Supporting Information

Experimental and Computational Details

(POP)Rh pincer hydride complexes: unusual reactivity and selectivity in oxidative addition and olefin insertion reactions.

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General Information: All manipulations were carried out under argon, using standard Schlenk or glovebox techniques. Anhydrous grade hexane, pentane, benzene, octane, and toluene were bubbled with argon before use. C_6D_6, toluene-*d8*, *tert*-butylethylene (TBE), 1-hexene, and 1-octene were dried over NaK and vacuum distilled. Fluorobenzene was freeze-pump-thawed and distilled over CaH_2. Norbornene (NBE) was purified by sublimation. Et_2O and THF were distilled from sodium benzophenone under argon. $(CD_3)_2CO$ was dried over B_2O_3 and vacuum distilled. CD_2Cl_2 was dried over 4Å molecular sieves, freeze-pump-thawed, and stored over 4Å molecular sieves. ^1H, ^{13}C, and ^{31}P NMR were recorded on 300, 400, or 500 MHz Varian spectrometers and are reported in ppm. ^1H and ^{31}C NMR were referenced to the residual solvent signals. ^{31}P NMR were referenced to an external standard of 85% H_3PO_4. ^{tBu}xanPOP and di-*tert*-butylphosphine were purchased from Strem. 2,5-bis(hydroxymethyl)furan is commercially available from Pennakem and $[Rh(NBD)Cl]_2$ from Johnson-Matthey. ^{iPr}xanPOP[1], 2,5-bis(chloromethyl)furan[2] and $[Rh(COE)_2Cl]_2$[3] were prepared according to the literature.

Synthesis of Complexes

Synthesis of 2,5-bis((di-*tert*-butylphosphino)methyl)furan, ^{tBu}furPOP: 907 mg (5.40 mmol, 1.00 equiv) freshly prepared 2,5-bis(chloromethyl)furan was dissolved in 5.0 mL THF at room temperature. 2.00 mL (10.8 mmol, 2.00 equiv) di-*tert*-butylphosphine was added and the solution was stirred for 24 h at room temperature, leading to the formation of a yellow precipitate. The supernatant was removed via cannula filtration, and the precipitate was washed with pentane. The precipitate was suspended in MeOH and stirred with 1.00 mL Et_3N overnight. The supernatant was removed, dried in vacuo and the process was repeated twice to yield 1.04 g (2.70 mmol, 50%) of ^{tBu}furPOP as a tan oil which solidified upon standing. ^{1}H NMR (300 MHz, C_6D_6): δ 6.10 (s, 2H), 2.73 (s, 4H), 1.05 (d, $^2J_{PH}$ = 11 Hz, 36H). ^{13}C NMR (75 MHz, C_6D_6): δ 153.28 (d, J_{PC} = 18.3 Hz), 107.54 (d, J_{PC} = 7.7 Hz), 31.48 (d, J_{PC} = 24.9 Hz), 29.70 (d, J_{PC} = 13.8 Hz), 21.24 (d, J_{PC} = 25.9 Hz). ^{31}P NMR (121 MHz, C_6D_6): δ 27.6 (s).

(^{tBu}furPOP)RhCl: 23 mg (0.06 mmol) ^{tBu}furPOP and 20 mg (0.03 mmol) $[Rh(COE)_2(Cl)_2]_2$ were dissolved in 2 mL benzene and stored at room temperature overnight. The solvent was removed in vacuo and the light orange residue was extracted with 5 mL pentane. Removal of the pentane in vacuo afforded the title compound in 87% yield. Orange crystals suitable for X-ray diffraction were obtained by recrystallization from pentane. ^{1}H NMR (500 MHz, C_6D_6): δ 5.51 (s, 2H), 2.26 (s, 4H), 1.44 (vt, J_{PH} = 5.16 Hz, 36H). ^{13}C NMR (125 MHz, C_6D_6): δ 158.77, 104.82, 35.34 (t, J_{PC} = 5.1 Hz), 29.30 (t, J_{PC} = 3.7 Hz), 21.52 (t, J_{PC} = 2.8 Hz). ^{31}P NMR (C_6D_6, 202 MHz): δ 56.9 (d, J_{RhP} = 141 Hz).

***cis*-(^{tBu}furPOP)Rh(H)$_2$Cl:** 15 mg (0.04 mmol) (^{tBu}furPOP)RhCl is dissolved in 1 mL C_6D_6 in a J-Young tube to give a light orange solution. The solution is frozen, and the headspace evacuated and refilled with 1 atm H_2. The solution is gently warmed to room temperature, and the tube is shaken on an agitator table for 24 h. NMR indicates the formation of the *cis* and *trans* hydrides in a 7:3 ratio. The solvent replaced with toluene-d_8 and the mixture is heated under 1 atm H_2 at 110°C for 2h, yielding the *cis* dihydride quantitatively.

Alternatively, 77 mg (0.2 mmol) ^{tBu}furPOP and 0.1 mmol $[Rh(NBD)Cl]_2$ were dissolved in 5 mL toluene and refluxed for 48 h under H_2 bubbling, yielding a red solution. The solvent was removed in vacuo and the residue redissolved in 2 mL benzene. Addition of 2 mL pentane caused the precipitation of 54 mg of a yellow solid, 51% yield of the title compound. Data for the *cis* complex: ^{1}H NMR (400 MHz, C_6D_6): δ 6.77 (s, 2H), 3.64 (s, 4H), 1.33 (vt, J_{PH} = 5.3 Hz), -22.40 (m, 2H). ^{13}C NMR (100 MHz, C_6D_6): δ 148.98, 107.59, 27.01 (m), 26.79 (m), 22.93. ^{31}P NMR (162 MHz, C_6D_6) δ 73.4 (d, J_{RhP} = 120 Hz). Selected data for the *trans* complex: ^{1}H NMR (400 MHz, C_6D_6): δ -22.59 (dt, J_{PH} = 16 Hz, J_{RhH} = 24 Hz).

(^{tBu}xanPOP)RhCl: 30 mg (0.06 mmol) ^{tBu}xanPOP and 20 mg (0.03 mmol) $[Rh(COE)_2Cl]_2$ were dissolved in 2 mL benzene and stored at room temperature overnight. The solvent was removed in vacuo and the light orange residue was extracted with 5 mL pentane. Removal of the pentane in vacuo afforded the title compound in 93% yield. Dark orange rods suitable for X-ray diffraction were obtained by slow evaporation from pentane. ^{1}H NMR (500 MHz, C_6D_6): δ 7.77 (m, 2H), 6.99 (m, 2H), 6.78 (m, 2H), 1.67 (vt, J_{PH} = 6.8 Hz, 36H), 1.15 (s, 6H). ^{13}C NMR (126 MHz, C_6D_6): δ 158.71, 133.90, 131.15, 125.65, 123.58, 37.44, 33.64, 32.32 ^{31}P NMR (202 MHz, C_6D_6): δ 48.8 (d, J_{RhP} = 141 Hz)

***cis*-(^{tBu}xanPOP)Rh(H)$_2$Cl:** 15 mg (^{tBu}xanPOP)RhCl is dissolved in 1 mL C_6D_6 in a J-Young tube to give an orange solution. The solution is frozen, and the headspace evacuated and refilled with 1 atm H_2. The solution is gently warmed to room temperature, and the tube is shaken for 24 h on an agitator table. During the reaction, the solution becomes yellow. NMR indicates full conversion into the title complex. Removal of the solvent affords the title compound as a yellow solid in quantitative yield. Orange needles suitable for X-ray diffraction were grown by slow diffusion of pentane into an acetone solution of the title compound.

Alternatively, a convenient one-pot preparation can be used for large scale reactions. 250 mg ^{tBu}xanPOP (0.50 mmol) and 175 mg $[Rh(COE)_2Cl]_2$ (0.50 mmol Rh) were dissolved in 5 mL benzene and stirred overnight. The resulting dark-red solution was gently bubbled with H_2 for 2 h at room temperature, causing the solution to become light orange. The solvent was removed in vacuo, affording the title

complex as a yellow solid in quantitative yield. ^{1}H NMR (C_6D_6, 300 MHz): δ 7.49-7.44 (m, 2H), 7.06 (dd, J = 3.2 Hz, J = 1.6 Hz, 2H), 6.86 (t, J_{PH} = 7.8 Hz, 2H), 1.76 (vt, J_{PH} = 7.0 Hz, 18H), 1.30 (vt, J_{PH} = 7.0 Hz, 18H), 1.23 (s, 3H), 1.20 (s, 3H), -17.02 (dtd, J_{RhH} = 23 Hz, J_{PH} = 14 Hz, J_{HH} = 9.2 Hz, 1H), -20.51 (dtd, J_{RhH} = 29 Hz, J_{PH} = 12 Hz, J_{HH} = 9.2 Hz, 1H). ^{13}C NMR (C_6D_6, 126 MHz): δ 156.03 (t, J_{PC} = 6.5 Hz), 133.89, 132.71, 132.23 (t, J_{PC} = 2.5 Hz), 124.94 (t, J_{PC} = 8.6 Hz), 123.40 (t, J_{PC} = 2.1 Hz), 38.00 (t, J_{PC} = 5.6 Hz), 36.37 (m), 34.68 (m), 32.21, 30.27, 29.78 (m). ^{31}P NMR (C_6D_6, 162 MHz): δ 79.1 (dt, J_{RhP} = 118 Hz, J_{HP} = 10 Hz). Analysis for $C_{31}H_{52}ClOP_2Rh$: calculated C 58.08, H 8.18. Found C 57.72, H 7.71.

[(^{tBu}xanPOP)Rh(H)$_2$]SbF$_6$/BF$_4$: 64 mg (0.15 mmol) *cis*-(^{tBu}xanPOP)Rh(H)$_2$Cl was dissolved in 3 mL acetone in a glass vial wrapped in aluminum foil. A solution of 34 mg (0.15 mmol) $AgSbF_6$ in 1 mL acetone was added dropwise and the reaction was stirred at room temperature. Over 30 min the reaction turns from yellow to orange and a grey precipitate forms. The solution is decanted, filtered to remove AgCl, and dried in vacuo to give the title complex as an orange solid in quantitative yield. The BF_4 salt is prepared similarly and has identical spectral data for the cation. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.85-7.80 (comp, 4H), 7.52 (m, 2H), 1.75 (s, 6H), 1.41 (vt, J_{PH} = 8.0 Hz, 36H), -21.53 (dt, J_{PH} = 12 Hz, J_{RhH} = 43 Hz). ^{13}C NMR (CD_2Cl_2, 100 MHz): δ 165.11, 133.70, 132.54, 126.48, 119.99, 36.96, 32.20, 30.81, 30.25. ^{31}P NMR (CD_2Cl_2, 162 MHz): δ 80.1 (dt, J_{HP} = 11 Hz, J_{RhP} = 111 Hz). Analysis for {[(^{tBu}xanPOP)Rh(H)$_2$] BF_4}*½(CH_2Cl_2), $C_{31.5}H_{53}BF_4OP_2Rh$: calculated C 51.48, H 7.57. Found C 51.80, H 6.79. Alternatively, H_2 is bubbled through an acetone solution of [(^{tBu}xanPOP)Rh(C_2H_4)]BF_4 or [(^{tBu}xanPOP)Rh(C_2H_4)]SbF_6 for 1 h. NMR shows quantitative formation of [(^{tBu}xanPOP)Rh(C_2H_4)]$^+$. Crystals suitable for X-ray diffraction were obtained by layering a solution of the title complex with pentane.

[(^{tBu}xanPOP)Rh(C_2H_4)]SbF$_6$/BF$_4$: 18 mg (0.025 mmol) $[Rh(COE)_2Cl]_2$ and 10 mg (0.05 mmol) $AgBF_4$ were dissolved in 2 mL acetone and stirred for 30 min at room temperature in a foil-wrapped vial. The solution is filtered and added to a solution of 25 mg (0.05 mmol) ^{tBu}xanPOP in 1 mL acetone. Ethylene is slowly passed through the solution for 24h. After removal of the solvent, the product is titurated with benzene to afford the title complex in 80% yield. The PF_6 salt is prepared similarly and has identical

spectral data for the cation. ^{1}H NMR (400 MHz, acetone-d_6): δ 8.11-8.04 (comp, 4H), 7.57 (m, 2H), 3.95 (m, 4H), 1.81 (s, 6H), 1.52 (vt, J_{PH} = 14 Hz, 36H). ^{13}C NMR (acetone-d_6, 100 MHz): δ 165.11, 134.54, 131.87, 130.04, 128.49, 126.18, 43.10, 38.47 (dt, J_{PC} = 6.6 Hz, J_{RhC} = 71 Hz), 32.90, 30.43, 29.95. ^{31}P NMR (acetone-d_6, 162 MHz): δ 55.3 (d, J_{RhP} = 158 Hz).

Alternatively, ethylene is bubbled through an acetone solution of [(^{tBu}xanPOP)Rh(H_2)]BF_4 or [(^{tBu}xanPOP)Rh(H_2)]SbF_6 for 12h, affording the title complex in near quantitative yield.

[(^{tBu}furPOP)Rh(H)$_2$]SbF_6: *cis*-(^{tBu}furPOP)Rh(H)$_2$Cl or a *cis/trans* mixture was converted into the title complex in quantitative yield, following the same procedure as for [(^{tBu}xanPOP)Rh(H)$_2$]SbF_6. The complex is a red solid. ^{1}H NMR (300 MHz, CD_2Cl_2): δ 6.26 (s, 2H), 3.28 (vt, J_{PH} = 3.3 Hz, 4H), 1.30 (vt, J_{PH} = 7.3 Hz, 36H), -20.12 (dt, J_{RhH} = 39 Hz, J_{PH} = 10 Hz, 2H). ^{13}C NMR (75 MHz, CD_2Cl_2): δ 127.76 (t, J_{PC} = 25 Hz), 108.89, 35.38 (t, J_{PC} = 8.3 Hz), 28.57 (t, J_{PC} = 3.3 Hz), 21.88 (t, J_{PC} = 6.6 Hz). ^{31}P NMR (CD_2Cl_2, 162 MHz): δ 83.9 (d, J_{RhP} = 113 Hz).

Attempted reaction of (^{tBu}PNP)RhCl with H_2: (^{tBu}PNP)RhCl was prepared according to the literature[4] and refluxed in toluene under H_2 bubbling for 48h. The title compound was recovered after removal of solvent. No hydrides were detected from 0 to -50 ppm in C_6D_6.

[*cis*-(^{tBu}xanPOP)Rh(H)$_2$(OH_2)]SbF_6: 10 mg of [(^{tBu}xanPOP)Rh(H)$_2$]SbF_6 was dissolved in undried CD_2Cl_2. Slow diffusion of pentane into this solution afforded crystals suitable for X-Ray diffraction. Selected NMR data: ^{1}H NMR (400 MHz, CD_2Cl_2): δ -9 ppm (br s).

(^{tBu}xanPOP)RhH: 20 mg *cis*-(^{tBu}xanPOP)Rh(H)$_2$Cl (0.031 mmol) was dissolved in 1 mL C_6D_6. 5 mg KO^{t}Bu was added and the orange solution immediately turned dark red. After 30 min, the solution was filtered through celite and characterized by NMR. The solvent was removed in vacuo, the residue extracted with pentane, and the pentane removed in vacuo to give the title complex as a red powder in 90% yield. ^{1}H NMR (300 MHz, C_6D_6): δ 7.78 (d, J = 6.6 Hz, 2H), 7.11 (d, J = 7.8 Hz, 2H), 6.90 (t, J = 7.5 Hz, 2H), 1.56 (vt, J_{PH} = 6.3 Hz, 36H), 1.28 (s, 6H), -18.95 (dt, J_{PH} = 18.9 Hz, J_{RhH} = 36.9 Hz, 1H). ^{13}C

NMR (75 MHz, C_6D_6): δ 157.19, 132.55 (m), 131.154, 126.28, 122.92, 121.647, 35.53 (m), 34.14, 33.09, 31.31 (m). ^{31}P NMR (121 MHz, C_6D_6): δ 78.0 (dd, J_{HP} = 18.3 Hz, J_{RhP} = 173 Hz).

(^{tBu}xanPOP)RhEt: 15 mg (0.025 mmol) (^{tBu}xanPOP)RhH was dissolved in C_6D_6 in a J-Young NMR tube. The solution was frozen, the headspace evacuated and replaced with 1 atm ethylene. The solution was allowed to thaw and NMR was immediately recorded (~1 min reaction time). ^{1}H NMR (300 MHz, C_6D_6): δ 7.81 (m, 2H), 7.08, (m, 2H), 6.86 (t, J = 6.0 Hz, 2H), 2.21 (qd, J = 7.5 Hz and J_{RhH} = 2.4 Hz, 2H), 1.85 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, C_6D_6): δ 158.69, 133.18, 132.03, 132.29, 131.27, 125.15, 38.01, 37.74, 34.54, 31.43, 30.68, 18.32. ^{31}P NMR (121 MHz, C_6D_6): δ 46.3 (d, J_{RhP} = 194 Hz)

(^{iPr}xanPOP)RhH$_2$Cl: To an orange solution of 70 mg (0.20 mmol) [Rh(COE)$_2$Cl]$_2$ in 2 mL pentane is added 88 mg (0.2 mmol) ^{iPr}xanPOP in 10 mL pentane. The reaction mixture immediately becomes dark red, and is stirred at 25°C for 12 hours, resulting in the quantitative formation of (^{iPr}xanPOP)RhCl (^{31}P NMR (C_6H_6, 121 MHz): δ 38 ppm, d, J_{RhP} = 147 Hz). An additional 5 mL pentane is added, and the solution is bubbled with H_2 at 25°C. After 4h, the solution had turned light orange. Removal of the solvent afforded the title complex, as a 1:1 mixture of the monomer and dimer in quantitative yield. Selected NMR data for the monomeric product: ^{1}H NMR (C_6D_6, 300 MHz): δ -17.46 (dtd, J_{HH} = 9.9 Hz, J_{PH} = 15 Hz, J_{RhH} = 24 Hz, 1H), -20.07 (dtd, J_{HH} = 9.9 Hz, J_{PH} = 14 Hz, J_{RhH} = 28 Hz, 1H). ^{31}P NMR (121 MHz, C_6D_6): δ 67.0 (dt, J_{HP} = 14 Hz, J_{RhP} = 115 Hz). Selected NMR data for the dimeric product: ^{1}H NMR (C_6D_6, 300 MHz): δ -22.03 (comp). ^{31}P NMR (121 MHz, C_6D_6): δ 61.5 (br d, J_{RhP} = 122 Hz).

[(^{iPr}xanPOP)Rh(H)$_2$]B(C$_6$F$_5$)$_4$: 0.1 mmol (^{iPr}xanPOP)RhH$_2$Cl was dissolved in 0.6 mL CD_2Cl_2 to give an orange solution. 0.1 mmol Li[B(C$_6$F$_5$)$_4$]*OEt$_2$ was added and the solution was kept at 25 °C for 12 h, yielding a red solution with a colorless precipitate. NMR indicated complete conversion into the title species, which was isolated as a red solid after filtration and drying in vacuo. ^{1}H NMR (CD_2Cl_2, 400 MHz): δ -23.93 (dt, J_{PH} = 15 Hz, J_{RhH} 44 Hz, 1H). ^{31}P NMR (CD_2Cl_2, 162 MHz): δ 79.3 (d, J_{RhP} = 206 Hz).

COMPUTATIONAL METHODS

DFT calculations[5] employed the M06-L exchange-correlation functionals[6] and the SDD-model effective core potentials/basis sets on all atoms.[7] Calculations were performed on the actual molecular species used in the experiments, where pincers retained their bulky *t*Bu groups on P, and on truncated model complexes (PR_2 = PH_2). Standard procedures were employed to obtain the geometries and electronic energies for stationary points on the potential energy surfaces. Normal mode analysis was performed for each species and the resulting set of vibrational frequencies was employed (without scaling) to determine zero-point energy corrections. Enthalpies (ΔH, $\Delta H^{\ddagger}$) and Gibbs' free energies (ΔG, $\Delta G^{\ddagger}$; T = 298.15 K, P = 1 atm) were obtained from the potential energies (ΔE, $\Delta E^{\ddagger}$) using standard thermodynamic corrections.[8] All calculations have been performed using the Gaussian09 collection of computer programs.[9]

Optimized geometries and absolute energies of molecular species relevant to the reactions of (^{tBu}xanPOP)RhX (X = Cl, H) and (^{tBu}xanPOP)Rh$^+$ with H_2.

(tBuxanPOP)RhH

Charge = 0 Multiplicity = 1
Rh,0,-0.000011,-1.240756,-0.0471
P,0,2.278441,-0.969848,-0.010203
O,0,0.000013,0.994239,-0.058758
P,0,-2.278458,-0.969795,-0.010197
C,0,1.23439,1.697382,-0.030842
C,0,2.409255,0.908884,-0.014509
C,0,3.639255,1.584297,0.040529
C,0,3.703891,2.982854,0.05867
C,0,2.520727,3.724281,0.027005
C,0,1.261077,3.100353,-0.011889
C,0,-1.234348,1.697411,-0.030852
C,0,-2.409233,0.908939,-0.014526
C,0,-3.639218,1.584384,0.040485
C,0,-3.703819,2.982944,0.058621
C,0,-2.520637,3.72434,0.026973
C,0,-1.261002,3.100383,-0.011903
C,0,0.000048,3.96022,-0.03388
H,0,4.555059,1.00613,0.075586
H,0,4.663724,3.484397,0.099228
H,0,2.568978,4.809587,0.038013
H,0,-4.555037,1.006242,0.075524
H,0,-4.663641,3.484509,0.09916
H,0,-2.568862,4.809648,0.037975
C,0,0.000053,4.895387,1.203668
C,0,0.000066,4.826029,-1.321476
H,0,0.00004,4.314397,2.129599
H,0,0.882921,5.541285,1.202017
H,0,-0.882796,5.54131,1.202007
H,0,0.88566,5.468333,-1.352617
H,0,0.000062,4.195848,-2.214737
H,0,-0.885509,5.468358,-1.352626
C,0,3.262955,-1.533121,-1.59368
C,0,3.203105,-1.503306,1.625688
C,0,-3.203115,-1.503243,1.625693
C,0,-3.263017,-1.533089,-1.593631
C,0,2.720379,-2.93273,1.942126
H,0,3.072759,-3.661569,1.205574
H,0,3.103561,-3.232713,2.926608
H,0,1.62598,-2.971454,1.953463
C,0,4.736331,-1.469802,1.577011
H,0,5.129993,-0.469434,1.366406
H,0,5.13077,-1.773646,2.556105
H,0,5.138225,-2.167154,0.834112
C,0,2.681121,-0.554924,2.721403
H,0,3.015335,-0.914666,3.702532
H,0,3.049397,0.467221,2.584604
H,0,1.583001,-0.531281,2.716216
C,0,2.326908,-1.182036,-2.766878
H,0,2.174966,-0.098474,-2.841921

H,0,2.770259,-1.533218,-3.708129
H,0,1.344656,-1.64996,-2.631155
C,0,4.629466,-0.874862,-1.833181
H,0,4.52864,0.196719,-2.030225
H,0,5.324082,-1.014253,-0.999483
H,0,5.087036,-1.328655,-2.722817
C,0,3.410584,-3.061846,-1.498506
H,0,4.136319,-3.353588,-0.730819
H,0,2.449412,-3.534835,-1.268968
H,0,3.766959,-3.452797,-2.459722
C,0,-3.410619,-3.061813,-1.498418
H,0,-3.767048,-3.452789,-2.459605
H,0,-2.449426,-3.534782,-1.268929
H,0,-4.136302,-3.353548,-0.730677
C,0,-4.629554,-0.874864,-1.833059
H,0,-4.528764,0.196721,-2.030104
H,0,-5.08716,-1.328665,-2.722673
H,0,-5.324124,-1.014275,-0.999323
C,0,-2.327027,-1.181999,-2.766875
H,0,-2.770417,-1.533194,-3.708103
H,0,-2.175105,-0.098434,-2.841934
H,0,-1.34476,-1.649906,-2.631197
C,0,-4.736342,-1.469788,1.576981
H,0,-5.130033,-0.469429,1.366391
H,0,-5.138188,-2.167135,0.834049
H,0,-5.130795,-1.773671,2.556056
C,0,-2.681167,-0.554827,2.721396
H,0,-1.583047,-0.531147,2.716213
H,0,-3.049477,0.467305,2.584581
H,0,-3.015374,-0.914566,3.702529
C,0,-2.720355,-2.93265,1.942143
H,0,-1.625954,-2.971342,1.9535
H,0,-3.103545,-3.232641,2.92662
H,0,-3.072702,-3.661502,1.205586
H,0,-0.000028,-2.827641,-0.054658

SCF Done: E(RM06L) = -2078.96163130 A.U. after 1 cycles

Zero-point correction= 0.737926 (Hartree/Particle)
Thermal correction to Energy= 0.778230
Thermal correction to Enthalpy= 0.779174
Thermal correction to Gibbs Free Energy= 0.670495
Sum of electronic and zero-point Energies= -2078.223705
Sum of electronic and thermal Energies= -2078.183402
Sum of electronic and thermal Enthalpies= -2078.182457
Sum of electronic and thermal Free Energies= -2078.291136

(tBuxanPOP)RhCl

Charge = 0 Multiplicity = 1
Rh,0,-0.0000101478,-1.1933887044,0.0387982936
P,0,2.2995179313,-0.9556548407,0.005640696
O,0,0.0000050415,0.9760434429,0.031691394
P,0,-2.2995303599,-0.9556203577,0.0056408202
C,0,1.2385354504,1.6907824958,0.0038834154

C,0,2.4180333252,0.913754047,-0.0313761367
C,0,3.645907062,1.5967636326,-0.0325140784
C,0,3.7023655898,2.9941334647,-0.0042536111
C,0,2.5138283365,3.7253425649,0.0228521101
C,0,1.257669022,3.0937477331,0.0260617636
C,0,-1.2385136117,1.6907998796,0.0038016508
C,0,-2.4180207301,0.9137881756,-0.0315292716
C,0,-3.6458810631,1.5968200445,-0.0329449982
C,0,-3.7023195784,2.9941921747,-0.0047658271
C,0,-2.5137746065,3.7253821317,0.0225156272
C,0,-1.2576264586,3.0937660545,0.0259307178
C,0,0.0000257232,3.9530787869,0.0666468841
H,0,4.5670042662,1.0271110681,-0.0503165036
H,0,4.6593897058,3.5021046201,-0.0020160333
H,0,2.5530226868,4.8105732136,0.0464181773
H,0,-4.5669867452,1.0271873233,-0.0509030233
H,0,-4.6593356417,3.5021794718,-0.0027276558
H,0,-2.552954285,4.8106146294,0.0460182496
C,0,-0.000034661,4.7914833408,1.3723317278
C,0,0.0000960732,4.9134200898,-1.151756461
H,0,-0.0000919525,4.1429821068,2.2522835498
H,0,0.8849678761,5.4333427061,1.4170963822
H,0,-0.8850234789,5.4333680419,1.416999491
H,0,0.8830379424,5.5588368774,-1.1363755318
H,0,0.0001451481,4.3520510568,-2.0896426479
H,0,-0.882842767,5.558843292,-1.1364717613
C,0,3.188784715,-1.57572306,-1.6090805734
C,0,3.2836172732,-1.4584291048,1.6093513158
C,0,-3.2835692193,-1.4583080134,1.6094205032
C,0,-3.1888789734,-1.5757757803,-1.6089801178
C,0,2.8477468017,-2.8933206046,1.9649814673
H,0,3.1688368606,-3.6252430535,1.2189649112
H,0,3.2959494633,-3.1683162264,2.9288337625
H,0,1.7589390546,-2.9671073595,2.0434136696
C,0,4.8121075625,-1.3876059033,1.488654763
H,0,5.1681700592,-0.3763701852,1.2663810072
H,0,5.2571178774,-1.6866620069,2.4468422559
H,0,5.1954405673,-2.069682533,0.7231133326
C,0,2.790677064,-0.5063487659,2.7158937872
H,0,3.1796505083,-0.847891156,3.6828746663
H,0,3.129255337,0.522398696,2.5532312806
H,0,1.6942685972,-0.5077488146,2.7665565101
C,0,2.1530963405,-1.3507711818,-2.728841122
H,0,1.88247933,-0.2912817167,-2.8210064607
H,0,2.5756462247,-1.6832587571,-3.6859052994
H,0,1.2382481746,-1.9172072112,-2.5248359641
C,0,4.489700944,-0.8431069383,-1.9663691457
H,0,4.3079247284,0.2113117028,-2.1954676169
H,0,5.2438973108,-0.9065513298,-1.1752604985
H,0,4.9162465476,-1.3070303114,-2.8656152352
C,0,3.4413372747,-3.0855202288,-1.4502910303
H,0,4.2377701133,-3.2940720492,-0.7273535397
H,0,2.5312558157,-3.6089267367,-1.1381039489
H,0,3.75799339,-3.4940213759,-2.418268631
C,0,-3.4414557985,-3.0855567319,-1.4500696326
H,0,-3.7581685418,-3.4941178609,-2.4180031399

H,0,-2.5313703719,-3.6089608273,-1.1378899926
H,0,-4.2378574063,-3.2940394117,-0.7270771574
C,0,-4.4897991028,-0.8431372531,-1.9662104632
H,0,-4.3080181954,0.2113000965,-2.1952276836
H,0,-4.9163573852,-1.306999901,-2.8654815867
H,0,-5.2439861102,-0.9066320903,-1.1750970539
C,0,-2.1532429325,-1.3509046336,-2.7288067214
H,0,-2.5758472935,-1.6834395569,-3.6858304033
H,0,-1.8826131117,-0.2914245947,-2.821046348
H,0,-1.2383942207,-1.9173445374,-2.5248168351
C,0,-4.8120640242,-1.387469174,1.4887850831
H,0,-5.1681255134,-0.3762265375,1.2665511961
H,0,-5.195430183,-2.0695234433,0.7232389627
H,0,-5.2570421745,-1.6865445318,2.4469811119
C,0,-2.7905547672,-0.5062078203,2.7159147814
H,0,-1.6941427698,-0.5076155177,2.7665121572
H,0,-3.1291359484,0.5225396417,2.5532594779
H,0,-3.1794727667,-0.8477322522,3.6829243938
C,0,-2.8477146213,-2.8931984087,1.9650683182
H,0,-1.7589047571,-2.9670035196,2.0434616204
H,0,-3.2958869372,-3.1681633672,2.9289433206
H,0,-3.168849091,-3.6251308312,1.219079224
Cl,0,-0.0000448115,-3.6121410841,-0.1605636179

SCF Done: E(RM06L) = -2538.60143553 A.U. after 3 cycles

Zero-point correction= 0.732929 (Hartree/Particle)
Thermal correction to Energy= 0.774519
Thermal correction to Enthalpy= 0.775463
Thermal correction to Gibbs Free Energy= 0.663985
Sum of electronic and zero-point Energies= -2537.868507
Sum of electronic and thermal Energies= -2537.826917
Sum of electronic and thermal Enthalpies= -2537.825973
Sum of electronic and thermal Free Energies= -2537.937451

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dihydrogen

Charge = 0 Multiplicity = 1
H,0,0.,0.,0.0025489349
H,0,0.,0.,0.7474510651

SCF Done: E(RM06L) = -1.16824931834 A.U. after 1 cycles

Zero-point correction= 0.009924 (Hartree/Particle)
Thermal correction to Energy= 0.012284
Thermal correction to Enthalpy= 0.013228
Thermal correction to Gibbs Free Energy= -0.001569
Sum of electronic and zero-point Energies= -1.158326
Sum of electronic and thermal Energies= -1.155965
Sum of electronic and thermal Enthalpies= -1.155021
Sum of electronic and thermal Free Energies= -1.169818

(tBuxanPOP)Rh-H-H-H

Charge = 0 Multiplicity = 1
Rh,0,0.0001187538,-1.2667873654,0.0123638939
P,0,2.2921342826,-0.9598788093,0.1135619257
O,0,-0.0000512846,1.0074048885,-0.2921368695
P,0,-2.2920356357,-0.9602987578,0.1127100645
C,0,1.2193679798,1.6832637604,0.0131946595
C,0,2.3606540432,0.9060411782,0.2823880856
C,0,3.5353587573,1.5964041172,0.6348830996
C,0,3.5651209884,2.9935968949,0.7044997949
C,0,2.4229328727,3.7328121431,0.3688752885
C,0,1.2346996903,3.0886142073,-0.0031298215
C,0,-1.2197305515,1.6830430317,0.0126459042
C,0,-2.3609925152,0.9056201838,0.2813612046
C,0,-3.5359899824,1.5957720659,0.6332701233
C,0,-3.5660725882,2.9929632635,0.702764016
C,0,-2.423864417,3.732381787,0.3676500574
C,0,-1.2353268516,3.0883901228,-0.0037313062
C,0,-0.0002550094,3.8164245788,-0.5272181778
H,0,4.4304095848,1.0280392116,0.8688647274
H,0,4.4763396915,3.5022630073,0.9970175823
H,0,2.4606703445,4.8162454777,0.388462319
H,0,-4.4310216869,1.0272379517,0.8669126985
H,0,-4.4775428269,3.5014681172,0.9947762481
H,0,-2.4618200679,4.8158104267,0.3871289282
C,0,-0.000483603,5.3073149663,-0.1707626055
C,0,0.0001374023,3.6711713935,-2.0802718978
H,0,-0.0007595301,5.4677643116,0.9116750613
H,0,0.87667803,5.8034413654,-0.5954359322
H,0,-0.8775338372,5.8032826828,-0.595854842
H,0,0.8907939671,4.1480868338,-2.5019809
H,0,0.0002376407,2.6167371857,-2.3758524335
H,0,-0.8903380189,4.1480353703,-2.5024186516
C,0,3.3279773096,-1.2400201684,-1.5224470523
C,0,3.2069732755,-1.6924506581,1.6756121369
C,0,-3.2072506445,-1.6928531258,1.6745303246
C,0,-3.3271633266,-1.2408180455,-1.5236902762
C,0,2.6259393392,-3.1093090639,1.8652289187
H,0,2.8235863573,-3.7550732047,1.0022703379
H,0,3.0883973962,-3.5679886365,2.7487494128
H,0,1.5430718512,-3.0640251943,2.0110866471
C,0,4.7366507272,-1.7911017898,1.5700822136
H,0,5.2164822414,-0.8211212965,1.4034934708
H,0,5.1222086467,-2.1909914608,2.5168581025
H,0,5.0491863893,-2.4746474404,0.7740553422
C,0,2.8211625127,-0.8321187141,2.8914813652
H,0,3.1379091402,-1.3513257883,3.804676495
H,0,3.3050097747,0.1494867943,2.8733505901
H,0,1.7364621704,-0.687891624,2.9313123585
C,0,2.5441948921,-0.5272037793,-2.640699597
H,0,2.5496132519,0.5610004306,-2.4963928546
H,0,3.0241251017,-0.7430076424,-3.603639184
H,0,1.5063219907,-0.8706092415,-2.6746013092
C,0,4.7588485346,-0.677656392,-1.5233462108

H,0,4.765782177,0.4051751699,-1.3623615179
H,0,5.4138719538,-1.1475426498,-0.7889040562
H,0,5.1961229913,-0.8584574342,-2.5143647801
C,0,3.3285426998,-2.7580752271,-1.7698360678
H,0,3.933000079,-3.290742485,-1.0254715463
H,0,2.3069952577,-3.1527368964,-1.7403729341
H,0,3.7534438525,-2.9706613611,-2.7584776578
C,0,-3.3274292275,-2.7589098786,-1.7708771313
H,0,-3.7519078544,-2.9716617194,-2.7596675973
H,0,-2.3058490375,-3.1534492803,-1.7409686519
H,0,-3.9321151239,-3.2915638791,-1.0266929498
C,0,-4.7581238245,-0.6786645128,-1.5252815772
H,0,-4.7652745372,0.4042302983,-1.3647095126
H,0,-5.1950404121,-0.8599154456,-2.5163781312
H,0,-5.4133340008,-1.1483617686,-0.7908881894
C,0,-2.5430273234,-0.5280743199,-2.641726881
H,0,-3.022608272,-0.7440399099,-3.6048050911
H,0,-2.5485650349,0.5601391774,-2.4975446415
H,0,-1.505126018,-0.8714360185,-2.6752016887
C,0,-4.736881718,-1.7916979291,1.5685760738
H,0,-5.2167794795,-0.821769523,1.4018483218
H,0,-5.0491023809,-2.4752798028,0.7724598238
H,0,-5.122664951,-2.1916259442,2.5152409636
C,0,-2.8219157881,-0.8323162292,2.8904098868
H,0,-1.7372369871,-0.6880558629,2.9305798859
H,0,-3.3057720586,0.1492795529,2.8719468427
H,0,-3.1389866741,-1.3514153342,3.8035509202
C,0,-2.6260689551,-3.1096121062,1.8644550358
H,0,-1.5432228435,-3.0641903529,2.0104229707
H,0,-3.0885648247,-3.5681968987,2.7480070261
H,0,-2.8235680778,-3.755543724,1.0015883964
H,0,0.0002728041,-2.8013834071,0.2126629718
H,0,0.0004891608,-1.7110900827,-1.5916614408
H,0,-0.0001955153,-1.0095157061,1.6841198983

SCF Done: E(RM06L) = -2080.14333814 A.U. after 3 cycles

Zero-point correction= 0.753984 (Hartree/Particle)
Thermal correction to Energy= 0.794681
Thermal correction to Enthalpy= 0.795625
Thermal correction to Gibbs Free Energy= 0.686996
Sum of electronic and zero-point Energies= -2079.389354
Sum of electronic and thermal Energies= -2079.348657
Sum of electronic and thermal Enthalpies= -2079.347713
Sum of electronic and thermal Free Energies= -2079.456342

(tBuxanPOP)Rh-Cl-H-H, H's cis

Charge = 0 Multiplicity = 1
Rh,0,0.0001869985,-1.2567482572,0.3560697427
P,0,2.319242503,-0.9715100989,0.1538342642
O,0,-0.0001308818,0.9760891959,-0.1431301043
P,0,-2.3189485838,-0.9722606057,0.1533784772
C,0,1.2309639345,1.6734319853,-0.0150936565
C,0,2.4052912855,0.8943173295,0.0842848028

C,0,3.6367438304,1.563764913,0.145688522
C,0,3.7026299225,2.9615508726,0.1140809472
C,0,2.5196727088,3.6991066457,0.0377791803
C,0,1.2606936305,3.0759050272,-0.0202383389
C,0,-1.2314779743,1.6730316559,-0.0153358859
C,0,-2.4055712182,0.893539302,0.083837616
C,0,-3.637253269,1.562593996,0.1449959293
C,0,-3.703583035,2.9603578705,0.1133670859
C,0,-2.52084844,3.6982937892,0.0372830495
C,0,-1.2616630542,3.0754943099,-0.0205059229
C,0,-0.0006225855,3.9347706142,-0.0697825909
H,0,4.5487290283,0.9819132257,0.2396359419
H,0,4.6608277363,3.464680178,0.1633457961
H,0,2.5682971706,4.7841328391,0.0282130578
H,0,-4.5490688556,0.9804493944,0.2387814656
H,0,-4.6619521284,3.4631790286,0.1624460411
H,0,-2.569814271,4.7833054335,0.0277178568
C,0,-0.0009383117,4.8900451862,1.1534362363
C,0,-0.0006228329,4.7731287806,-1.3744376857
H,0,-0.0009070147,4.3208545006,2.0861929447
H,0,0.8810706993,5.5367530351,1.141915895
H,0,-0.8832251428,5.5363732054,1.1417450505
H,0,0.8845547449,5.415334707,-1.418545424
H,0,-0.0004070177,4.1254826787,-2.2554955475
H,0,-0.8860179677,5.4150208025,-1.4187483762
C,0,3.0236216313,-1.4825735433,-1.5967149671
C,0,3.4708999795,-1.5620950072,1.6237341326
C,0,-3.4707574752,-1.5632605462,1.6229937475
C,0,-3.022774831,-1.4834894835,-1.5973580464
C,0,2.7648859777,-2.8186026831,2.1759192462
H,0,2.667306654,-3.6024357755,1.4155433956
H,0,3.3556722987,-3.2192212013,3.0092868594
H,0,1.7641840268,-2.565891663,2.5386564437
C,0,4.9083021826,-1.9160156487,1.2167361635
H,0,5.4567750685,-1.0530532,0.8242837186
H,0,5.4385545503,-2.2613370511,2.1134914931
H,0,4.9495172226,-2.724134172,0.479127908
C,0,3.5027869579,-0.4836550084,2.7222319467
H,0,3.9614963416,-0.9273506047,3.6153987474
H,0,4.1047633438,0.3831462337,2.4345536097
H,0,2.4963056685,-0.1482493538,2.9838665649
C,0,2.1243480489,-0.7836876247,-2.6355449445
H,0,2.2840705973,0.3004716915,-2.629210037
H,0,2.3790956033,-1.1582982444,-3.6346982581
H,0,1.0648341312,-0.9783085943,-2.4504468554
C,0,4.4718640951,-1.0568130235,-1.8938850608
H,0,4.6052306399,0.0253426425,-1.7968008424
H,0,5.2094963129,-1.5637595394,-1.2721731323
H,0,4.6926577514,-1.3140465679,-2.9381534276
C,0,2.8735393475,-3.0098030636,-1.7035856894
H,0,3.536744586,-3.5338332302,-1.0051774097
H,0,1.8428028984,-3.3159343489,-1.4963443507
H,0,3.1349671417,-3.333398927,-2.7184897559
C,0,-2.8721704407,-3.0106669792,-1.7042497002
H,0,-3.1333277085,-3.334311078,-2.7192090293
H,0,-1.8413701209,-3.3164648369,-1.4968438517

H,0,-3.5353201936,-3.5349361464,-1.0059673329
C,0,-4.4710888914,-1.0582220648,-1.8948512013
H,0,-4.6048931908,0.0238683027,-1.7976410516
H,0,-4.691503274,-1.3153760803,-2.9392192783
H,0,-5.208693161,-1.5655410445,-1.2734142195
C,0,-2.1235016173,-0.7842508954,-2.6359630592
H,0,-2.3778487006,-1.1589569165,-3.6351816477
H,0,-2.2836638919,0.2998432242,-2.6296565292
H,0,-1.0639568105,-0.9784556989,-2.4506119322
C,0,-4.9079380358,-1.9176428566,1.2156181253
H,0,-5.4566195837,-1.0548330572,0.8231202987
H,0,-4.9486877397,-2.7257036082,0.4779159254
H,0,-5.4382841277,-2.2632360331,2.112214006
C,0,-3.5032852722,-0.4848802828,2.7215304671
H,0,-2.4969844918,-0.1491238339,2.9834110739
H,0,-4.1055080859,0.3817211656,2.4337588074
H,0,-3.9620418342,-0.9287801511,3.6145710872
C,0,-2.7644654867,-2.819557871,2.1753082603
H,0,-1.7639323176,-2.5665308317,2.5382983326
H,0,-3.3553237671,-3.2203931233,3.0085208684
H,0,-2.6664504444,-3.6033394295,1.414932835
H,0,0.0003851153,-2.7501102977,0.7587304053
H,0,0.0004369301,-1.9652390366,-1.0372670348
Cl,0,-0.0002601074,-0.2174771211,2.7358496056

SCF Done: E(RM06L) = -2539.79959978 A.U. after 4 cycles

Zero-point correction= 0.750333 (Hartree/Particle)
Thermal correction to Energy= 0.792592
Thermal correction to Enthalpy= 0.793536
Thermal correction to Gibbs Free Energy= 0.681034
Sum of electronic and zero-point Energies= -2539.049267
Sum of electronic and thermal Energies= -2539.007008
Sum of electronic and thermal Enthalpies= -2539.006064
Sum of electronic and thermal Free Energies= -2539.118565

(tBuxanPOP)Rh-H-Cl-H, H's trans

Charge = 0 Multiplicity = 1
Rh,0,0.0000597823,-1.1532505429,-0.1384742291
P,0,2.3173752321,-0.9475102671,-0.1008102223
O,0,-0.0000516806,0.9960859158,0.0266996616
P,0,-2.3172748184,-0.9477392096,-0.1010360394
C,0,1.2403972215,1.6996669198,-0.0142854498
C,0,2.4184809074,0.9243807705,-0.1005402924
C,0,3.6458818532,1.6072755073,-0.091211064
C,0,3.7019781743,3.0026155129,-0.0104621477
C,0,2.5151959726,3.7319918551,0.0632055951
C,0,1.2592552258,3.1007875405,0.0619251914
C,0,-1.2405677636,1.6995460898,-0.0143891025
C,0,-2.4185719528,0.924145694,-0.1007351624
C,0,-3.6460376748,1.6069257167,-0.0914614594
C,0,-3.7022698224,3.0022608036,-0.010715966

C,0,-2.5155629474,3.7317510423,0.0630185962
C,0,-1.259563237,3.1006660214,0.0618249763
C,0,-0.0001992401,3.9543191715,0.1640927933
H,0,4.5668156447,1.040193438,-0.1369351118
H,0,4.659172466,3.5099326025,-0.000683746
H,0,2.5568894163,4.8149797254,0.1308716128
H,0,-4.5669182748,1.0397619493,-0.1372315774
H,0,-4.6595126244,3.5094874384,-0.000994859
H,0,-2.5573651203,4.8147342678,0.1306889728
C,0,-0.0002912889,4.6935481946,1.5289340344
C,0,-0.000202517,5.0009658559,-0.9808940488
H,0,-0.0002945001,3.9818730398,2.3586886343
H,0,0.885241425,5.3298673183,1.6205787975
H,0,-0.8858903909,5.3297853223,1.6205013636
H,0,0.8811900355,5.645229063,-0.9195004952
H,0,-0.000138367,4.5090512341,-1.9568826867
H,0,-0.8816604138,5.6451468363,-0.9195735814
C,0,3.3528975057,-1.6105404618,-1.6171650273
C,0,3.1893709524,-1.4365081998,1.5803947261
C,0,-3.1893666122,-1.4368571108,1.5800796682
C,0,-3.3525752526,-1.6108896558,-1.6175060903
C,0,2.7113577501,-2.8566377595,1.9384336274
H,0,3.0887352972,-3.6127899533,1.2456123856
H,0,3.0738725412,-3.1047856452,2.9443477856
H,0,1.6186180064,-2.9088972676,1.9317285822
C,0,4.7244418095,-1.380953285,1.5433298868
H,0,5.0999045907,-0.37589383,1.3199433473
H,0,5.1042154875,-1.6549709628,2.5360337032
H,0,5.1536647969,-2.0856736843,0.8253194449
C,0,2.6716039314,-0.4573095912,2.6501828328
H,0,3.0145438393,-0.8014455109,3.63358783
H,0,3.0480947761,0.5598471625,2.4947255115
H,0,1.5761772478,-0.4390993612,2.6563157307
C,0,2.4818987165,-1.4381829167,-2.8730900897
H,0,2.1978907141,-0.3923163869,-3.0318840785
H,0,3.0592035395,-1.7780107001,-3.7432666399
H,0,1.5641652008,-2.0254679313,-2.7986690604
C,0,4.6905711088,-0.8876232953,-1.8499464736
H,0,4.5354590414,0.1466660347,-2.1710003977
H,0,5.3460468392,-0.8933191737,-0.9746540583
H,0,5.2197277034,-1.4053543713,-2.6603293076
C,0,3.5856473789,-3.1162205983,-1.3848890103
H,0,4.3018375497,-3.3087884084,-0.5798421838
H,0,2.6468794609,-3.6320815808,-1.1589317912
H,0,3.9988290215,-3.5471401435,-2.3054303393
C,0,-3.5851761286,-3.1165949262,-1.3852552289
H,0,-3.9982026149,-3.5475603676,-2.3058461003
H,0,-2.6463713334,-3.6323404728,-1.1591901823
H,0,-4.3014318518,-3.309244158,-0.5802885186
C,0,-4.6903037556,-0.8881250254,-1.8504337424
H,0,-4.5352673075,0.1461672523,-2.1715143498
H,0,-5.2193304417,-1.4059396794,-2.6608478737
H,0,-5.3458623349,-0.8938532013,-0.9752018169
C,0,-2.4814683543,-1.4384341202,-2.8733438428
H,0,-3.0586419799,-1.7783427275,-3.7435762028
H,0,-2.1975840061,-0.3925314118,-3.0321172396

H,0,-1.5636684059,-2.0256024606,-2.7988336761
C,0,-4.7244447005,-1.3814978125,1.54287137
H,0,-5.1000083155,-0.3764916591,1.3194228022
H,0,-5.1535167334,-2.086287634,0.8248384951
H,0,-5.1042759213,-1.6555368536,2.535548286
C,0,-2.6718176677,-0.4575976865,2.6499167095
H,0,-1.5763931593,-0.4392329207,2.6561459994
H,0,-3.0484361741,0.5595069374,2.4944335928
H,0,-3.0147911135,-0.8017824377,3.6332924409
C,0,-2.7111883346,-2.8569193714,1.9381588547
H,0,-1.6184400458,-2.9090307325,1.9315570737
H,0,-3.0737597988,-3.1051193376,2.944040097
H,0,-3.0883977191,-3.6131193371,1.2453013518
H,0,0.0001149598,-0.9046208097,-1.774828149
Cl,0,0.0001841595,-3.5540162953,-0.5130361185
H,0,-0.0000801557,-1.3964336602,1.5303389863

SCF Done: E(RM06L) = -2539.75623615 A.U. after 3 cycles

Zero-point correction= 0.748274 (Hartree/Particle)
Thermal correction to Energy= 0.790144
Thermal correction to Enthalpy= 0.791088
Thermal correction to Gibbs Free Energy= 0.679842
Sum of electronic and zero-point Energies= -2539.007962
Sum of electronic and thermal Energies= -2538.966092
Sum of electronic and thermal Enthalpies= -2538.965148
Sum of electronic and thermal Free Energies= -2539.076394

(tBuxanPOP)Rh+

Charge = 1 Multiplicity = 1
Rh,0,-0.0000022209,-1.0176362059,0.085219743
P,0,2.2799085567,-0.7357677852,0.0826407999
O,0,-0.0000026192,1.1572128133,-0.1031784597
P,0,-2.2799132514,-0.7357691403,0.08264469
C,0,1.2206630603,1.8591155616,-0.0711571387
C,0,2.3890195448,1.0865523933,0.0180160335
C,0,3.6141166646,1.7553155498,0.0774245546
C,0,3.6755160906,3.1391170667,0.0200089125
C,0,2.5015088471,3.8637395352,-0.089537252
C,0,1.2470089201,3.2494480804,-0.1262202377
C,0,-1.2206684438,1.8591150782,-0.0711552727
C,0,-2.3890245904,1.0865514388,0.0180195792
C,0,-3.6141217674,1.7553146925,0.0774279352
C,0,-3.6755215551,3.1391161618,0.0200116511
C,0,-2.5015146127,3.8637388711,-0.0895351992
C,0,-1.2470146473,3.2494476371,-0.1262187899
C,0,-0.0000030765,4.1058902408,-0.2370468498
H,0,4.5281999154,1.1812197597,0.1721595375
H,0,4.6315344182,3.6478079852,0.0603943256
H,0,2.5506000356,4.9461742946,-0.1438682601
H,0,-4.5282050127,1.181219173,0.1721630848

H,0,-4.6315399927,3.6478068691,0.0603970062
H,0,-2.5506060805,4.9461735926,-0.1438667394
C,0,-0.0000026902,5.1537339212,0.8902093336
C,0,-0.0000040422,4.8184497637,-1.6017010313
H,0,-0.0000020352,4.6785601896,1.873883011
H,0,0.8766108751,5.8007492571,0.8270959694
H,0,-0.8766166428,5.8007488305,0.8270969347
H,0,0.8820517046,5.4547509167,-1.707794585
H,0,-0.0000043058,4.1010007193,-2.4259163189
H,0,-0.8820602868,5.4547503989,-1.7077935876
C,0,3.144593325,-1.3624234708,-1.4723775554
C,0,3.0879733802,-1.290104349,1.6971965402
C,0,-3.0879706432,-1.2901053365,1.6972060318
C,0,-3.1445955233,-1.3624240787,-1.4723766852
C,0,2.4738728568,-2.6586527834,2.0210461481
H,0,2.7297983902,-3.4256923195,1.2871667001
H,0,2.8364710597,-3.0033959072,2.9948527151
H,0,1.3799787378,-2.593926257,2.0833419501
C,0,4.6097827879,-1.3940149905,1.681975382
H,0,5.0952503873,-0.4410711764,1.4588309251
H,0,4.9584358669,-1.7022838176,2.6735707553
H,0,4.9714762588,-2.1400269105,0.97079809
C,0,2.6365085968,-0.294397541,2.7700228008
H,0,2.9133215566,-0.6767084208,3.7574732761
H,0,3.1014818148,0.6866325689,2.6500818221
H,0,1.5483808361,-0.1591767642,2.7589594351
C,0,2.2193228736,-0.9444387366,-2.6217492023
H,0,2.1169588254,0.1433343995,-2.688112002
H,0,2.6328093244,-1.2954018721,-3.5728733102
H,0,1.216659106,-1.3708889783,-2.5082785141
C,0,4.5403717864,-0.8002381515,-1.733030757
H,0,4.517368479,0.2734232719,-1.9290416937
H,0,5.2426842458,-0.991176552,-0.9197948812
H,0,4.9499316576,-1.2780348914,-2.6295116488
C,0,3.1963727675,-2.8897523396,-1.3956882238
H,0,3.9050331187,-3.2462878397,-0.6442594759
H,0,2.2152020082,-3.3241010256,-1.1760895522
H,0,3.5211309288,-3.2914974249,-2.3605708219
C,0,-3.1964054404,-2.8897514746,-1.3956754923
H,0,-3.5211528159,-3.2914980342,-2.3605611108
H,0,-2.2152469015,-3.3241167371,-1.1760549289
H,0,-3.905086599,-3.2462684987,-0.644257888
C,0,-4.5403585833,-0.8002122827,-1.7330566406
H,0,-4.5173294024,0.273446308,-1.9290799083
H,0,-4.9499147355,-1.278010255,-2.6295385826
H,0,-5.2426878831,-0.9911260731,-0.9198301403
C,0,-2.2193025458,-0.9444696238,-2.6217410714
H,0,-2.6327829672,-1.2954361882,-3.5728665066
H,0,-2.1169177331,0.1433008454,-2.6881151406
H,0,-1.2166481235,-1.3709369705,-2.5082523614
C,0,-4.6097799238,-1.394021546,1.6819995291
H,0,-5.0952533359,-0.4410823731,1.4588485002
H,0,-4.9714781597,-2.1400437696,0.9708361692
H,0,-4.9584221862,-1.7022794835,2.6736021047
C,0,-2.6365021478,-0.2943947464,2.7700270444
H,0,-1.5483747581,-0.1591716966,2.7589571222

H,0,-3.1014781077,0.6866340275,2.6500858491
H,0,-2.9133087192,-0.6767034271,3.7574801707
C,0,-2.4738633689,-2.6586504081,2.0210569608
H,0,-1.3799691148,-2.5939199757,2.0833448756
H,0,-2.8364537426,-3.0033907967,2.9948674027
H,0,-2.7297912663,-3.4256937866,1.287182415

SCF Done: E(RM06L) = -2077.71595038 A.U. after 1 cycles

Zero-point correction= 0.720477 (Hartree/Particle)
Thermal correction to Energy= 0.761116
Thermal correction to Enthalpy= 0.762061
Thermal correction to Gibbs Free Energy= 0.650693
Sum of electronic and zero-point Energies= -2076.995473
Sum of electronic and thermal Energies= -2076.954834
Sum of electronic and thermal Enthalpies= -2076.953890
Sum of electronic and thermal Free Energies= -2077.065257

(tBuxanPOP)Rh+, SQP, H apical

Charge = 1 Multiplicity = 1
Rh,0,0.0020887359,-1.2397126496,-0.0096136167
P,0,-2.2977516475,-0.9446788175,-0.0448578068
O,0,-0.0000534775,1.011147994,0.125026047
P,0,2.3008952685,-0.9392815804,-0.0625083914
C,0,-1.219170531,1.6879976257,0.0143969909
C,0,-2.3806767206,0.8956913156,-0.0575444782
C,0,-3.6063179228,1.5613491798,-0.1497679477
C,0,-3.6764316331,2.9459790241,-0.1586140588
C,0,-2.5091122689,3.6860929673,-0.0812561154
C,0,-1.2540887986,3.0793747092,-0.0011563038
C,0,1.2166538491,1.6908554569,0.0057713865
C,0,2.3794806879,0.9012873997,-0.074586045
C,0,3.6028749519,1.5698453086,-0.1753363667
C,0,3.6696740775,2.9546386571,-0.1843397022
C,0,2.5011915808,3.6919939684,-0.098677577
C,0,1.2481929616,3.082313612,-0.0098651707
C,0,-0.0035946179,3.9372945129,0.0972280947
H,0,-4.5199212932,0.9833470443,-0.2123440012
H,0,-4.6368955155,3.4436567773,-0.2236254822
H,0,-2.5677798518,4.7692957858,-0.0792833767
H,0,4.5173686973,0.9940182716,-0.2445447559
H,0,4.6284878141,3.4545832702,-0.2559815272
H,0,2.5573167135,4.7753329723,-0.0969843673
C,0,-0.0087188358,4.9799159156,-1.0338878759
C,0,0.0002779636,4.6569429075,1.4584829122
H,0,-0.0115847919,4.501028657,-2.0157095038
H,0,-0.8845900441,5.6275147758,-0.9705131758
H,0,0.8660924322,5.6295123384,-0.9765970187
H,0,-0.8831477675,5.2918211852,1.5638349029
H,0,0.0039903137,3.943986443,2.2868942011
H,0,0.882909476,5.2939084924,1.5577166063
C,0,-3.056254862,-1.4531668727,1.6073170841
C,0,-3.2565111524,-1.5645026641,-1.5506143984
C,0,3.249499608,-1.5556146067,-1.5760968728

C,0,3.0730256144,-1.4474856167,1.5834349034
C,0,-2.7619314061,-2.9859955098,-1.8465693597
H,0,-2.9610606973,-3.6823170358,-1.0294629036
H,0,-3.2822102749,-3.3639122705,-2.7321523243
H,0,-1.6893332613,-3.0067445352,-2.0493715875
C,0,-4.7760968304,-1.5932334773,-1.3824478854
H,0,-5.2086238071,-0.6095651719,-1.191185137
H,0,-5.2238475708,-1.9576401946,-2.3127351255
H,0,-5.0966326359,-2.2719751821,-0.5896045927
C,0,-2.8791470865,-0.6579113851,-2.7250652631
H,0,-3.2712999397,-1.0901270113,-3.6506367697
H,0,-3.2924181672,0.3482062166,-2.6259891623
H,0,-1.7937378581,-0.5692767119,-2.839166553
C,0,-1.9931013193,-1.0529384982,2.6375617691
H,0,-1.7677120817,0.0187629204,2.6107545936
H,0,-2.3423110657,-1.2887617648,3.6480944978
H,0,-1.0626526792,-1.613153612,2.4819523703
C,0,-4.3762828535,-0.7749780018,1.9641894178
H,0,-4.2641784247,0.3049774272,2.0797746022
H,0,-5.1661577137,-0.9653216277,1.235451437
H,0,-4.725595085,-1.1668216476,2.9253393491
C,0,-3.2139436265,-2.9747210873,1.6228348703
H,0,-4.015573732,-3.317736395,0.9651600143
H,0,-2.2896571896,-3.4840851505,1.3338511029
H,0,-3.4687905531,-3.3003646906,2.6363165954
C,0,3.2346298117,-2.9686562393,1.5963333776
H,0,3.4977080578,-3.2945837246,2.607618848
H,0,2.3095188669,-3.480063462,1.3136750772
H,0,4.0322820445,-3.3090509012,0.9324923459
C,0,4.393977106,-0.7663795398,1.9312121608
H,0,4.2800277292,0.3131404809,2.049009694
H,0,4.7515232543,-1.1585304595,2.8892041658
H,0,5.178806034,-0.9538265663,1.1962870419
C,0,2.0165038828,-1.0509914329,2.6219164749
H,0,2.3738739888,-1.2865963742,3.6296447775
H,0,1.7879063046,0.0200963282,2.5976310381
H,0,1.0865181383,-1.6137555819,2.4727790473
C,0,4.7703965604,-1.5806078127,-1.4196447835
H,0,5.2018544032,-0.5959358798,-1.231138177
H,0,5.0987387488,-2.2589826889,-0.6296894478
H,0,5.2119158175,-1.9433325583,-2.3535605159
C,0,2.8608142614,-0.649012977,-2.7468418975
H,0,1.7743349738,-0.5631357162,-2.8525643407
H,0,3.2722081075,0.3580977183,-2.6500430052
H,0,3.2470122426,-1.0794132743,-3.6757571982
C,0,2.7561812051,-2.9780834006,-1.86942587
H,0,1.6820432888,-3.0013752805,-2.063631512
H,0,3.2702819738,-3.3538368662,-2.7595260449
H,0,2.9636490599,-3.674668939,-1.0546329473
H,0,0.0035917985,-2.7840441593,-0.1043079534
H,0,-0.003765815,-1.4074340567,-1.5268735047

SCF Done: E(RM06L) = -2078.95091020   A.U. after   1 cycles

Zero-point correction=   0.737429 (Hartree/Particle)
Thermal correction to Energy=   0.778545

Thermal correction to Enthalpy= 0.779489
Thermal correction to Gibbs Free Energy= 0.668729
Sum of electronic and zero-point Energies= -2078.213481
Sum of electronic and thermal Energies= -2078.172365
Sum of electronic and thermal Enthalpies= -2078.171421
Sum of electronic and thermal Free Energies= -2078.282181

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