SUPPORTING INFORMATION

Cleavage of Both C(sp^3)-C(sp^2) Bonds of Alkylidenecyclopropanes: Formation of Ethylene-Osmium-Vinylidene Complexes

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Experimental Section

General Methods and Instrumentation. All reactions were carried out under argon with rigorous exclusion of air using Schlenk-tube techniques. 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. All reagents were obtained from commercial suppliers and used without further purification, with the exception of phenylacetylene, which was distilled. The starting materials [OsTp(κ^1-$OCMe_2)_2(P^iPr_3)]BF_4$ (**1**),[1] benzylidenecyclopropane,[2] and 3-

phenylpropylidenecyclopropane[3] were prepared according to the published methods. ^{1}H, $^{31}P\{^{1}H\}$, and $^{13}C\{^{1}H\}$ NMR spectra were recorded on either a Varian Gemini 2000, a Bruker ARX 300, a Bruker Avance 300 MHz or a Bruker Avance 400 MHz instrument. Chemical shifts (expressed in parts per million) are referenced to residual solvent peaks (^{1}H, $^{13}C\{^{1}H\}$) or external H_3PO_4 ($^{31}P\{^{1}H\}$). Coupling constants, *J*, are given in hertz. Spectral assignments were achieved by ^{1}H-^{1}H COSY, $^{1}H\{^{31}P\}$, ^{13}C APT, ^{1}H-^{13}C HSQC, and ^{1}H-^{13}C HMBC experiments. Infrared spectra were recorded on a Spectrum One spectrometer as neat solids. C, H and N analyses were carried out in a Perkin- Elmer 2400 CHNS/O analyzer or a Fisons EA-1108 apparatus. High-resolution electrospray mass spectra were acquired using a MicroTOF-Q hybrid quadrupole time-of-flight spectrometer (Bruker Daltonics, Bremen, Germany).

Preparation of [OsTp(η^2-CH_2=CH_2)(=C=CHPh)(P^iPr_3)]BF_4 (2): Method a. Benzylidenecyclopropane (71 mg, 0.55 mmol) in 18 mL of fluorobenzene was added to a Schlenk flask with **1** (300 mg, 0.39 mmol). After 30 min the brownish solution was passed through Celite and the solvent removed *in vacuo*. The addition of dichloromethane (1 mL) and diethyl ether (10 ml) caused the apparition of a sticky solid which was washed with further portions of diethyl ether (4 x 7 mL) and vacuum-dried. Brown solid. Yield: 215 mg (71 %). **Method b.** A yellow solution of [OsTp(κ^1-$OCMe_2$)(η^2-CH_2=CH_2)(P^iPr_3)]BF_4 (**4**) (330 mg, 0.45 mmol) in 8 mL of dichloromethane was treated with phenylacetylene (74 μL, 0.67 mmol). The color of the solution turned immediately to brown. After stirring 2 h at room temperature it was concentrated to ca. 1 mL. Diethyl ether (10 mL) was added, resulting in the precipitation of a brown solid which was washed with diethyl ether (3 x 7 mL) and vacuum-dried. Yield: 272 mg (81 %). **Method c.** A solution of [OsTp(κ^1-

$OCMe_2$)(=C=CHPh)(P^iPr_3)]BF_4 (**5**) (100 mg, 0.12 mmol) in 5 mL of dichloromethane was connected to an ethylene reservoir and the argon atmosphere was replaced by ethylene (1 atm). After 90 min, the solution was concentrated to ca. 0.5 mL, diethyl ether (8 mL) was added and the oily residue was washed with diethyl ether (3 x 8 mL) and dried *in vacuo*. Brown solid. Yield: 66 mg (69 %). Anal. Calcd for $C_{28}H_{41}B_2F_4N_6OsP$: C, 43.09; H, 5.29; N, 10.77. Found: C, 42.61; H, 5.75; N, 10.46. IR (ATR, cm^{-1}): *v*(BH) 2502 (w), *v*(C=C) 1633 (m), *v*(BF_4) 1046 (vs). ^{1}H NMR (400 MHz, CD_2Cl_2, 298 K): 8.35 (d, 1H, Tp), 7.98 (d, 1H, Tp), 7.96 (d, 1H, Tp), 7.65 (d, 1H, Tp), 7.59 (d, 1H, Tp), 7.57 (d, 1H, Tp), 7.11 (dd, J_{H-H} = 7.6, J_{H-H} = 7.6, 2H, m-Ph), 6.96 (t, J_{H-H} = 7.6, 1H, p-Ph), 6.50 (t, 1H, Tp), 6.48 (t, 1H, Tp), 6.43 (d, J_{H-H} = 7.6, 1H, o-Ph), 6.11 (t, 1H, Tp), 3.94 and 3.77 (m, 2H each, part ABCD of an ABCDX (X = ^{31}P) spin system, CH_2=CH_2), 3.28 (d, J_{H-P} = 3.2, 1H, =CHPh), 2.79 (m, 3H, PCH), 1.30 (dd, J_{H-P} = 13.6, J_{H-H} = 7.2, 9H, PCHC*H*$_3$), 1.01 (dd, J_{H-P} = 13.8, J_{H-H} = 7.2, 9H, PCHC*H*$_3$), all coupling constants for the pyrazolyl proton resonances were about 2 Hz. ^{31}P{^{1}H} NMR (161.98 MHz, CD_2Cl_2, 298 K): –6.8 (s). ^{13}C{^{1}H} NMR (75.48 MHz, CD_2Cl_2, 298 K): 326.8 (d, J_{C-P} = 10, Os=C), 148.2 (s, Tp), 145.5 (d, J_{C-P} = 2, Tp), 141.9, 139.7, 139.2, 136.3 (all s, Tp), 129.0 (s, m-Ph), 127.9 (s, o-Ph), 127.4 (s, p-Ph), 115.5 (s, =CHPh), 108.6, 108.0 (both s, Tp), 107.0 (d, J_{C-P} = 2, Tp), 59.0 (d, J_{C-P} = 2, CH_2=CH_2), 26.6 (d, J_{C-P} = 26, PCH),19.5 (d, J_{C-P} = 2, PCHC*H*$_3$), 19.4 (d, J_{C-P} = 3, PCHC*H*$_3$). HRMS (electrospray, *m*/*z*): calcd. for $C_{26}H_{37}BN_6OsP$ $[M - C_2H_4]^+$ 667.2525, found: 667.2504.

Preparation of the BPh_4 Salt of 2: Benzylidenecyclopropane (47 mg, 0.36 mmol) in fluorobenzene (15 mL) was added to a Schlenk flask with **1**-BPh_4 (200 mg, 0.20 mmol). After 1 h the solvent was removed *in vacuo*. Dichloromethane (15 mL) was added and the mixture filtered through Celite and concentrated to ca. 1 mL. Subsequent addition of diethyl ether (10 mL) caused the formation of an oil which was washed with diethyl

ether (3 x 10 mL) and vacuum-dried. Dark purple solid. Yield: 114 mg (56 %). The ^{31}P and ^{1}H NMR data were identical to those reported for **2** except the additional ^{1}H signals of BPh_4^-.

Preparation of [OsTp(η^2-CH_2=CH_2)(=C=$CHCH_2CH_2Ph$)(P^iPr_3)]BF_4 (3): This complex was prepared as described for **2** (method a), starting from 150 mg of **1** (0.20 mmol) and 37 mg of 3-phenylpropylidenecyclopropane (0.23 mmol). Pink solid. Yield: 126 mg (80 %). Anal. Calcd for $C_{30}H_{45}B_2F_4N_6OsP$: C, 44.57; H, 5.61; N, 10.39. Found: C, 44.72; H, 5.19; N, 10.49. IR (ATR, cm^{-1}): *ν*(BH) 2488 (w), *ν*(C=C) 1672 (m), *ν*(BF_4) 1043 (vs). ^{1}H NMR (400 MHz, CD_2Cl_2, 298 K): 8.06 (d, 1H, Tp), 7.90 (d, 1H, Tp), 7.89 (d, 1H, Tp), 7.57 (d, 1H, Tp), 7.51 (d, 1H, Tp), 7.48 (d, 1H, Tp), 7.31 (dd, J_{H-H} = 7.2, J_{H-H} = 7.2, 2H, m-Ph), 7.24 (t, J_{H-H} = 7.2, 1H, p-Ph), 7.14 (d, J_{H-H} = 7.2, 1H, o-Ph), 6.42 (t, 1H, Tp), 6.41 (t, 1H, Tp), 6.20 (t, 1H, Tp), 3.62 and 3.49 (m, 2H each, ABCD of an ABCDX (X = ^{31}P) spin system, CH_2=CH_2), 2.97 (m, 1H, CHC*H*$_2$), 2.89 (m, 1H, CHC*H*$_2$), 2.62 (m, 5H, 3H PCH + 2H C*H*$_2$Ph), 2.21 (ddd, J_{H-H} = 8.2, J_{H-H} = 8.2, J_{H-P} = 3.6, 1H, CH), 1.17 (dd, J_{H-P} = 13.6, J_{H-H} = 7.0, 9H, PCHC*H*$_3$), 0.91 (dd, J_{H-P} = 13.6, J_{H-H} = 7.0, 9H, PCHC*H*$_3$), all coupling constants for the pyrazolyl proton resonances were about 2 Hz. $^{31}P\{^{1}H\}$ NMR (161.98 MHz, CD_2Cl_2, 298 K): –4.0 (s). $^{13}C\{^{1}H\}$ NMR (75.48 MHz, CD_2Cl_2, 298 K): 319.6 (d, J_{C-P} = 9, Os=C), 147.4, 144.8, 142.2 (all s, Tp), 141.2 (s, Cipso), 139.7, 139.1, 136.0 (all s, Tp), 129.2 (s, o-Ph), 129.0 (s, m-Ph), 126.9 (s, p-Ph), 108.6 (s, =CH), 108.4, 107.9 (both s, Tp), 57.1 (d, J_{C-P} = 2, Tp), 57.1 (d, J_{C-P} = 2, CH_2=CH_2), 39.5 (s, CH_2Ph), 26.4 (d, J_{C-P} = 26, PCH), 19.5 (d, J_{C-P} = 2, PCHC*H*$_3$), 19.3 (d, J_{C-P} = 2, PCHC*H*$_3$), 17.3 (d, J_{C-P} = 1, CHC*H*$_2$). HRMS (electrospray, *m*/*z*): calcd. for $C_{28}H_{41}BN_6OsP$ [M – C_2H_4]$^+$ 695.2838, found: 695.2837.

Preparation of [OsTp(κ^1-$OCMe_2$)(η^2-CH_2=CH_2)(P^iPr_3)]BF_4 (4): A solution of **1** (300 mg, 0.39 mmol) in 7 mL of acetone was connected to an ethylene reservoir and the

argon atmosphere was replaced by ethylene (1 atm). After 2 h the resulting yellow solution was concentrated to ca. 0.5 mL. Diethyl ether (7 mL) was added, causing the precipitation of a yellow solid which was washed with diethyl ether (2 x 7 mL) and vacuum-dried. Yield: 251 mg (87 %). Anal. Calcd for $C_{23}H_{41}B_2F_4N_6OOsP$: C, 37.51; H, 5.61; N, 11.41. Found: C, 37.43; H, 5.49; N, 11.37. IR (ATR, cm^{-1}): *ν*(BH) 2495 (w), *ν*(CO) 1637 (m), *ν*(BF_4) 1034 (vs). ^{1}H NMR (400 MHz, CD_3COCD_3, 298 K): 8.30 (d, 1H Tp), 8.18 (d, 1H, Tp), 8.00 (m, 4H, Tp), 6.66 (t, 1H, Tp), 6.44 (t, 1H, Tp), 6.41 (t, 1H, Tp), 4.30 and 4.21 (m, 2H each, part ABCD of an ABCDX (X = ^{31}P) spin system, CH_2=CH_2), 2.99 (m, 3H, PCH), 2.21 (s, 6H, $(CH_3)_2CO$), 1.36 (dd, J_{H-P} = 12.0, J_{H-H} = 7.2, 9H, PCHC*H*$_3$), 1.20 (dd, J_{H-P} = 12.4, J_{H-H} = 7.2, 9H, PCHC*H*$_3$), all coupling constants for the pyrazolyl proton resonances were about 2 Hz. ^{31}P{^{1}H} NMR (161.98 MHz, CD_3COCD_3, 298 K): –23.3 (s). ^{13}C{^{1}H} NMR (100.63 MHz, CD_3COCD_3, 298 K): 207.1 (s, CO), 149.2, 148.1 (all s, Tp), 142.9 (d, J_{C-P} = 2, Tp), 139.7, 139.1, 137.8, 109.3, 108.7 (all s, Tp), 108.3 (d, J_{C-P} = 2, Tp), 57.2 (s, CH_2=CH_2), 30.8 (s, (*C*$H_3)_2CO$), 27.4 (d, J_{C-P} = 25, PCH), 21.2 (s, PCH*C*H_3), 21.1(d, J_{C-P} = 3, PCH*C*H_3). HRMS (electrospray, *m*/*z*): calcd. for $C_{20}H_{35}BN_6OsP$ [M – $(CH_3)_2CO]^+$ 593.2367, found: 593.2405; calcd. for $C_{18}H_{31}BN_6OsP$ [M – $(CH_3)_2CO$ – $C_2H_4]^+$ 565.2064, found: 565.2097.

Preparation of **[OsTp(*κ*^{1}-OCMe$_2$)(=C=CHPh)(P^{i}Pr$_3$)]BF$_4$ (5):** Phenylacetylene (22 μL, 0.20 mmol) was added to a solution of **1** (120 mg, 0.16 mmol) in 8 mL of acetone and stirred at room temperature for 90 min. This solution was then concentrated to ca. 1 mL. Subsequent addition of diethyl ether (10 mL) caused the apparition of a brown oil which was washed with diethyl ether (3 x 7 mL) and dried *in vacuo*. Light brown solid. Yield: 88 mg (69 %). Anal. Calcd for $C_{29}H_{43}B_2F_4N_6OOsP$: C, 42.97; H, 5.35; N, 10.37.

Found: C, 42.90; H, 5.37; N, 10.19. IR (ATR, cm^{-1}): *ν*(BH) 2515 (w), *ν*(CO) 1628 (m), *ν*(BF_4) 1039 (vs). ^{1}H NMR (400 MHz, CD_3COCD_3, 298 K): 8.38 (d, 1H, Tp), 8.31 (d, 1H, Tp), 8.16 (d, 1H, Tp), 8.05 (d, 1H, Tp), 8.01 (d, 1H, Tp), 7.66 (d, 1H, Tp), 7.25 (dd, J_{H-H} = 7.8, J_{H-H} = 7.8, 2H, m-Ph), 6.96 (tt, J_{H-H} = 7.8, J_{H-H} = 1.2, 1H, p-Ph), 6.82 (dd, J_{H-H} = 7.8, J_{H-H} = 1.2, 2H, o-Ph), 6.75 (t, 1H, Tp), 6.48 (t, 1H, Tp), 6.36 (t, 1H, Tp), 3.38 (d, J_{H-P} = 2.8, 1H, CHPh), 2.96 (m, 3H, PCH), 2.21 (s, 6H, $(CH_3)_2CO$), 1.34 (dd, J_{H-P} = 13.2, J_{H-H} = 7.2, 9H, PCHC*H*$_3$), 1.33 (dd, J_{H-P} = 13.4, J_{H-H} = 7.2, 9H, PCHC*H*$_3$), all coupling constants for the pyrazolyl proton resonances were about 2 Hz. ^{31}P{^{1}H} NMR (121.49 MHz, CD_3COCD_3, 298 K): –2.1 (s). ^{13}C{^{1}H} NMR (75.48 MHz, CD_3COCD_3, 298 K): 323.4 (d, J_{C-P} = 11, Os=C), 206.7 (s, CO), 150.7, 146.6, 146.1, 140.9, 139.7, 137.8 (all s, Tp), 130.1 (s, m-Ph), 127.8 (s, o-Ph), 127.3 (s, p-Ph), 126.7 (s, Cipso), 117.0 (s, CHPh), 109.8, 109.3 (both s, Tp), 108.8 (d, J_{C-P} = 2, Tp), 31.6 (s, (*C*$H_3)_2CO$), 27.5 (d, J_{C-P} = 27, PCH), 21.0 (s, PCHC*H*$_3$), 20.5 (d, J_{C-P} = 2, PCHC*H*$_3$). HRMS (electrospray, m/z): calcd. for $C_{26}H_{37}BN_6OsP$ $[M-(CH_3)_2CO]^+$ 667.2525, found: 667.2555.

Structural Analysis of Complexes 2, 4, and 5. Crystals suitable for the X-ray diffraction study were obtained by slow diffusion of diethyl ether (**2**, **4**) or pentane (**5**) into concentrated solutions of the complexes in fluorobenzene (**2**) or acetone (**4**, **5**). 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 40 mA. Data were collected over the complete sphere by a combination of four sets. Each frame exposure time was 10 s covering 0.3^o in ω. Data were corrected for absorption by using a multiscan method applied with the SADABS program.[4] The structures of all compounds were solved by the Patterson method. 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 hydrogen atoms were observed or calculated and refined freely or using a restricted riding model. All the highest electronic residuals were observed in close proximity of the Os centers and make no chemical sense.

Crystal data for **2**: $C_{28}H_{41}BN_6OsP$ x $C_{24}H_{20}B$ x $C_4H_{10}O$, M_W 1086.98, violet, irregular block (0.10 x 0.10 x 0.08), triclinic, space group *P*-1, *a*: 13.1940(12) Å, *b*: 13.2046(12) Å, *c*: 17.0692(15) Å, α: 92.519(2)°, β: 96.857(2)°, γ: 118.8300(10)°, *V* = 2568.9(4) Å^3, *Z* = 2, D_{calc}: 1.405 g cm^{-3}, *F*(000): 1116, *T* = 120(2) K, μ = 2.558 mm^{-1}. 24537 measured reflections (2θ: 3–58°, ω scans 0.3°), 12077 unique (R_{int} = 0.0298); min./max. transm. factors 0.697/0.822. Final agreement factors were R_1 = 0.0351 (10826 observed reflections, $I > 2\sigma(I)$) and wR_2 = 0.0770; data/restraints/parameters 12077 /0/635; GoF = 1.048. Largest peak and hole 1.554 and –0.620 e/ Å^3.

Crystal data for **4**: $C_{23}H_{41}BN_6OOsP$ x BF_4, M_W 736.41, yellow, irregular block (0.14 x 0.10 x 0.08), monoclinic, space group *P*2(1)/c, *a*: 10.832(3) Å, *b*: 16.129(5) Å, *c*: 16.280(5) Å, β: 97.185(5)°, *V* = 2822.0(14) Å^3, *Z* = 4, D_{calc}: 1.733 g cm^{-3}, *F*(000): 1464, *T* = 100(2) K, μ = 4.631 mm^{-1}. 34973 measured reflections (2θ: 3–58°, ω scans 0.3°), 7041 unique (R_{int} = 0.0543); min./max. transm. factors 0.516/0.697. Final agreement factors were R_1 = 0.0298 (5103 observed reflections, $I > 2\sigma(I)$) and wR_2 = 0.0514; data/restraints/parameters 7041/1/370; GoF = 0.838. Largest peak and hole 1.881 and –0.955 e/ Å^3.

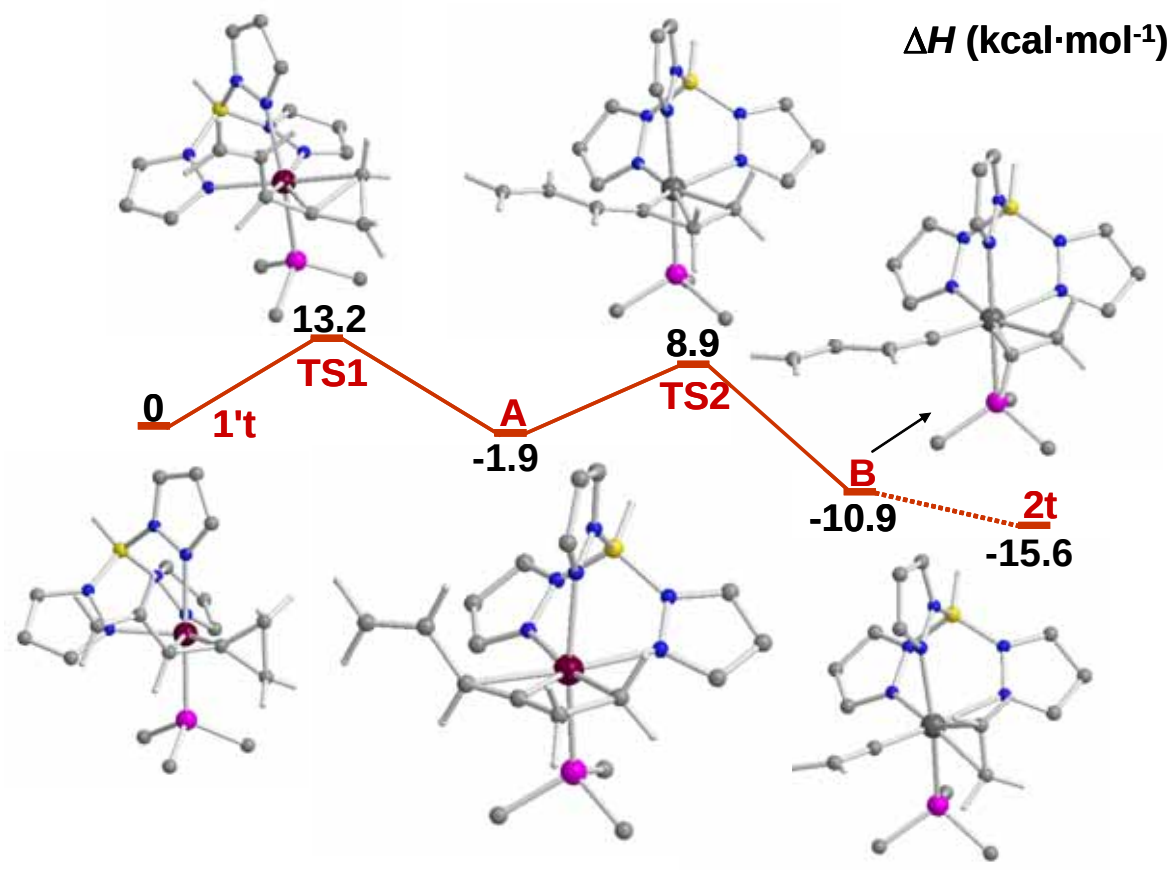
Crystal data for **5**: $C_{29}H_{43}BN_6OOsP$ x BF_4 x C_3H_6O, M_W 868.56, red, irregular prism (0.18 x 0.10 x 0.08), monoclinic, space group *P*2(1)/n, *a*: 12.9099(15) Å, *b*: 16.726(2) Å, *c*: 17.744(2) Å, β: 100.233(2)°, *V* = 3770.5(8) Å^3, *Z* = 4, D_{calc}: 1.530 g cm^{-3}, *F*(000): 1744, *T* = 100(2) K, μ = 3.481 mm^{-1}. 39542 measured reflections (2θ: 3–58°, ω scans 0.3°), 9314 unique (R_{int} = 0.0866); min./max. transm. factors 0.446/ 0.770. Final

agreement factors were R_1 = 0.0384 (7807 observed reflections, I > 2σ(I)) and wR_2 = 0.0849; data/restraints/parameters 9314/0/449; GoF = 1.042. Largest peak and hole 1.863 and –1.356 e/ $Å^3$.

Computational details and orthogonal coordinates of the model complexes. The theoretical calculations were carried out on the model complexes by optimizing the structures at the b3pw91-DFT levels with the Gaussian 03 program.[6] The basis sets used were LANL2DZ basis and pseudopotentials for Os, and 6-31G(d,p) for the rest of atoms.

The transition states have been found by carry out potential energy surfaces of the processes following the reaction coordinates, optimized the maxima, and confirmed by frequency calculations. The connections between the starting and final reactants have been checked by slightly perturbing the TS geometry towards the minima geometries and reoptimizing.

The numerical values shown in the schemes corresponds to calculated enthalpies.[7]



1't

Os	-0.31061800	-0.05051200	-0.34650100
P	-2.25106400	1.18627200	0.14926000
N	1.52122700	-1.05079600	-0.85538000
N	2.67480500	-0.58493100	-0.31860400
N	0.78441900	1.70562200	-0.69843400
N	2.05561400	1.81324100	-0.25008900
N	0.39474700	0.06921700	1.55738100
N	1.69616400	0.38836900	1.75975500
B	2.65229800	0.65700000	0.57931700
H	3.74775700	0.93099600	0.97586300
C	-0.39916100	-2.94551700	0.99348600
C	-1.30377800	-1.95593200	0.41534600
H	-2.15880400	-1.70238100	1.03871700
C	-1.42335700	-1.73672600	-0.97809900
C	-1.35130300	-2.62704700	-2.16447400
H	-1.39327000	-3.70248800	-2.00647000
H	-0.79519600	-2.32357300	-3.04861100
C	-2.60385100	-1.79481000	-1.88532900
H	-2.79021600	-0.99613400	-2.59951500
H	-3.50111400	-2.30196400	-1.53758600
C	1.85502900	-2.09245900	-1.63410500
H	1.09682500	-2.64209300	-2.16617400
C	3.23446000	-2.30261200	-1.60037600
H	3.79960800	-3.06068100	-2.12059300
C	3.71599500	-1.32027400	-0.75121000
H	4.72088200	-1.09157700	-0.42699300
C	0.53773900	2.79910300	-1.44417700
H	-0.42249100	2.93720100	-1.91686300
C	1.66468600	3.61731300	-1.48062300
H	1.78121200	4.55910200	-1.99449600
C	2.60265400	2.95433800	-0.70049700
H	3.61582200	3.21928700	-0.43466300
C	-0.17300500	-0.09597800	2.76081500
H	-1.20896500	-0.38275200	2.84252300
C	0.76903700	0.13792400	3.76215900
H	0.62071300	0.08386200	4.82962800
C	1.93774100	0.44091500	3.08314200
H	2.92446800	0.68976300	3.44506400
H	0.43164000	-3.27801500	0.37658200
C	-1.94390800	2.66011800	1.19960000
H	-1.25185100	3.33888300	0.69700100
H	-2.87805800	3.18906300	1.40849000
H	-1.48792500	2.35012500	2.14310700
C	-3.65571100	0.37577600	1.02135100
H	-4.47639800	1.08999100	1.13617100
H	-4.01730600	-0.48110500	0.44808100
H	-3.36033100	0.03531100	2.01676500
C	-3.14323200	1.89401100	-1.30017000
H	-3.97936600	2.51322600	-0.96126600
H	-2.48696200	2.51171500	-1.91634100
H	-3.53850300	1.08752000	-1.92146000
C	-0.56685800	-3.47257200	2.21466300
H	0.10407900	-4.23270500	2.60148300
H	-1.39273400	-3.17925900	2.85874000

SCF Done: E(RB+HF-PW91) = -1487.44104970 A.U. after 1 cycle

Zero-point correction=	0.442535 (Hartree/Particle)
Thermal correction to Energy=	0.470340
Thermal correction to Enthalpy=	0.471284
Thermal correction to Gibbs Free Energy=	0.386118
Sum of electronic and zero-point Energies=	-1486.998515
Sum of electronic and thermal Energies=	-1486.970710
Sum of electronic and thermal Enthalpies=	-1486.969765
Sum of electronic and thermal Free Energies=	-1487.054931

negative frequencies 0

A

Os	-0.34916300	-0.16976100	-0.41080700
P	-2.43582000	0.61518400	0.43844400
N	1.68317800	-0.53124300	-0.95282100
N	2.68861200	0.01989100	-0.23676000
N	0.37981100	1.85595000	-0.32457000
N	1.52681100	2.13086400	0.34010100
N	0.41203300	-0.37673800	1.65201500
N	1.57112700	0.23239300	1.98758300
B	2.38545500	0.98703400	0.92821600
H	3.39814700	1.42073900	1.39664600
C	0.08815900	-3.36718100	-0.07369600
C	-0.95761100	-2.34631500	-0.22974400
H	-1.82491400	-2.49078300	0.41579300
C	-1.14103000	-1.57398100	-1.38023700
C	-0.82731800	0.24138300	-2.49219700
H	0.08309700	0.44787700	-3.05972300
H	-1.54769500	1.04346000	-2.66252100
C	-1.40949000	-1.16440600	-2.76095500
H	-2.47604100	-1.21084600	-3.02221200
H	-0.89231500	-1.79048000	-3.50217700
C	2.24147000	-1.21418800	-1.96178300
H	1.62705700	-1.73783800	-2.67979400
C	3.63259800	-1.11505400	-1.89422300
H	4.35921500	-1.55794200	-2.55789100
C	3.87119800	-0.31740700	-0.78739900
H	4.79517700	0.03759700	-0.35507000
C	-0.04125700	3.00218000	-0.87839900
H	-0.93231400	3.02135300	-1.48704700
C	0.83535300	4.03906500	-0.55903300
H	0.76889300	5.07544500	-0.85257200
C	1.81997100	3.43730100	0.21062600
H	2.70912300	3.84566100	0.66868100
C	-0.01124400	-1.03249400	2.74008900
H	-0.91566900	-1.62101100	2.70660300
C	0.87813600	-0.83975000	3.80003000
H	0.81264100	-1.23769100	4.80109700
C	1.87281800	-0.03196500	3.27380400
H	2.77183200	0.36810500	3.71954700
H	0.94791200	-3.30454600	-0.73458200
C	-2.23633300	1.82896900	1.79379500
H	-1.67590700	2.69623700	1.44015300
H	-3.21775600	2.15489100	2.15007200
H	-1.68491100	1.37110200	2.61731600
C	-3.57195900	-0.63335400	1.16437800
H	-4.46494600	-0.13235200	1.54969400
H	-3.88284500	-1.35689700	0.40609200
H	-3.09583200	-1.16667100	1.98999600
C	-3.55290000	1.46160400	-0.74630100
H	-4.46891100	1.77504400	-0.23707600
H	-3.07379600	2.34483200	-1.17272700
H	-3.81629100	0.78209500	-1.56045900
C	0.01643200	-4.34524100	0.83618500
H	0.79994500	-5.09030400	0.92460700
H	-0.82943900	-4.44101600	1.51266300

SCF Done: E(RB+HF-PW91) = -1487.44310425 A.U. after 1 cycle

Zero-point correction=	0.441761 (Hartree/Particle)
Thermal correction to Energy=	0.469404
Thermal correction to Enthalpy=	0.470348
Thermal correction to Gibbs Free Energy=	0.386100
Sum of electronic and zero-point Energies=	-1487.001344
Sum of electronic and thermal Energies=	-1486.973701
Sum of electronic and thermal Enthalpies=	-1486.972757
Sum of electronic and thermal Free Energies=	-1487.057004

negative frequencies 0

B

Os	-0.22672100	0.14218200	-0.41357900
P	-1.22646300	2.19218900	0.20380000
N	0.77567700	-1.69537700	-0.88112900
N	1.92517200	-2.01960000	-0.24560400
N	1.80168500	1.00952500	-0.28927800
N	2.79602200	0.27531800	0.25760200
N	0.21030100	-0.33627300	1.58966900
N	1.38771300	-0.91270500	1.91902300
B	2.49080500	-1.10856700	0.85494100
H	3.47058800	-1.59014100	1.34630700
C	-3.70052200	-1.99060700	0.62146500
C	-3.01628600	-1.40985700	-0.53119900
H	-3.47379900	-1.54571600	-1.51300400
C	-1.88076500	-0.73643800	-0.47150000
C	0.05574300	0.75458500	-2.52470400
H	0.89755200	0.17857700	-2.89814400
H	0.14793700	1.83230600	-2.59555900
C	-1.21828500	0.17846900	-2.53705000
H	-2.10645600	0.80246700	-2.53335000
H	-1.35446500	-0.82700200	-2.92178400
C	0.48494200	-2.70981900	-1.70590900
H	-0.41339800	-2.69760400	-2.30434000
C	1.46363900	-3.70197300	-1.61473400
H	1.50974000	-4.63647100	-2.15246700
C	2.35683800	-3.22264900	-0.67147700
H	3.26425200	-3.65128900	-0.27170600
C	2.35558500	2.15708800	-0.70866500
H	1.75848100	2.91137500	-1.19942100
C	3.72175900	2.16990100	-0.42509200
H	4.43569100	2.95030100	-0.63932700
C	3.95710300	0.95106700	0.19251300
H	4.86503800	0.52024300	0.58881700
C	-0.54200800	-0.30879100	2.70140100
H	-1.54287200	0.09506500	2.67705400
C	0.16099500	-0.86699200	3.76782700
H	-0.17139700	-0.98847800	4.78729500
C	1.38381500	-1.23236000	3.22492500
H	2.25004900	-1.69334300	3.67649600
H	-3.20547300	-1.89131100	1.58440300
C	-0.37614400	3.06992300	1.57131500
H	0.65838400	3.27852000	1.28998400
H	-0.88634200	4.01014000	1.79936200
H	-0.36158500	2.44281100	2.46496200
C	-2.96748100	2.08898300	0.77945900
H	-3.34049300	3.08062100	1.05082000
H	-3.59476900	1.67090800	-0.01122400
H	-3.05036800	1.43240300	1.64837400
C	-1.35952600	3.50854300	-1.07777700
H	-1.87591900	4.37798200	-0.66059900
H	-0.37220200	3.83194500	-1.41582200
H	-1.92720300	3.15661000	-1.94315700
C	-4.87126700	-2.63563700	0.53904600
H	-5.33935700	-3.05936300	1.42092500
H	-5.39268500	-2.76426300	-0.40567900

SCF Done: E(RB+HF-PW91) = -1487.45736422 A.U. after 1 cycle

Zero-point correction=	0.440613 (Hartree/Particle)
Thermal correction to Energy=	0.469243
Thermal correction to Enthalpy=	0.470187
Thermal correction to Gibbs Free Energy=	0.382940
Sum of electronic and zero-point Energies=	-1487.016751
Sum of electronic and thermal Energies=	-1486.988121
Sum of electronic and thermal Enthalpies=	-1486.987177
Sum of electronic and thermal Free Energies=	-1487.074425

negative frequencies 0

2t

Os	0.22813900	-0.12273800	-0.46510100
P	1.12627700	-2.20682800	0.37175100
N	-0.68437100	1.80281900	-0.71551800
N	-1.86769200	2.06953400	-0.11732900
N	-1.81773000	-0.95254900	-0.46511600
N	-2.80389600	-0.25075900	0.13863500
N	-0.15703200	0.38769900	1.56184000
N	-1.39544700	0.78455000	1.93503100
B	-2.48483100	1.06168900	0.86816300
H	-3.46918900	1.51003200	1.38115200
C	3.98578200	1.71018400	0.32534900
C	3.06944100	1.25470800	-0.71528000
H	3.36728600	1.41500400	-1.75625300
C	1.90059600	0.66179800	-0.54816700
C	-0.00450200	-0.00264500	-2.66596800
H	0.57636200	0.82449000	-3.05882700
H	-1.07069500	0.04000200	-2.86779400
C	0.60321100	-1.23170600	-2.39382700
H	0.01429500	-2.13928600	-2.44630300
H	1.66807300	-1.35820400	-2.56521700
C	-0.30392000	2.91000600	-1.36278300
H	0.63037600	2.93482500	-1.90323400
C	-1.25807500	3.91504900	-1.18820400
H	-1.23963100	4.91826500	-1.58547500
C	-2.22966300	3.34000000	-0.38640300
H	-3.14830900	3.74262700	0.01471800
C	-2.39201600	-2.04688400	-0.98961500
H	-1.80751300	-2.77103500	-1.53728300
C	-3.76153700	-2.05431200	-0.72289800
H	-4.48931800	-2.79582300	-1.01468600
C	-3.97805900	-0.89223100	0.00167300
H	-4.88160700	-0.48046500	0.42730500
C	0.63325500	0.48380200	2.64188800
H	1.68198000	0.23821600	2.57600600
C	-0.10506600	0.92953300	3.73690100
H	0.24415100	1.10526200	4.74279000
C	-1.38588500	1.11636100	3.23816700
H	-2.28610000	1.47422400	3.71616000
H	3.65311700	1.59281700	1.35425800
C	0.21864100	-2.82467700	1.84180100
H	-0.83068300	-2.97705700	1.57728700
H	0.64845900	-3.77501800	2.17091100
H	0.26514800	-2.10710100	2.66182000
C	2.87463700	-2.11236300	0.91439400
H	3.20391400	-3.07989300	1.30373900
H	3.50473000	-1.82613500	0.06917500
H	2.99799200	-1.35887400	1.69449000
C	1.15234900	-3.71864100	-0.67390400
H	1.56364200	-4.54240900	-0.08351100
H	0.14297500	-3.99593200	-0.98607900
H	1.77560600	-3.58290900	-1.55944400
C	5.17922500	2.26556700	0.07831300
H	5.82155800	2.59610200	0.88733100
H	5.54751300	2.40999900	-0.93383200

SCF Done: E(RB+HF-PW91) = -1487.46508407 A.U. after 1 cycle

Zero-point correction=	0.441054 (Hartree/Particle)
Thermal correction to Energy=	0.469463
Thermal correction to Enthalpy=	0.470408
Thermal correction to Gibbs Free Energy=	0.383116
Sum of electronic and zero-point Energies=	-1487.024030
Sum of electronic and thermal Energies=	-1486.995621
Sum of electronic and thermal Enthalpies=	-1486.994676
Sum of electronic and thermal Free Energies=	-1487.081968

negative frequencies 0

TS1

Os	0.29770100	0.38282900	-0.22163100
P	2.39806500	-0.57366000	0.32707500
N	-1.81719200	0.53139200	-0.62406600
N	-2.64266300	-0.43213700	-0.14197300
N	-0.13372700	-1.58059100	-1.01833100
N	-1.10123600	-2.33519000	-0.44774700
N	-0.33824900	-0.29654800	1.68535600
N	-1.31357800	-1.22157000	1.80905900
B	-2.07750600	-1.68455200	0.56088800
H	-2.95199800	-2.44755500	0.85416000
C	-0.68361200	3.47769000	0.07616100
C	0.38900800	2.52201700	0.38810400
H	0.83573000	2.68204700	1.37253400
C	1.30219000	1.98198900	-0.55271400
C	0.92044400	1.37370300	-2.20043900
H	0.12055800	1.93087300	-2.68035500
H	1.26905300	0.52993100	-2.79157200
C	2.11432400	2.26639200	-1.70867800
H	3.06634500	1.75394500	-1.82626100
H	2.16885900	3.31319000	-2.00881200
C	-2.56899600	1.34649100	-1.37442800
H	-2.13563800	2.19496100	-1.87694100
C	-3.89874800	0.92158500	-1.37142900
H	-4.73838900	1.37944000	-1.87122800
C	-3.89733100	-0.21443200	-0.58212200
H	-4.69555000	-0.88739800	-0.30494600
C	0.35528400	-2.28006100	-2.05117600
H	1.13070300	-1.86570800	-2.67780300
C	-0.29382900	-3.51375700	-2.14699100
H	-0.12177600	-4.29716700	-2.86908100
C	-1.21930000	-3.49964000	-1.11614900
H	-1.95929200	-4.22818100	-0.81819700
C	0.00118400	0.08804900	2.92273500
H	0.75913900	0.84190500	3.07479900
C	-0.76159700	-0.60593000	3.86653200
H	-0.72111900	-0.51913900	4.94149700
C	-1.58981000	-1.42131100	3.11337900
H	-2.35781400	-2.12066600	3.40968300
H	-0.92055500	3.63372800	-0.97406300
C	2.22770200	-2.15043500	1.24378900
H	1.66660400	-2.86764600	0.64091800
H	3.21878700	-2.56053500	1.45907300
H	1.69423000	-1.98599400	2.18170500
C	3.48225600	0.43788700	1.40935600
H	4.38969400	-0.11564300	1.66783200
H	3.76459600	1.36334900	0.90103700
H	2.95793200	0.69598500	2.33184000
C	3.54314000	-1.05531600	-1.02934500
H	4.47998600	-1.42226300	-0.59946400
H	3.10217300	-1.85722000	-1.62425300
H	3.77180100	-0.21447100	-1.68632000
C	-1.32131300	4.20874900	0.99645900
H	-2.07381700	4.93800400	0.71584900
H	-1.10845800	4.10534700	2.05742000

SCF Done: E(RB+HF-PW91) = -1487.41777902 A.U. after 1 cycle

Zero-point correction=	0.440829 (Hartree/Particle)
Thermal correction to Energy=	0.468130
Thermal correction to Enthalpy=	0.469074
Thermal correction to Gibbs Free Energy=	0.384902
Sum of electronic and zero-point Energies=	-1486.976950
Sum of electronic and thermal Energies=	-1486.949649
Sum of electronic and thermal Enthalpies=	-1486.948705
Sum of electronic and thermal Free Energies=	-1487.032877

negative frequencies 1

TS2

Os	0.30894800	-0.06495500	-0.25932900
P	1.65457300	-1.93188700	0.29503700
N	-0.88266300	1.65503600	-0.66833900
N	-2.16347000	1.71882400	-0.23195300
N	-1.51634100	-1.19600400	-0.67964900
N	-2.71345700	-0.71912600	-0.27375300
N	-0.56336400	-0.07514400	1.61858900
N	-1.84946600	0.31163500	1.79964100
B	-2.76722100	0.56018000	0.57172300
H	-3.88325400	0.80984700	0.92434700
C	2.58601300	2.68704800	0.68538200
C	2.64962700	2.00317100	-0.58375000
H	3.43086200	2.33104400	-1.27620700
C	1.88060100	0.93929800	-0.94463400
C	0.64474200	-0.55258000	-2.32725000
H	-0.16508800	-0.08842000	-2.89258700
H	0.74696000	-1.60068000	-2.59711500
C	1.94563700	0.25119700	-2.30840700
H	2.83902300	-0.37578200	-2.41201200
H	1.96771100	1.01012700	-3.10441200
C	-0.63883200	2.79166400	-1.33894000
H	0.33387100	2.96611900	-1.77253400
C	-1.77367100	3.60399800	-1.33413800
H	-1.89064400	4.57733900	-1.78527800
C	-2.71712600	2.88459400	-0.61895100
H	-3.73939500	3.11820100	-0.35849800
C	-1.75295200	-2.32603600	-1.35934000
H	-0.94057200	-2.88501600	-1.79820600
C	-3.12291500	-2.59134800	-1.38691700
H	-3.62527400	-3.42526400	-1.85267400
C	-3.69557300	-1.54406600	-0.68160400
H	-4.72693900	-1.33022600	-0.44121800
C	0.00113600	-0.17039300	2.84301300
H	1.03601000	-0.45555200	2.95037300
C	-0.92662300	0.17206900	3.81707600
H	-0.78101400	0.20387000	4.88598700
C	-2.08979200	0.46128600	3.10807600
H	-3.06804100	0.76457400	3.45283500
H	1.78897600	2.38538400	1.36593200
C	0.84439500	-3.16883800	1.38733600
H	-0.03779100	-3.56999200	0.88141800
H	1.53487400	-3.98837800	1.60624000
H	0.51782200	-2.71893900	2.32593700
C	3.21424600	-1.50569800	1.16787000
H	3.77701000	-2.40943100	1.41935900
H	3.81901900	-0.86791500	0.51851200
H	3.01749800	-0.94687200	2.08561400
C	2.28459200	-3.03723500	-1.03629200
H	2.92308300	-3.80382100	-0.58733900
H	1.45948200	-3.53867600	-1.54764600
H	2.87206300	-2.48626800	-1.77302800
C	3.42961500	3.66914700	1.05230200
H	3.32004000	4.19172900	1.99683300
H	4.25376000	3.97681500	0.41343900

SCF Done: E(RB+HF-PW91) = -1487.42422733 A.U. after 1 cycle

Zero-point correction=	0.440222 (Hartree/Particle)
Thermal correction to Energy=	0.467701
Thermal correction to Enthalpy=	0.468645
Thermal correction to Gibbs Free Energy=	0.383831
Sum of electronic and zero-point Energies=	-1486.984006
Sum of electronic and thermal Energies=	-1486.956527
Sum of electronic and thermal Enthalpies=	-1486.955583
Sum of electronic and thermal Free Energies=	-1487.040396

negative frequencies 1

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