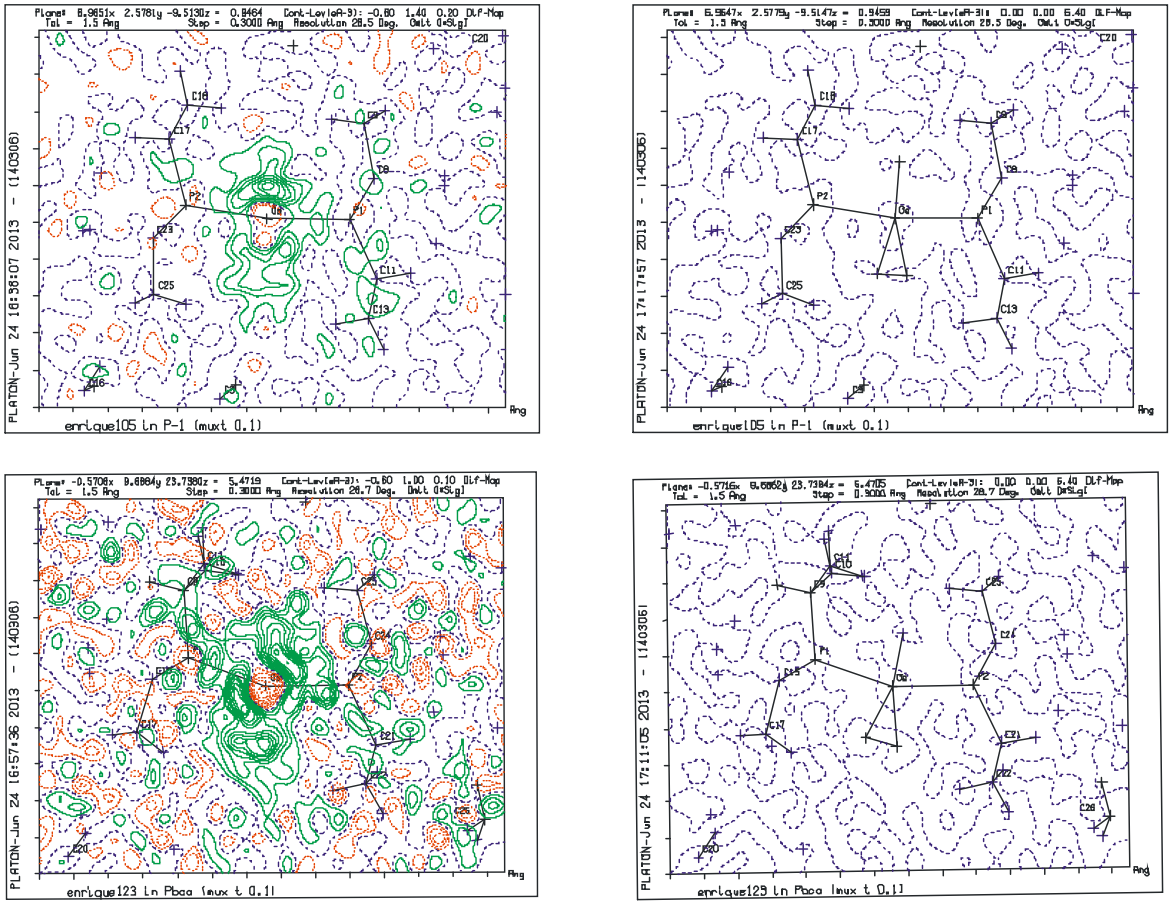


Fig S2 Difference Fourier maps for **2** (top) and **4** (bottom) in the P-Os-P plane without hydrides (left) and with hydrides (right).

Crystal data for **2** (CCDC 936598): $C_{25}H_{57}BO_3OsP_2S$, M_W 700.72, red, irregular block (0.16 x 0.12 x 0.08), triclinic, space group P$\bar{1}$, *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) Å^3, *Z* = 2, D_{calc}: 1.481 g cm^{-3}, F(000): 716, T = 100(2) K, μ: 4.248 mm^{-1}. 19347 measured reflections (2θ: 3-58°, ω scans 0.3°), 7308 unique (R_{int} = 0.0271); min./max. transm. Factors 0.673/0.862. Final agreement factors were R^1 = 0.0239 (6790 observed reflections, I > 2σ(I)) and wR^2 = 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/ Å^3.

Crystal data for **4** (CCDC 936599): $C_{27}H_{59}BOOsP_2S$, 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) Å^3, *Z* = 8, D_{calc}: 1.456 g cm^{-3}, F(000): 2848, T = 100(2) K, μ 4.208 mm^{-1}). 74109 measured reflections (2θ: 3-58°, ω scans 0.3°), 7829 unique (R_{int} = 0.0365); min./max. transm. Factors 0.668/0.862. Final agreement factors were R^1 = 0.0219 (6448 observed reflections, I > 2σ(I)) and wR^2 = 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/ Å^3.

Crystal data for **6** (CCDC 93660): $C_{25}H_{47}BO_3OsP_2S$, M_W 690.64, orange, irregular block (0.22 x 0.15 x 0.05), monoclinic, space group $P2_1/n$, *a*: 16.2977(7) Å, *b*: 10.9590(5) Å, *c*: 16.8715(7) Å, β: 106.1190(10)°, *V* = 2894.9(2) Å^3, *Z* = 4, D_{calc}: 1.585 g cm^{-3}, F(000): 1392, T = 100(2) K, μ: 4.611 mm^{-1}. 34451 measured reflections (2θ: 3-58°, ω scans 0.3°), 7005 unique (R_{int} = 0.0322); min./max. transm. Factors 0.673/0.862. Final agreement factors were R^1 = 0.0237 (6132 observed reflections, I > 2σ(I)) and wR^2 = 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/ Å^3.

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 levels[8] with the Gaussian 09 program[9] 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 $\mathbf{B_1}$, $\mathbf{B_2}$ and $\mathbf{C_1}$, $\mathbf{C_2}$ 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.

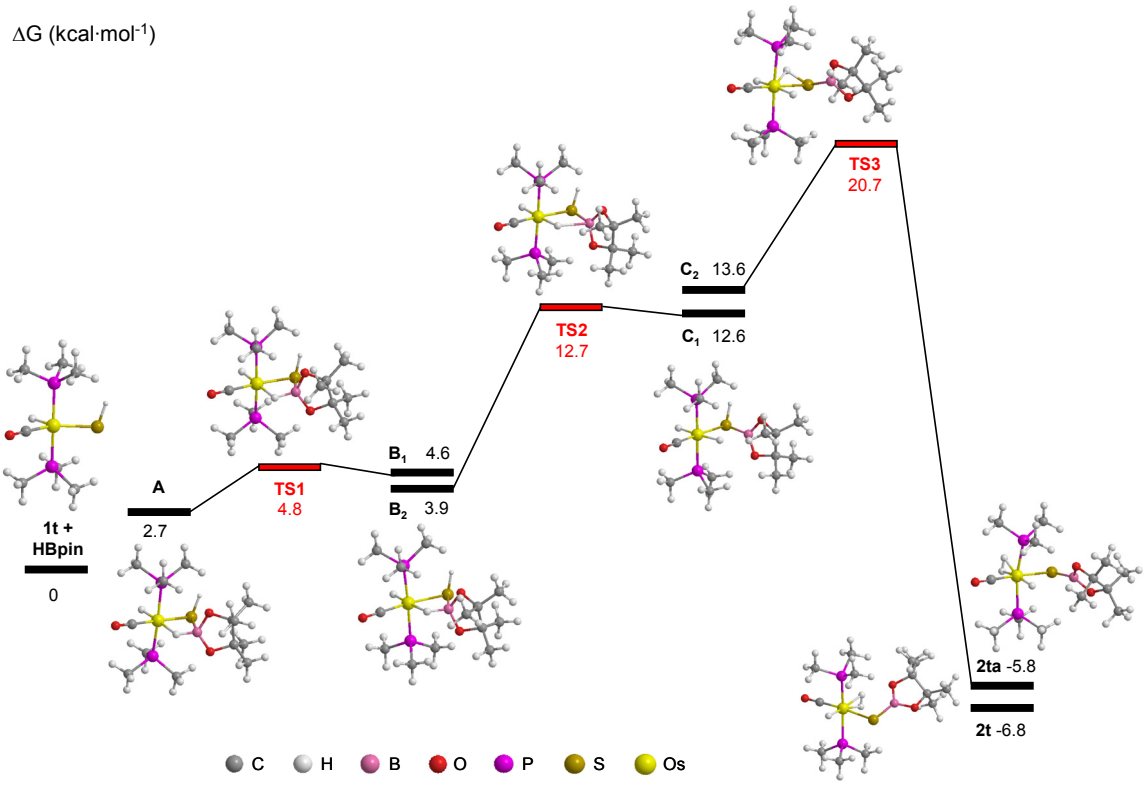
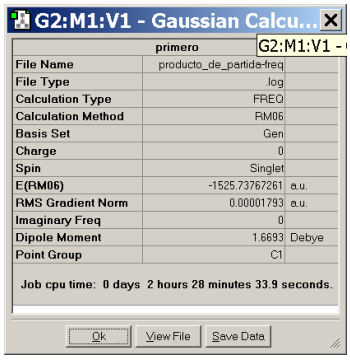


Fig. S3 Energy profile (ΔG, kcal•mol^{-1}) for the formation of OsH(SBpin)(η^2-H_2)(CO)(PMe_3)$_2$ (**2t**) from OsH(SH)(CO)(PMe_3)$_2$ (**1t**) and HBpin. Drawings of **B_1**and **C_2**are omitted for clarity.

1t

Os	-0.00500000	0.06206500	-0.00419000
H	-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
O	-0.02691900	2.97125000	-0.82184900
C	-0.01944400	1.85997100	-0.44930100
C	3.16813900	1.63227300	0.38575800
H	2.76457700	2.10999200	1.28465700
C	2.94871700	-0.94904800	1.59744100
H	4.04361300	-0.93774200	1.65778400
C	3.29452200	-0.72947400	-1.22469000
H	2.93751500	-1.75175300	-1.39088800
C	-3.17527600	1.57306400	0.53804900
H	-2.95838300	2.29856100	-0.25275200
C	-2.96436600	-1.09709100	1.50052100
H	-2.60955800	-2.12105900	1.34620700
C	-3.30275700	-0.59643800	-1.29813800
H	-4.37668100	-0.64320200	-1.08080300
H	-3.12982700	0.09179900	-2.13180100
H	-2.94941100	-1.58699500	-1.60285800
H	-4.06005700	-1.09145600	1.54715500
H	-2.55518100	-0.73865400	2.45083400
H	-2.77240400	1.96570800	1.47743000
H	-4.26053800	1.44658500	0.62901900
H	4.25428800	1.52152100	0.48572700
H	2.94394800	2.27777600	-0.46961000
H	4.37041300	-0.74494500	-1.01295200
H	3.10924400	-0.15401500	-2.13723800

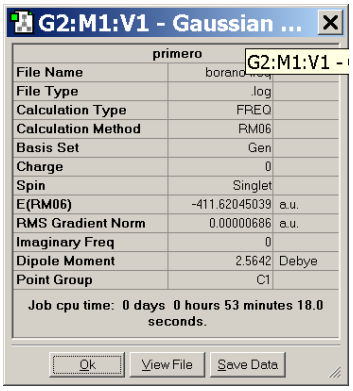


H	2.59460200	-1.98113400	1.50469800
H	2.52544700	-0.52311300	2.51281500
H	-1.14556300	-2.68817000	-0.65241400

Zero-point correction= 0.255915 (Hartree/Particle)
Thermal correction to Energy= 0.276535
Thermal correction to Enthalpy= 0.277479
Thermal correction to Gibbs Free Energy= 0.206536
Sum of electronic and zero-point Energies= -1525.481757
Sum of electronic and thermal Energies= -1525.461137
Sum of electronic and thermal Enthalpies= -1525.460193
Sum of electronic and thermal Free Energies= -1525.531136

HBpin

H	0.00033700	3.11260200	-0.00011900
O	-1.06258400	1.18285000	0.41926000
O	1.06271900	1.18260800	-0.41963800
B	0.00015300	1.92712600	-0.00019800
C	-0.77780800	-0.18678700	0.05459500
C	-1.47429200	-0.43374900	-1.27522300
H	-2.53708700	-0.19522000	-1.16277600
H	-1.38773300	-1.47952700	-1.59142700
H	-1.06673400	0.20635700	-2.06580900
C	-1.34678900	-1.10409800	1.11623800
H	-0.98127400	-0.84934700	2.11487100
H	-1.09008000	-2.14954800	0.90301300
H	-2.43865100	-1.01948900	1.12542800
C	0.77780400	-0.18689400	-0.05460200
C	1.47414700	-0.43348300	1.27534700
H	2.53696200	-0.19503900	1.16296300
H	1.38747500	-1.47915600	1.59185900
H	1.06646800	0.20686400	2.06568000
C	1.34672400	-1.10459500	-1.11593700
H	0.98139100	-0.84996400	-2.11466200
H	1.08975600	-2.14993800	-0.90249900
H	2.43861100	-1.02025100	- 1.12500600

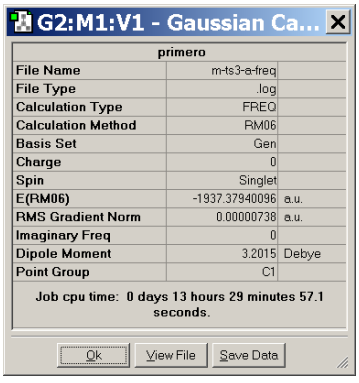


Zero-point correction= 0.190443 (Hartree/Particle)
Thermal correction to Energy= 0.199818
Thermal correction to Enthalpy= 0.200762
Thermal correction to Gibbs Free Energy= 0.157627
Sum of electronic and zero-point Energies= -411.430007
Sum of electronic and thermal Energies= -411.420632
Sum of electronic and thermal Enthalpies= -411.419688
Sum of electronic and thermal Free Energies= -411.462823

A

Os	1.16579700	0.12976100	0.01004300
H	2.45476900	0.35073300	0.95719600
H	-0.33061200	-0.16821500	-1.18255000
P	1.78474900	-2.15378600	0.00089200
P	0.72103700	2.44047500	0.25705300
S	-0.11735500	-0.55611500	2.05756200
O	-2.13677700	-1.39613000	-0.79497500
O	-2.18345000	0.83779100	-0.28305800
O	2.86161500	0.86062800	-2.39429300
B	-1.43099800	-0.24372600	-0.64178900
C	-3.46036500	-1.15784300	-0.25799300
C	-3.49672800	-1.76689500	1.13325500
H	-3.27139100	-2.83603600	1.04886500
H	-4.48782200	-1.66384900	1.59018500
H	-2.73994300	-1.32108900	1.78738100
C	-4.46604900	-1.86136300	-1.14719700
H	-4.37516000	-1.55807200	-2.19369600
H	-5.48908000	-1.65474000	-0.80770900
H	-4.30448100	-2.94291700	-1.09200600
C	-3.56516800	0.40886000	-0.27544500
C	-4.18224900	0.96408800	-1.54951000
H	-4.04851300	2.05142400	-1.56022400
H	-5.25495700	0.74893700	-1.61112800
H	-3.69067600	0.55512200	-2.43951500
C	-4.23656100	1.01007100	0.94111400
H	-3.69426300	0.75716400	1.85771300
H	-5.27100300	0.65619400	1.03317100
H	-4.25977900	2.10175300	0.84520200
C	2.19811000	0.55728000	-1.47816100
C	2.88758100	-2.69707700	-1.35729000
H	3.80562700	-2.10042300	-1.33802300
C	2.71319600	-2.67906800	1.48701600
H	2.94660500	-3.75008400	1.45300900
C	0.42692700	-3.38041600	-0.07440300
H	-0.27287300	-3.18230500	0.74513500
C	2.23557500	3.43187500	0.53722700
H	2.93544900	3.24410100	-0.28422100
C	-0.39351100	3.05221400	1.57601200
H	-1.38405000	2.60525600	1.43470000
C	0.01295900	3.25172800	-1.22795400
H	-0.08049600	4.33536100	-1.08664900
H	0.66173900	3.05251900	-2.08789400
H	-0.97425500	2.82038700	-1.42249100
H	-0.47221300	4.14472800	1.52542700
H	-0.00391500	2.76546900	2.55848600
H	2.70954800	3.10715500	1.46874900
H	2.01190500	4.50419500	0.58972800
H	3.14278800	-3.75873800	-1.25674800
H	2.39419900	-2.53243100	-2.32080800
H	0.81452000	-4.40351000	0.00209100
H	-0.12307800	-3.25896900	-1.01305400
H	2.11440100	-2.45315900	2.37547300
H	3.64041300	-2.10015100	1.54578500
H	-0.63149500	0.61943600	2.47248900

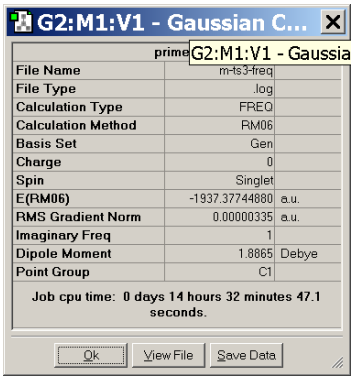
Zero-point correction= 0.449847 (Hartree/Particle)
Thermal correction to Energy= 0.480545
Thermal correction to Enthalpy= 0.481490
Thermal correction to Gibbs Free Energy= 0.389695
Sum of electronic and zero-point Energies= -1936.929554
Sum of electronic and thermal Energies= -1936.898856
Sum of electronic and thermal Enthalpies= -1936.897911
Sum of electronic and thermal Free Energies= -1936.989706



TS1

Os	-1.15850000	0.15495200	-0.02850600
H	-2.42312800	0.42122300	-1.02696400
H	0.31106600	-0.21318500	1.05125600
P	-1.89388300	-2.09539900	0.00298700
P	-0.61882300	2.44464700	-0.28784700
S	0.31239800	-0.65802400	-1.89702400
O	2.04189700	-1.46550500	0.61044700
O	2.16210800	0.77649300	0.09936700
O	-2.85898600	0.98486800	2.33468900
B	1.33149500	-0.31961600	0.30814100
C	3.41065000	-1.21504400	0.24761300
C	3.63728500	-1.74295600	-1.16281800
H	3.33393200	-2.79585500	-1.19021100
H	4.69456800	-1.68105500	-1.44706700
H	3.03359400	-1.21003400	-1.90301800
C	4.30217200	-1.97154200	1.21352500
H	4.05916600	-1.74500200	2.25525200
H	5.35904500	-1.73343500	1.03664700
H	4.16966300	-3.04851100	1.06322900
C	3.50963300	0.34324100	0.35783500
C	3.85857700	0.82382800	1.76000400
H	3.73555100	1.91233100	1.80037900
H	4.89472200	0.58926400	2.03078600
H	3.19118400	0.38006200	2.50782600
C	4.42714500	0.99475500	-0.65690100
H	4.10088500	0.79026700	-1.68146400
H	5.45914500	0.64063400	-0.53904700
H	4.42366400	2.08106500	-0.50974200
C	-2.20615600	0.64800500	1.42390800
C	-3.07695100	-2.54629900	1.32526800
H	-3.96339300	-1.90732900	1.25395700
C	-2.78412500	-2.60445500	-1.51167300
H	-3.07528900	-3.66088900	-1.46808600
C	-0.61282100	-3.39538200	0.16369100
H	0.12874400	-3.27572700	-0.63425200
C	-2.09145800	3.51372400	-0.49178800
H	-2.76465600	3.35937200	0.35819500
C	0.44893400	2.99699800	-1.67003500
H	1.42945300	2.51731100	-1.57646400
C	0.20423200	3.20005200	1.16496100
H	0.37465800	4.27376100	1.01964300
H	-0.42853500	3.04869300	2.04653600
H	1.15986300	2.68746900	1.32091500
H	0.57163500	4.08601700	-1.63694900
H	-0.00564400	2.71832500	-2.62692600
H	-2.62263100	3.22233200	-1.40314000
H	-1.81249300	4.57276600	-0.54775800
H	-3.37933800	-3.59669100	1.23983500
H	-2.61426100	-2.38075100	2.30366200
H	-1.05915800	-4.39558800	0.10669400
H	-0.08924800	-3.27379200	1.11741000
H	-2.13371500	-2.43235300	-2.37541100
H	-3.67473800	-1.97840100	-1.62452500
H	0.77355100	0.50267600	-2.40775900

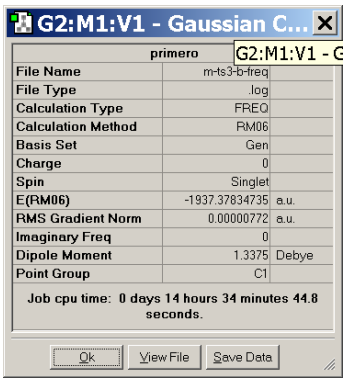
Zero-point correction= 0.448809 (Hartree/Particle)
Thermal correction to Energy= 0.478570
Thermal correction to Enthalpy= 0.479514
Thermal correction to Gibbs Free Energy= 0.391081
Sum of electronic and zero-point Energies= -1936.928640
Sum of electronic and thermal Energies= -1936.898879
Sum of electronic and thermal Enthalpies= -1936.897934
Sum of electronic and thermal Free Energies= -1936.986368



B_1

Os	-1.17036800	0.13857600	-0.04887200
H	-2.48024900	0.36093100	-1.01649500
H	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
O	2.05869400	-1.44674700	0.42135300
O	2.22221000	0.80721900	-0.09482200
O	-2.83179900	0.89238800	2.36000300
B	1.34841500	-0.30013200	0.02975900
C	3.44405600	-1.15722100	0.21029200
C	3.82037800	-1.56524600	-1.20952200
H	3.49746900	-2.60032300	-1.36820900
H	4.90378100	-1.51358500	-1.37250300
H	3.32262600	-0.94178800	-1.95905300
C	4.25923900	-1.96139800	1.20376400
H	3.88631500	-1.83397700	2.22393500
H	5.31630000	-1.66690400	1.17237800
H	4.19846000	-3.02653000	0.95369900
C	3.48895600	0.38498000	0.42970200
C	3.52530500	0.76407200	1.90515400
H	3.37882300	1.84683000	1.99703000
H	4.48486200	0.51048200	2.37117500
H	2.72268300	0.26251500	2.45869000
C	4.59676900	1.10101800	-0.31514000
H	4.51280700	0.96220600	-1.39688300
H	5.58020800	0.73836200	0.01061100
H	4.54849300	2.17594000	-0.10651100
C	-2.19470500	0.58387400	1.42816200
C	-3.15008600	-2.53663400	1.22519700
H	-4.01985900	-1.89689800	1.04297500
C	-2.56912300	-2.73326200	-1.55489200
H	-2.84726800	-3.79158500	-1.48310600
C	-0.56881100	-3.40061700	0.36600300
H	0.22938400	-3.34303100	-0.38177600
C	-2.19477200	3.49401600	-0.42298600
H	-2.84060500	3.31090800	0.44251300
C	0.32989000	3.04008400	-1.67601100
H	1.32078600	2.57809100	-1.60215000
C	0.15868200	3.16983600	1.16292100
H	0.31177900	4.24963000	1.04703400
H	-0.43793900	2.97970500	2.06184600
H	1.12541100	2.66302300	1.26432300
H	0.43475200	4.13028000	-1.62674800
H	-0.13490200	2.77093100	-2.63087300
H	-2.74734000	3.21219100	-1.32454800
H	-1.93507900	4.55861900	-0.46425800
H	-3.44683000	-3.58872900	1.14153400
H	-2.78839600	-2.34306600	2.24019100
H	-1.00568400	-4.40675600	0.36231800
H	-0.11199500	-3.19401200	1.33898300
H	-1.84249700	-2.59615900	-2.36227700
H	-3.45338400	-2.13125600	-1.78620800
H	0.75508600	0.56508800	-2.43660600

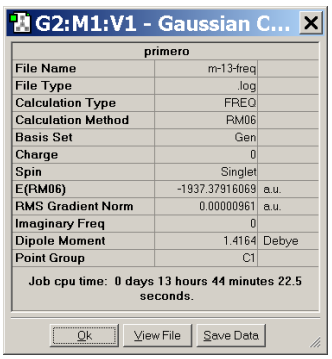
Zero-point correction= 0.449283 (Hartree/Particle)
Thermal correction to Energy= 0.479357
Thermal correction to Enthalpy= 0.480301
Thermal correction to Gibbs Free Energy= 0.391685
Sum of electronic and zero-point Energies= -1936.929064
Sum of electronic and thermal Energies= -1936.898990
Sum of electronic and thermal Enthalpies= -1936.898046
Sum of electronic and thermal Free Energies= -1936.986663



B_2

Os	1.18538000	0.07463400	-0.11867700
H	2.50139900	0.25403500	-1.08845800
H	-0.36550200	-0.17699700	0.81493200
P	0.97884800	2.43340300	-0.04479400
P	1.50757900	-2.26648100	-0.14172400
S	-0.47681200	0.08249900	-2.00425200
O	-2.15516600	0.98315700	0.25339000
O	-2.09025300	-1.32037100	-0.05055200
O	2.98618500	0.22861600	2.30407400
B	-1.33704200	-0.12307700	-0.06096800
C	-3.50799800	0.52313800	0.14342500
C	-3.98133400	0.74061700	-1.28920200
H	-3.81175200	1.79078100	-1.55546900
H	-5.05120000	0.52644200	-1.40035800
H	-3.42131400	0.12248600	-1.99817700
C	-4.37038600	1.32995300	1.09348900
H	-3.96294500	1.32946700	2.10853200
H	-5.39377200	0.93407900	1.12332200
H	-4.42134600	2.36968900	0.75081600
C	-3.36596100	-0.98510600	0.50983300
C	-3.28315100	-1.21765100	2.01434200
H	-2.96857800	-2.25273400	2.19049500
H	-4.24872000	-1.06647700	2.51165900
H	-2.54221500	-0.55357300	2.47461600
C	-4.42394900	-1.88514600	-0.09509400
H	-4.39875100	-1.85698800	-1.18802500
H	-5.42576800	-1.58945100	0.24259800
H	-4.25352100	-2.92061200	0.22070600
C	2.28977200	0.16642600	1.36480600
C	2.57300900	3.32824300	-0.10826000
H	3.06424800	3.11568500	-1.06270800
C	-0.02819200	3.28304600	-1.31439500
H	-0.00550800	4.36725200	-1.15339700
C	0.22922800	3.04271500	1.50928500
H	-0.77846200	2.61829700	1.58465900
C	3.24941300	-2.79510200	-0.33127500
H	3.84572700	-2.31632500	0.45316500
C	0.63005100	-3.31948300	-1.35757700
H	-0.45068100	-3.19212200	-1.22437300
C	1.02140600	-3.06080600	1.43607800
H	1.20675800	-4.14162500	1.42387500
H	1.58521800	-2.60405100	2.25678100
H	-0.04505300	-2.87067400	1.60143900
H	0.88761700	-4.37302600	-1.19723000
H	0.90700600	-3.03701200	-2.37890300
H	3.62572600	-2.45017200	-1.29922200
H	3.35427900	-3.88416100	-0.25745800
H	2.43059500	4.40960800	0.00380500
H	3.21754800	2.95832400	0.69649800
H	0.17683600	4.13802400	1.53095400
H	0.82601700	2.68961400	2.35746600
H	-1.06082100	2.92356000	-1.23780000
H	0.35196200	3.05049300	-2.31414000
H	-0.56365000	-1.22870300	-2.30851100

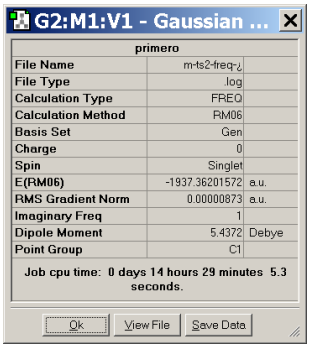
Zero-point correction= 0.449234 (Hartree/Particle)
Thermal correction to Energy= 0.479432
Thermal correction to Enthalpy= 0.480376
Thermal correction to Gibbs Free Energy= 0.391336
Sum of electronic and zero-point Energies= -1936.929926
Sum of electronic and thermal Energies= -1936.899729
Sum of electronic and thermal Enthalpies= -1936.898784
Sum of electronic and thermal Free Energies= -1936.987824



TS2

Os	1.18538000	0.07463400	-0.11867700
H	2.50139900	0.25403500	-1.08845800
H	-0.36550200	-0.17699700	0.81493200
P	0.97884800	2.43340300	-0.04479400
P	1.50757900	-2.26648100	-0.14172400
S	-0.47681200	0.08249900	-2.00425200
O	-2.15516600	0.98315700	0.25339000
O	-2.09025300	-1.32037100	-0.05055200
O	2.98618500	0.22861600	2.30407400
B	-1.33704200	-0.12307700	-0.06096800
C	-3.50799800	0.52313800	0.14342500
C	-3.98133400	0.74061700	-1.28920200
H	-3.81175200	1.79078100	-1.55546900
H	-5.05120000	0.52644200	-1.40035800
H	-3.42131400	0.12248600	-1.99817700
C	-4.37038600	1.32995300	1.09348900
H	-3.96294500	1.32946700	2.10853200
H	-5.39377200	0.93407900	1.12332200
H	-4.42134600	2.36968900	0.75081600
C	-3.36596100	-0.98510600	0.50983300
C	-3.28315100	-1.21765100	2.01434200
H	-2.96857800	-2.25273400	2.19049500
H	-4.24872000	-1.06647700	2.51165900
H	-2.54221500	-0.55357300	2.47461600
C	-4.42394900	-1.88514600	-0.09509400
H	-4.39875100	-1.85698800	-1.18802500
H	-5.42576800	-1.58945100	0.24259800
H	-4.25352100	-2.92061200	0.22070600
C	2.28977200	0.16642600	1.36480600
C	2.57300900	3.32824300	-0.10826000
H	3.06424800	3.11568500	-1.06270800
C	-0.02819200	3.28304600	-1.31439500
H	-0.00550800	4.36725200	-1.15339700
C	0.22922800	3.04271500	1.50928500
H	-0.77846200	2.61829700	1.58465900
C	3.24941300	-2.79510200	-0.33127500
H	3.84572700	-2.31632500	0.45316500
C	0.63005100	-3.31948300	-1.35757700
H	-0.45068100	-3.19212200	-1.22437300
C	1.02140600	-3.06080600	1.43607800
H	1.20675800	-4.14162500	1.42387500
H	1.58521800	-2.60405100	2.25678100
H	-0.04505300	-2.87067400	1.60143900
H	0.88761700	-4.37302600	-1.19723000
H	0.90700600	-3.03701200	-2.37890300
H	3.62572600	-2.45017200	-1.29922200
H	3.35427900	-3.88416100	-0.25745800
H	2.43059500	4.40960800	0.00380500
H	3.21754800	2.95832400	0.69649800
H	0.17683600	4.13802400	1.53095400
H	0.82601700	2.68961400	2.35746600
H	-1.06082100	2.92356000	-1.23780000
H	0.35196200	3.05049300	-2.31414000
H	-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 Energy= 0.388320
Sum of electronic and zero-point Energies= -1936.916164
Sum of electronic and thermal Energies= -1936.886498
Sum of electronic and thermal Enthalpies= -1936.885553
Sum of electronic and thermal Free Energies= -1936.973696



C_1

Os	1.23826800	0.07469200	-0.11137800
H	2.43339900	0.24306800	-1.32866700
H	-0.14771800	-0.11438500	0.91175300
P	1.00721100	2.41144800	-0.02689400
P	1.49940300	-2.25469900	-0.07687100
S	-0.42735200	0.06851800	-2.05541400
O	-2.40527400	1.01697000	-0.28662800
O	-2.47330100	-1.25760600	-0.63529400
O	3.21448300	0.20584000	2.15644000
B	-1.82841600	-0.07850000	-0.85170100
C	-3.63385500	0.55462000	0.32841300
C	-4.75801400	0.94823900	-0.61665800
H	-4.72053800	2.03083100	-0.77612400
H	-5.74141300	0.69399500	-0.20492300
H	-4.64977600	0.45942200	-1.59157000
C	-3.79477700	1.25383700	1.66080100
H	-2.92027300	1.10342100	2.30057500
H	-4.68464300	0.88511400	2.18628100
H	-3.91940700	2.33013000	1.49784500
C	-3.42335200	-0.99584900	0.43190500
C	-2.76808900	-1.44454900	1.72778100
H	-2.51597300	-2.50785400	1.63554300
H	-3.44748900	-1.32937200	2.58005100
H	-1.84091000	-0.89328400	1.92434100
C	-4.66885500	-1.81716700	0.17419900
H	-5.08484900	-1.63568200	-0.82051300
H	-5.43736700	-1.59145200	0.92416300
H	-4.42624900	-2.88223700	0.25145300
C	2.44309700	0.16110400	1.27214300
C	2.58300500	3.34060000	0.07883300
H	3.18431900	3.10921900	-0.80587000
C	0.16259400	3.26694400	-1.41655100
H	0.19622300	4.35370000	-1.27423600
C	0.07159100	3.06129500	1.40842600
H	-0.95002500	2.67018500	1.34235500
C	3.17564600	-2.88448700	-0.46818300
H	3.89000800	-2.41213500	0.21506900
C	0.44472100	-3.31262500	-1.15055800
H	-0.61384800	-3.09820100	-0.95637500
C	1.19630300	-3.02095700	1.56234500
H	1.38270800	-4.10207900	1.55030300
H	1.85027900	-2.54817000	2.30304900
H	0.15965400	-2.82336700	1.85393600
H	0.64028400	-4.37242100	-0.94848200
H	0.66636400	-3.12040300	-2.20734900
H	3.43791400	-2.58136700	-1.48651200
H	3.24119500	-3.97518700	-0.37052500
H	2.41146900	4.42199100	0.14454400
H	3.13876200	3.00671600	0.96154700
H	0.05352200	4.15806700	1.42943200
H	0.52679700	2.68005800	2.32872100
H	-0.88554600	2.94855800	-1.46184700
H	0.65279700	3.00681000	-2.36060100
H	-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 Energy= 0.388397
Sum of electronic and zero-point Energies= -1936.915919
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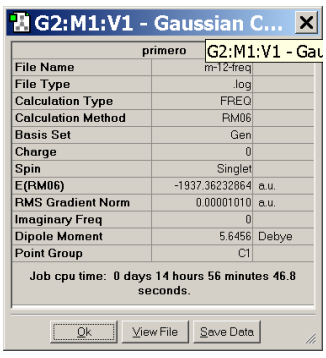
Sum of electronic and thermal Enthalpies= -1936.884805
Sum of electronic and thermal Free Energies= -1936.973931



C_2

Os	-1.24200700	0.08320200	-0.06974400
H	-2.34487100	0.22964500	-1.37731800
H	0.07953000	-0.12369200	1.02972700
P	-1.69957500	-2.22328300	0.00640500
P	-0.91328900	2.40289800	-0.15310700
S	0.43682800	-0.46610600	-1.92648300
O	2.40166400	-1.40552400	-0.16266900
O	2.70491000	0.78494500	-0.78177300
O	-3.26728400	0.66816400	2.07768500
B	1.94189900	-0.33944300	-0.85786900
C	3.66635800	-1.00294300	0.41697200
C	4.75038900	-1.61561600	-0.45459800
H	4.59370300	-2.69820500	-0.49975900
H	5.75055300	-1.42913600	-0.04734100
H	4.70961700	-1.22615900	-1.47817300
C	3.73650900	-1.55983000	1.82255100
H	2.85222600	-1.28313700	2.40431700
H	4.63409600	-1.19920900	2.34047800
H	3.78566500	-2.65312700	1.77986000
C	3.61093300	0.56048700	0.33556500
C	2.96631000	1.21416000	1.54580200
H	2.85264300	2.28529600	1.33802100
H	3.58693200	1.10661900	2.44235300
H	1.96918700	0.79633500	1.73855100
C	4.93407000	1.22384700	0.02153000
H	5.35320900	0.87575200	-0.92622800
H	5.65913100	1.02556200	0.82081200
H	4.79389300	2.30783400	-0.04550900
C	-2.48026400	0.42190000	1.24181300
C	-2.87550300	-2.74699900	1.30958200
H	-3.81819300	-2.20386900	1.18890900
C	-2.45575700	-2.95837200	-1.49623300
H	-2.61935600	-4.03771400	-1.38621400
C	-0.29742500	-3.37080600	0.30716000
H	0.45513500	-3.26242700	-0.48145000
C	-2.41979100	3.35940400	-0.57942600
H	-3.21100600	3.09853400	0.13212700
C	0.31147600	3.12914000	-1.31688600
H	1.30763200	2.70672600	-1.13777800
C	-0.44013300	3.19738200	1.43166000
H	-0.37642800	4.28860500	1.33931100
H	-1.19357300	2.94065800	2.18450800
H	0.52035700	2.79495900	1.76767500
H	0.34906200	4.21836200	-1.19651400
H	0.01065000	2.91131500	-2.34938600
H	-2.75570100	3.06093000	-1.57720400
H	-2.24209600	4.44174300	-0.54866200
H	-3.06375600	-3.82591100	1.25794800
H	-2.46121300	-2.49504600	2.29122800
H	-0.63631000	-4.41363800	0.34486700
H	0.17924400	-3.09494000	1.25379000
H	-1.80093100	-2.77482600	-2.35505400
H	-3.40765600	-2.45319700	-1.68697600
H	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 Energy= 0.388735
Sum of electronic and zero-point Energies= -1936.914153
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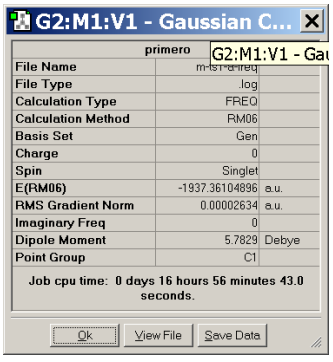
Sum of electronic and thermal Enthalpies= -1936.883089
Sum of electronic and thermal Free Energies= -1936.972314



TS3

Os	-1.30834100	0.11841000	-0.10684300
H	-2.33106800	0.17346500	-1.49520700
H	-0.22474900	-0.15970200	1.19305200
P	-1.83705300	-2.17010100	0.14230900
P	-0.65863000	2.39654600	-0.19525700
S	0.48658600	-0.75029100	-1.88625100
O	2.73841200	-1.48938300	-0.51754500
O	2.34966400	0.74932300	-0.23900100
O	-3.61012200	1.01793700	1.61416100
B	1.91593600	-0.42931100	-0.78213100
C	3.93160000	-0.94132200	0.08813500
C	4.93730200	-0.73046100	-1.03330400
H	5.08119500	-1.68017500	-1.55870700
H	5.90890300	-0.39907500	-0.64912500
H	4.57772700	0.00760000	-1.75914200
C	4.46608400	-1.93939900	1.09222700
H	3.69936300	-2.23554700	1.81308200
H	5.32213000	-1.52145900	1.63672400
H	4.80516600	-2.83927500	0.56817100
C	3.40131000	0.39047200	0.69679200
C	2.75883900	0.19175100	2.06058400
H	2.24620200	1.11002600	2.36583300
H	3.51353000	-0.04616400	2.81892600
H	2.00539600	-0.60397700	2.03788200
C	4.40883800	1.51805500	0.74323300
H	4.77789300	1.77654900	-0.25321800
H	5.26371100	1.24427100	1.37430300
H	3.94551500	2.41158100	1.17676600
C	-2.71015200	0.66284100	0.95592100
C	-3.08800800	-2.52635100	1.43020500
H	-4.01878200	-2.00349000	1.18764300
C	-2.50986000	-3.04833100	-1.31646600
H	-2.71494000	-4.10261400	-1.09356900
C	-0.44661000	-3.25099400	0.64558700
H	0.35615900	-3.18072100	-0.09598900
C	-2.08124600	3.54216500	-0.35781500
H	-2.76334200	3.40594900	0.48756500
C	0.41282000	2.97369300	-1.56871600
H	1.38016400	2.46464500	-1.52218400
C	0.21030900	3.07730000	1.26555400
H	0.32594600	4.16572600	1.19440300
H	-0.35368300	2.82082300	2.16815900
H	1.19576900	2.60392100	1.32193800
H	0.56688300	4.05642900	-1.48904200
H	-0.06720800	2.75009600	-2.52770000
H	-2.62573400	3.29509500	-1.27486200
H	-1.75006100	4.58707000	-0.39225900
H	-3.28247100	-3.60205100	1.51126900
H	-2.72543200	-2.14648200	2.39131500
H	-0.76802300	-4.29560900	0.73835900
H	-0.05929500	-2.89451000	1.60578000
H	-1.78658300	-2.98322300	-2.13594900
H	-3.43058300	-2.54838700	-1.63285500
H	-0.53658100	0.38509700	-1.77898000

Zero-point correction= 0.442591 (Hartree/Particle)
Thermal correction to Energy= 0.472946
Thermal correction to Enthalpy= 0.473890
Thermal correction to Gibbs Free Energy= 0.382202
Sum of electronic and zero-point Energies= -1936.900631
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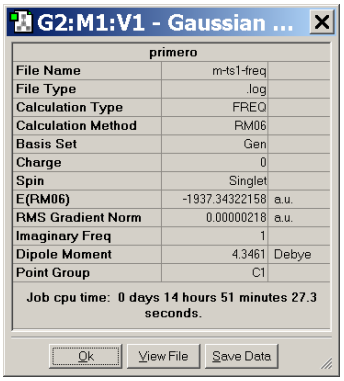
Sum of electronic and thermal Enthalpies= -1936.869331
Sum of electronic and thermal Free Energies= -1936.961019



2ta

Os	-1.42681400	0.05466800	-0.15191000
H	-2.53285100	-0.32211200	-1.56619400
H	-0.33297800	-0.00680400	1.06561000
P	-1.41972600	-2.31576000	0.09217600
P	-0.92761600	2.38089500	-0.16970400
S	0.43562300	-0.41679500	-1.80940300
O	2.91545300	-1.18205800	-0.77180000
O	2.21641100	0.84376900	0.02120900
O	-3.63207200	0.49303300	1.87703300
B	1.91037300	-0.23569200	-0.79525800
C	4.03424300	-0.60917200	-0.07435600
C	4.95112900	0.00046100	-1.12546300
H	5.20743800	-0.77346100	-1.85638100
H	5.88013000	0.38375800	-0.68689000
H	4.45235700	0.81649100	-1.66045400
C	4.75702600	-1.70988000	0.67374400
H	4.07458500	-2.28011100	1.31143900
H	5.56215500	-1.29819300	1.29573600
H	5.20581400	-2.40564000	-0.04347400
C	3.34603800	0.45806600	0.82523700
C	2.79841300	-0.12408100	2.12154500
H	2.12712200	0.60729900	2.58562800
H	3.59981100	-0.35910300	2.83198000
H	2.21749600	-1.03505600	1.93454500
C	4.18476800	1.68380600	1.12168400
H	4.44898700	2.22503700	0.20892200
H	5.10835800	1.40519600	1.64504400
H	3.62741400	2.36829200	1.77185800
C	-2.79211300	0.32036000	1.08160300
C	-2.70923700	-3.00810500	1.19455500
H	-3.70001900	-2.75368600	0.80357000
C	-1.61498400	-3.31072300	-1.42911800
H	-1.51418800	-4.38127800	-1.21498900
C	0.11350000	-2.99681700	0.82167300
H	0.97282300	-2.71640900	0.20077700
C	-2.40117600	3.47291700	-0.20259800
H	-3.04767600	3.24003800	0.65032000
C	0.08670400	3.04370400	-1.53475700
H	1.07138600	2.56964800	-1.49916300
C	-0.03782100	2.97073900	1.31211300
H	0.08763300	4.05977400	1.29042900
H	-0.59378700	2.67894600	2.20908500
H	0.94078500	2.48006100	1.32014200
H	0.18611600	4.13165100	-1.43780500
H	-0.37624800	2.79259800	-2.49413900
H	-2.96849800	3.28983000	-1.12156200
H	-2.11489300	4.53079700	-0.16057200
H	-2.61925400	-4.09780900	1.27539200
H	-2.61190000	-2.56145900	2.18975300
H	0.05332500	-4.08948000	0.89398200
H	0.24308700	-2.57197700	1.82309500
H	-0.84364300	-2.99862400	-2.14094100
H	-2.60106500	-3.11859300	-1.86569200
H	-2.38096400	0.52020400	-1.65092200

Zero-point correction= 0.448617 (Hartree/Particle)
Thermal correction to Energy= 0.478897
Thermal correction to Enthalpy= 0.479841
Thermal correction to Gibbs Free Energy= 0.390152
Sum of electronic and zero-point Energies= -1936.944713
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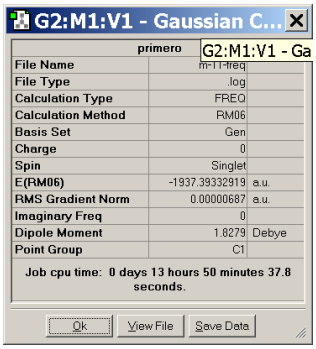
Sum of electronic and thermal Enthalpies= -1936.913488
Sum of electronic and thermal Free Energies= -1937.003177



2t

Os	-1.31789200	0.19461500	-0.06983100
H	-0.44481700	-0.55000700	-1.50437300
H	-2.16564000	0.48383300	1.30883300
P	-2.36241300	-1.93915600	0.01748800
P	-0.37892900	2.33004400	0.37735100
S	0.38585000	-0.94775200	1.42370300
O	3.08735900	-1.46345800	0.92133400
O	2.23817300	0.20704500	-0.39432800
O	-3.53652900	1.42984200	-1.72194100
B	1.96377400	-0.72849100	0.60160800
C	4.07469200	-1.18981200	-0.08281700
C	3.91231200	-2.24276500	-1.17153900
H	3.98691200	-3.23366900	-0.71173400
H	4.68811300	-2.15943900	-1.94189000
H	2.92950300	-2.16576100	-1.65195800
C	5.45405100	-1.29121100	0.53450700
H	5.54063400	-0.67709400	1.43489000
H	6.22523700	-0.98134900	-0.18254000
H	5.65401100	-2.33008300	0.81825200
C	3.67001000	0.23391200	-0.55826100
C	4.20668100	1.33177500	0.35068400
H	3.72519500	2.28181100	0.08959800
H	5.29010200	1.45774900	0.24121400
H	3.98493100	1.11590000	1.40280400
C	3.99835400	0.54668900	-2.00341500
H	3.49136200	-0.13582600	-2.69115900
H	5.07994500	0.48121700	-2.17815000
H	3.68348400	1.56828800	-2.24643700
C	-2.67301300	0.95464600	-1.09258200
C	-3.97007800	-2.08659200	-0.84749600
H	-3.83622200	-1.87576800	-1.91362000
C	-1.41439400	-3.35236600	-0.65452600
H	-1.94032300	-4.30022900	-0.48902300
C	-2.77636200	-2.49572800	1.70762100
H	-1.86189300	-2.51076800	2.30891200
C	-1.64354400	3.62061200	0.67845700
H	-2.26071400	3.31861000	1.53064600
C	0.63895700	3.08509500	-0.94509900
H	1.46490000	2.39923300	-1.16438200
C	0.68283200	2.48753800	1.85348800
H	1.00248700	3.52884600	1.98144800
H	0.12374300	2.15368300	2.73298600
H	1.55401800	1.83561900	1.74500300
H	1.03023300	4.06461500	-0.64383400
H	0.02516400	3.20027400	-1.84515100
H	-2.29386000	3.71330100	-0.19761900
H	-1.17816700	4.59134100	0.88753000
H	-4.39200000	-3.09128800	-0.72594400
H	-4.66880800	-1.34846200	-0.43984600
H	-3.22724900	-3.49501200	1.69048200
H	-3.47552600	-1.78151600	2.15343200
H	-0.43904400	-3.37680200	-0.15678600
H	-1.26012700	-3.20623700	-1.72921200
H	-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 Energy= 0.387841
Sum of electronic and zero-point Energies= -1936.944982
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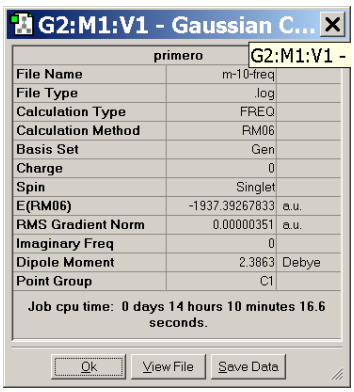
Sum of electronic and thermal Enthalpies= -1936.913429
Sum of electronic and thermal Free Energies= -1937.004838



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(3) $d_{H\text{-}H} = 1.42 - 0.0167\ (J_{H,D})$. See: Maltby, P. A.; Schlaf, M.; Steinbeck, M.; Lough, A. J.; Morris, R. H.; Klooster, W. T.; Koetzle, T. F.; Srivastava, R. C. *J. Am. Chem. Soc*. **1996**, *118*, 5396.

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