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Synthesis, Structural Properties and Reactivity of Ruthenocene-based Pincer Pd(II) Tetrahydroborate

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Supplementary Information

Experimental Section

All manipulations were performed under a dry argon atmosphere using standard Schlenk technique. Commercially available argon (99.9%) was additionally purified from traces of oxygen and moisture by sequential passage through Ni/Cr catalyst column and 4 Å molecular sieves. The HPLC grade solvents (Acros Organics) were used for sample preparation after additional purification by standard procedures. Dichloromethane (DCM) and toluene were dehydrated over CaH_2 and Na/benzophenone, respectively. All solvents were freshly distilled under argon prior to use. Deuterated were distilled and degassed by three freeze–pump–thaw cycles prior to use. {2,5-Bis(di-*tert*-butylphosphinomethyl)ruthenocen-1-yl}palladium chloride ($^{tBu}PC^{Ru}P$)PdCl (where $^{tBu}PC^{Ru}P$ = κ^3-[{2,5-($^{t}Bu_2PCH_2$)$_2C_5H_2$}Ru(C_5H_5)]) was prepared as previously described.[1]

FTIR spectra (Figures S10–S11, S24, S38 and S45) were measured on Shimadzu IR Prestige 21 FTIR spectrometer. NMR spectra (Figures S4–S15, S25, S27–S28, S30–S31, S35–S39, S42–S44) were recorded on a Bruker Avance II 400 MHz and 500 MHz spectrometers. ^{1}H chemical shifts are reported in parts per million (ppm) downfield to tetramethylsilane (TMS) and were calibrated against the residual solvent resonance, while $^{31}P\{^{1}H\}$ signals were referenced to 85% H_3PO_4 and ^{11}B – to $BF_3{\cdot}Et_2O$. **Elemental analyses** were carried out in the Laboratory of Microanalysis of INEOS RAS. Because the automatic CH analyzer cannot be used for the Ru-containing compounds due to formation of volatile oxides, the classic manual technique was used. The sample was burned in a stream of oxygen at 950 °C followed by trapping CO_2 and water by the Ascaris (asbestos impregnated with NaOH) and Anhydrone (anhydrous magnesium perchlorate), respectively, and the

analysis of the mass changes. Attempted high-resolution MS analysis of this series of complexes revealed easy ($^{tBu}PC^{Ru}P$)Pd-X → ($^{tBu}PC^{Ru}P$)Pd^+ + X^- dissociation (X = BH_4^-, $OC(O)H^-$, $OC(O)OH^-$), the only ions observed at the conditions required for ionization being ($^{tBu}PC^{Ru}P$)Pd^+ (m/z 653.12) and its adduct with acetonitrile (used as a solvent) ($^{tBu}PC^{Ru}P$)$Pd(NCCH_3)^+$ (m/z 694.15) for all compounds.

X-ray diffraction. Single crystals of **1** (Figure S1), **2** (Figure S22), **4** (Figure S32) and **5** (Figure S39) were obtained by slow solvent evaporation from toluene/hexane mixture. X-ray diffraction experiments were carried out with a SMART APEX2 DUO CCD diffractometer for the compound **2** and **4** with a SMART APEX2 CCD diffractometer for **1** and **5**, using graphite-monochromated Mo-K_α radiation (lλ = 0.71073 Å, ω-scans) at 120 K. The structures were solved by direct method and refined by the full-matrix least-squares against F^2 in anisotropic approximation for non-hydrogen atoms. Hydrogen atoms of the borohydride anion in **1** were found in difference Fourier synthesis and their coordinates and isotropic displacement parameters were refined freely. Hydrogen atoms of the borohydride anion in **2** and OH group in **5** were found in difference Fourier synthesis and refined isotropically in the riding model. Positions of other hydrogen atoms were calculated, and all of them were refined in isotropic approximation in the riding model. In **2**, the anion is, apparently, disordered by two positions. The best obtained model of this disorder resulted in R1 = 0.0465, wR2 = 0.1634 and GOOF= 1.147. Crystal data and structure refinement parameters for **1**, **2**, **4** and **5** are given in Table S1. All calculations were performed using the SHELXTL software.[2]

Full crystallographic data have been deposited with the CCDC as 1882669 (**1**), 1882671 (**2**), 1892812 (**4**), 1882670 (**5**). These data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

Preparation of ($^{tBu}PC^{Ru}P$)Pd($\eta^{1,2}$-BH_4) (1)

($^{tBu}PC^{Ru}P$)PdCl (100 mg, 0.145 mmol) was added to a suspension of $NaBH_4$ (50 mg, 1.32 mmol) in absolute EtOH (10 mL) at room temperature. The reaction mixture was refluxed for 1 h, then another portion of $NaBH_4$ (50 mg, 1.32 mmol) was added and the boiling was continued for 1 h. The reaction mixture was then cooled and evaporated *in vacuo* to a minimum volume. To the residue 10 ml of distilled H_2O was added, the resulting suspension was stirred at room temperature for 1 h. The reaction mass was extracted (3 × 10 ml) with hexane-CH_2Cl_2 (3:1). The solution was evaporated, and the residue was dried *in vacuo* at room temperature. The product is a pale yellow powder.

Yield: 93 mg (96%). The crystals suitable for XRD analysis were grown by slow solvent evaporation from toluene/hexane mixture under argon flow.

Anal. Calc. (%) for $C_{28}H_{51}BP_2RuPd$ (%): C 50.34, H 7.71. **Found:** C, 50.61; H, 7.90. **FTIR (KBr pellet, ν in cm^{-1}):** 3097, 2989, 2959, 2926, 2989, 2866, 2364 ($B–H_{term}^{as}$), 2292 ($B–H_{term}^{s}$), 1993 ($B–H_{br}–Pd$), 1840 ($B–H_{br}–Pd$), 1474, 1466, 1411, 1391, 1369, 1363, 1180, 1168, 1129, 1099, 1053.

NMR (298 K, C_6D_6, δ in ppm): ^{1}H: 0.20 (br m, 4H, BH_4^-), 1.18, (vt, J_{HP} = 13.2 Hz 18H, CH_3), 1.40 (vt, J_{HP} = 14.2 Hz, 18H, CH_3), 2.34 (dvt, J_{HH} = 16.7 Hz, J_{HP} = 8.8 Hz, 2H, CH_AH$_B$P), 2.64 (dvt, J_{HH} =16.7Hz, J_{HP} = 5.6 Hz, 2H, CH$_A$$H_B$P), 4.44 (s, 5H, C_5H_5), 4.65 (s, 2H, C_5H_2). ^{11}B{^{1}H}: −35.75 (br m). ^{31}P{^{1}H}: 89.91 (s).

NMR (298 K, toluene-d_8, δ in ppm): ^{1}H: 0.02 (br m, 4H, BH_4^-), 1.20, (vt, J_{HP} = 13.2 Hz 18H, CH_3), 1.41 (vt, J_{HP} = 14.2 Hz, 18H CH_3), 2.37 (dvt, J_{HH} =16.6 Hz, J_{HP} = 8.6 Hz, 2H, CH_AH$_B$P), 2.66 (dvt, J_{HH} = 16.6 Hz, J_{HP} = 5.4 Hz, 2H, CH$_A$$H_B$P), 4.39 (s, 5H, C_5H_5), 4.63 (s, 2H, C_5H_2). ^{11}B{^{1}H}: −35.85 (br m). ^{31}P{^{1}H}: 89.75 (s).

Preparation of (^{tBu}PC^{Ru}P)Pd(η^{1,2}-BD_4) (1-d_4)

Complex **1-d_4** was prepared by the same procedure using $NaBD_4$ instead of $NaBH_4$, EtOD as a solvent and D_2O for hydrolysis of excess $NaBD_4$. Yield: 21 mg (86%).

FTIR (KBr pellet, ν in cm^{-1}): 3096, 2988, 2960, 2899, 2868, 1775 ($B–D_{term}^{as}$), 1750 ($B–D_{term}^{s}$), 1680 ($B–D_{br}–Pd$), 1622 ($B–D_{br}–Pd$), 1474, 1466, 1411, 1391, 1369, 1337, 1319, 1300, 1266, 1180, 1168, 1140, 1129, 1099.

NMR (298 K, C_6D_6, δ in ppm): ^{2}H: 0.14 (s, BD_4^-), ^{1}H: 1.18, (vt, J_{HP} = 13.2 Hz, 18H, CH_3), 1.40 (vt, J_{HP} =14.2 Hz, 18H CH_3), 2.34 (dvt, J_{HH} =16.6 Hz, J_{HP} = 8.6 Hz, 2H, CH_AH$_B$P), 2.64 (dvt, J_{HH} =16.6 Hz, J_{HP} = 5.4 Hz, 2H, CH$_A$$H_B$P), 4.44 (s, 5H, C_5H_5), 4.66 (s, 2H, C_5H_2). ^{11}B{^{1}H}: −36.30 (br m). ^{31}P{^{1}H}: 89.83 (s).

Reaction of 1 and 1-d_4 with $(CF_3)_2$CHOH (HFIP).

Formation of {(^{tBu}PC^{Ru}P)Pd}$_2$(μ^2:η^{1,2}-BH_4) [B{OCH$(CF_3)_2$}$_4$] (2).

1 (3.5 mg, 0.0052 mmol) was weighed into standard NMR tube and dissolved in toluene-d_8 (0.5 mL). After addition of HFIP (15 μL, ca. 25 molar equiv.) by syringe the immediate formation of bubbles was observed. The reaction was monitored by ^{31}P NMR spectroscopy. After two days, the quantitative conversion of complex **1** into the product **2** was observed. The crystals suitable for XRD analysis were grown by slow solvent evaporation from toluene/hexane mixture under argon flow. Scaling-up the preparation of this complex seems to be a non-trivial task since the crystallization

relies on slow solvent evaporation and is sensitive to surface area - reaction mixture volume ratio, solvent vapor pressure etc. For this reason the element analysis was not performed for this compound.

FTIR (KBr, ν in cm^{-1}): 3422, 3097, 2963, 2920, 2871, 2416 (B–H_{term}^{as}), 2389 (B–H_{term}^{s}), 2029 (B–H_{br}^{s}), 1918 (B–H_{br}^{as}), 1474, 1381, 1372, 1292, 1262, 1216, 1180, 1138, 1101, 1054, 1020, 1000.

NMR (298 K, C_6D_6, δ in ppm): ^{1}H: −1.0 (br s, 4H, BH_4^-), 1.32–1.07, (m, 72H, CH_3), 1.40 (vt, J_{HP} = 14.2 Hz, 18H, CH_3), 2.34 (dvt, J_{HH} = 16.7Hz, J_{HP} = 8.8 Hz, 2H, CH_AH$_B$P), 2.64 (dvt, J_{HH} =16.7 Hz, J_{HP} = 5.6 Hz, 2H, CH$_A$$H_B$P), 4.44 (s, 5H, C_5H_5), 4.65 (s, 2H, C_5H_2). ^{11}B{^{1}H}: −39.0 (br m). ^{31}P{^{1}H}: δ_{centr} 90.58 (J_{PP} 329 Hz, δ_A 93.9, δ_B 87.3).

Formation of {(^{tBu}PC^{Ru}P)Pd}$_2$(μ^2:η^{1,2}-BD$_4$) [B{OCH(CF$_3$)$_2$}$_4$] (2-d$_4$)

Complex **2-d$_4$** was prepared by the same procedure using **1-d$_4$** instead **1**.

FTIR (KBr, ν in cm^{-1}): 1817 (B–D_{term}^{as}), 1592 (B–D_{br}), 1475, 1468, 1448, 1412, 1395, 1381, 1372, 1324, 1292, 1262, 1100, 1053, 1020, 997.

NMR (298 K, C_6D_6, δ in ppm): ^{31}P{^{1}H}: δ_{centr} 90.6 (J_{PP} 330 Hz, δ_A 94.0, δ_B 87.2).

Reaction of 1 with an excess pyridine

1 (6 mg, 0.0089 mmol) was weighed into standard NMR tube and dissolved in toluene-d$_8$ (0.5 mL), then pyridine (15 μL, ca. 25 molar equivalents) was added by syringe. The formation of (^{tBu}PC^{Ru}P)PdH (**3**) was monitored by ^{1}H NMR spectroscopy following the signal of C_5H_2 protons at 4.76 ppm. The rate constant was obtained from the difference between the integral area of C_5H_2 signals of **1** at 4.62 ppm and **3** at 4.76 ppm.

Preparation of (^{tBu}PC^{Ru}P)PdH (3)

To a solution of (^{tBu}PC^{Ru}P)PdCl (60 mg, 0.087 mmol) in 40 mL of absolute Et_2O at 0 °C was added $LiAlH_4$ (27 mg (0.71 mmol). The reaction mixture was stirred at this temperature for 1 h, then degassed distilled H_2O (0.07 ml, 3.89 mmol) was added and stirring was continued for 30 min. The supernatant solution was then decanted and evaporated in vacuum. The residue was extracted with pentane, the solution was filtered, concentrated in vacuum to a minimum volume and cooled to −15° C. The precipitated white crystals were separated and dried in vacuum. Yield: 52 mg (73%). According to the NMR data, the product has a purity of 80–85%.

NMR (298 K, C_6D_6, δ in ppm): ^{1}H: −2.92 (t, J_{HP} = 14.1 Hz, 1H, Pd*H*), 1.20, (vt, J_{HP} = 13.0 Hz 18H, CH_3), 1.31 (vt, J_{HP} = 13.8 Hz, 18H, CH_3), 2.69 (dvt, J_{HH} = 16.5 Hz, J_{HP} = 8.2 Hz, 2H, CH_AH$_B$P), 2.89 (dvt, J_{HH} = 16.5 Hz, J_{HP} = 5.6 Hz, 2H, CH$_A$$H_B$P), 4.44 (s, 5H, C_5H_5), 4.86 (s, 2H, C_5H_2 ^{31}P{^{1}H}: 107.27 (s).

Reaction of 3 with CO_2. Formation of (^{tBu}PC^{Ru}P)Pd(HCO$_2$) (4)

3 (7 mg, 0.01 mmol) was weighed into medium-walled NMR tube fitted with a resealable Teflon valve and dissolved in benzene-d$_6$ (0.5 mL). The tube was pressurized with 4 bar CO_2. The reaction was complete in less than 10 min, giving solution of **4**. The crystals suitable for XRD analysis were grown by slow solvent evaporation of benzene solution used for NMR measurements.

Anal. Calc. (%) for $C_{29}H_{48}P_2RuPd$ (%): C 49.89, H 6.93. **Found:** C, 50.61; H, 7.90.

FTIR (KBr, ν in cm^{-1}):

3097, 2959, 2943, 2924, 2899, 2867, 2761, 2669, 1620 (C=O), 1473 (C–O), 1393, 1370, 1316, 1263, 1181, 1100.

NMR (298 K, C_6D_6, δ in ppm): ^{1}H: 1.23, (vt, J_{HP} = 12.72 Hz, 18H, CH_3), 1.36 (vt, J_{HP} = 13.99 Hz, 18H, CH_3), 2.27 (dvt, J_{HH} = 16.69 Hz, J_{HP} = 8.42 Hz, 2H, CH_AH$_B$P), 2.53 (dvt, J_{HH} = 16.64 Hz, J_{HP} = 6.2 Hz, 2H, CH$_A$$H_B$P), 4.51 (s, 5H, C_5H_5), 4.65 (s, 2H, C_5H_2), 9.17 (s, 1H, *H*CO). ^{13}C{^{1}H}: 167.82 (s, *C*OO$^-$), 97.42 (vt, 2C*, J_{CP}* = 28.61 Hz, 2*C, 2,5*-C_5H_2), 72.88 (s, C_5H_5), 68.70 (vt, J_{CP} = 17.61 Hz 2*C, 3,4*-C_5H_2), 35.86 (vt, J_{CP} = 11 Hz, 1C *C*H$_2$P), 34.68 (vt, J_{CP} = 13.2 Hz, 1C *C*H$_2$P), 29.82 (vt, J_{CP} = 5.87 Hz, 9C, C(*C*H$_3$)$_3$), 29.59 (vt, J_{CP} = 8,07Hz, 9C, C(*C*H$_3$)$_3$), 25.26 (vt, J_{CP} = 21.3 Hz, 2C, *C*(CH$_3$)$_3$. ^{31}P{^{1}H}: 83.5 (s).

Characterization of (^{tBu}PC^{Ru}P)Pd(HCO$_3$) (5)

Slow evaporation of benzene solution of (^{tBu}PCRuP)PdH (**3**) under argon flow resulted in crystals which turned out being Pd(II) hydrocarbonate (**5**). The amount of this crystalline phase was enough for the spectroscopic (FTIR, NMR) characterisation and X-ray diffraction analysis (see the main text). it appears to be the most stable crystal phase in the mixture of hydride **3**, formate **4** and carbonate **5**, due to strong hydrogen bonding.

FTIR (KBr, ν in cm^{-1}): 3094, 2958, 2898, 2866, 2626, 2278, 1845, 1606 (C=O), 1466 (C–O), 1412 (C–O), 1392, 1371, 1355, 1264, 1180, 1162, 1099.

NMR (298 K, C_6D_6, δ in ppm, *J* in Hz): ^{1}H: 1.25, (vt, J_{HP} = 12.8 Hz, 18H, CH_3), 1.45 (vt, J_{HP} = 14.2 Hz, 18H, CH_3), 2.26 (dvt, J_{HH} = 16.6 Hz, J_{HP} = 8.5 Hz, 2H, CH_AH$_B$P), 2.51 (dvt, J_{HH} = 16.6 Hz, J_{HP} = 5.0 Hz, 2H, CH$_A$$H_B$P), 4.48 (s, 5H, C_5H_5), 4.62 (s, 2H, C_5H_2). ^{13}C{^{1}H}: 162.43 (s, *C*O$_2$OH), 109.89 (bt, 1C, *1*-C_5H_2), 97.52 (vt, J_{CP} = 29 Hz, 2*C, 2,5*-C_5H_2), 72.91 (s, C_5H_5), 67.63 (vt, J_{CP} = 17.3 Hz 2*C, 3,4*-C_5H_2), 35.49 (vt, J_{CP}

= 10.9Hz, 1C, *C*H_2P), 34.34 (vt, J_{CP} = 13.17 Hz, 1C, *C*H_2P), 29.55(vt, J_{CP} = 5.9 Hz, 9C, C(*C*H_3)$_3$), 29.36 (vt, J_{CP} = 7.27 Hz, 9C, C(*C*H_3)$_3$), 25.26 (vt, J_{CP} = 20.89 Hz, 2C, *C*$(CH_3)_3$). $^{31}P\{^1H\}$: 82.7 (s).

Computational details

The computations were carried out on "real" complexes without any ligand simplification. Full geometry optimizations were performed without symmetry constraints using the M06[3], B3LYP[4-6], BP86[7] and PBE0[8] methods implemented in Gaussian09 (Revision D.01)[9] software package. Effective core potentials (ECPs) and their associated SDD basis set supported with *f*-function polarization were used to represent the innermost electrons of the ruthenium and palladium atoms.[10] The basis sets used were 6-311++G(d,p) for the PCP ligand (with the exception of ^{t}Bu groups at phosphorus atoms[11]), BH_4^- fragment, palladium bound hydrogen and 6-31G for ^{t}Bu groups.[12, 13] The M06-optimized geometries quite well reproduced for all X-ray determined structures (**1**, **2**, **4**, **5**): the difference between the calculated and experimentally observed Pd–C, Pd–P and Pd···B bonds are less than 0.05 Å (Tables S5, S29, S37 and S41).

Frequency calculations were performed for all optimized complexes at the same level of theory to confirm a character of local minima on the potential energy surface and are reported without the use of scaling factors. The nature of all the stationary points on the potential energy surfaces was confirmed by an absence of any imaginary frequencies in vibrational analysis.[14] Transition state (TS) structures showed only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration using the Intrinsic Reaction Coordinate (IRC) method.[15] ZPVE correction was determined from the unscaled harmonic frequencies.[16, 17]

Inclusion of nonspecific solvent effects in the calculations was performed by using the SMD method.[18] The geometries of all species were optimized in toluene (ε = 2.4) or tetrahydrofurane (ε = 7.4) by SMD method. The calculations were carried out with ultrafine integration grid and very tight SCF option in order to improve the accuracy of the optimization procedure.

The Wiberg bond indices[19] (WBI) as measure of electron distribution between two atoms[20] and natural atomic charges were calculated using the natural-bond orbital (NBO) analysis[21] implemented in *Gaussian09*.[9] Topological analysis of the electron-density distribution function $\rho(r)$ was performed using the *AIMALL*[22] program package based on the wave function obtained by the M06 calculations. The delocalization index (DI)[23-25] is a measure of electrons that are shared or

exchanged between two atoms or basins, that obtained from the integration of the Fermi hole density, is directly related to the bond order.[26, 27] The X–Y bond ellipticity, ε_{X-Y}, was defined as $\varepsilon = (\lambda_1/\lambda_2 - 1)$, where λ_1 and λ_2 are the negative eigenvalues of the Hessian of the electron density at the bond critical point ordered such that $\lambda_1 < \lambda_2 < 0$. [28-30]

DHB Strength. The OH band shifts values, $\Delta\nu_{OH}$ ($\Delta\nu_{OH} = \nu_{OH}^{bond} - \nu_{OH}^{free}$), can be used to estimate the hydrogen bond formation enthalpy ($\Delta H°_{exp}$). Introduced by Iogansen for classical hydrogen bonds of organic acids and bases[31-33] the $\Delta Hº_{exp}/\Delta\nu_{OH}$ correlation (Eqn. S1) proved to be applicable to dihydrogen bonds.[34-36]

$$\Delta H^0 = -\frac{75 \cdot |\Delta\nu_{OH}|}{720 + |\Delta\nu_{OH}|} \qquad \text{(S1)}$$

The basicity factors (E_j), characterizing the proton accepting ability of the base participating in a hydrogen bond, can be calculated by the so-called "rule of factors" equation (Eqn. S2)[31-33] and are used to compare the properties of bases independent of a partner acid and solvent.

$$E_j = \frac{\Delta H^0}{\Delta H_{11}^0 \cdot P_i} \qquad \text{(S2)}$$

where ΔH_{11} is the enthalpy of the "standard" complex between phenol ($P_1 = 1.0$) and Et_2O ($E_1 = 1.0$) which is equal to –16.7 kJ/mol in toluene.[31]

DFT calculations of DHB complexes

According to DFT calculation ***syn*-1** in toluene interacts with proton donors (MeOH, TFE, HFIP) with formation monodentate (**Ia**) complexes on BH_{term} ligand and bifurcate DHB complexes (**IIa** and **IIab**) with coordination on two BH_{term} ligands or BH_{term} and BH_{br} ligands (Figures S16–S18, Table S9). Complexes **Ia** type characterized by short B–H_{term}···O–H distances (1.696–1.789 Å with O–H···H(B) angles 165–172°). Bifurcate complexes characterized by short B–H_{term}···O–H distances for primary interaction (1.719–1.939 Å with O–H···H(B) angles 145–173°) and longer B–H···O–H distances for the secondary contacts (1.954–2.258 Å with O–H···H(B) angles 147–123°). DHB formation causes typical elongation of O–H bond of proton donors (by 0.010–0.015 Å) and B–H bonds (0.003–0.008 Å) involved in DHB formation. It should be noted that in complexes **Ia** and **IIa** DHB formation causes elongation of Pd–H(B) (by 0.009–0.019 Å) and contraction of B–H(Pd) (by 0.004–0.019 Å).

Generally, the re-polarization of hydrogen atoms involved in DHB formation was anticipated.[37] During the DHB formation the increase of positive charge on the OH proton

($\Delta q^{NBO}_{[(O)H]}$ is 0.032 ÷ 0.047) of proton donors (MeOH, TFE, HFIP) and increase of negative charge for the BH_{term} ligand ($\Delta q^{NBO}_{[(B)Hterm]}$ is −0.002 ÷ −0.022) were observed (Table S10). It should be noted that for bifurcate DHB complexes of **IIab_anti** type (with coordination on BH_{term} and BH_{br} ligand) for some complexes the significant increase of negative charge was observed on BH_{br} ligand ($\Delta q^{NBO}_{[(B)Hbr}$ increased up to −0.081). The changes of Wiberg bond indices[19] (ΔWBI, Table S10) also reflect the depopulation of OH (ΔWIB_{OH} is −0.097 ÷ −0.147) and BH bonds (ΔWIB_{BHterm} is −0.011 ÷ −0.043) with simultaneous appearance of the electron density for the H···H contacts ($\Delta WIB_{H\cdots H}$ are 0.009 ÷ 0.030 for primary contact B–H_{term}···O–H and up to 0.007 for secondary B–H_{term}···O–H or B–H_{br}···O–H interactions). It should be noted that in all DHB complexes the depopulation of Pd–H(B) was observed (ΔWIB_{PdHbr} is −0.007 ÷ −0.041). This fact indicates the weakening of the interaction between palladium atom and the BH_4^- fragment as the result of DHB formation. Previously the same phenomenon was observed in the case of copper(I) tetrahydroborates.[38, 39]

The DHB formation between **1** and ROH also confirmed by energy donation (E^2, estimated from second-order perturbative analysis of donor-acceptor interactions, Table S10) from σ(B–H) to σ^*(O–H) (E^2 = 10.0–31.0 kJ/mol for the primary contact B–H_{term}···O–H and E^2 = 3.3–7.9 kJ/mol for thr B–H_{term}···O–H or B–H_{br}···O–H interactions). According to QTAIM analysis the (+3;−1) critical point (ρ_c = 0.02 a.u.) was found only for the B–H_{term}···O–H primary contact (Figures S19–S21, Table S11). The presence of B–H···O–H secondary interactions causes deviation of O–H···H(B) angles from linearity and reflected in the values of H···H bond ellipticity ($\varepsilon_{H\cdots H}$ = 0.17–0.26 for **Ia** and $\varepsilon_{H\cdots H}$ = 0.37–0.78 for **IIab** DHB complexes). Extremely high $\varepsilon_{H\cdots H}$ ellipticity values observed for **IIa** DHB complexes ($\varepsilon_{H\cdots H}$ = 1.17–8.31) correlate with the location the minima of molecular electrostatic potential (MEP) in **1** (Figure 3), which is located almost equidistantly from BH_{term} ligands.

Description of crystal structure of complex 2

In complex **2** two ruthenocene palladacycle fragments (**A**) and (**B**) are rotated by ca. 90° relative to each other (Figure S22). The structural parameters of ruthenocene palladacycle fragments are different: one (**A**) is similar to initial borohydride complex **1**, the structure of the second (**B**) is significantly distorted. In both fragments the palladium atoms have a distorted square-planar geometry with “gull wing” ” pincer arms conformation, with angles P(1)–Pd–P(2) 156.66(4) (**A**) and P(1A)–Pd–P(2A) 154.24(4) Å (**B**), being smaller compare to 160.58(2) in **1**.

The carbon atoms of methylene bridges are situated on the Cp-ring plane (**A**) C(15) 0.014 Å, C(6) 0.011 Å, (**B**) (C(15A) 0.042 Å, C(6A) 0.000 Å), for **1** (C(11) 0.009 Å C(12) 0.038 Å), the phosphorus atoms in fragment (**A**) rise above the plane on P(1) 0.251 Å and P (2) 0.483 Å, in fragment (**B**) on P(1A) 0.268 Å and P(2A) 0.178 Å, whereas these distances are 0.367 Å, 0.379 Å in **1**. Palladium atoms are deviated from the plane of the Cp-ring in the direction opposite to the ruthenium atom by 0.150 Å (**A**) and 0.132 Å (**B**). This deviation is much smaller compared to initial borohydride complex **1** (0.322 Å). At the same time the Cp-rings appear differently inclined in complexes **2** [4.05º (**A**), and 1.42º (**B**)], and **1** (2.42°), while the distance between the Cp rings centroids of **2** (3.623 Å (**A**) and 3.630Å (**B**)) is almost the same as in **1** (3.636 Å).

This disposition of two ruthenocene palladacycle fragments (**A**) and (**B**) in **2** rotated by ca. 90° relative to each other (Figure S22) leads to non-equivalence of phosphorus nuclei in palladacycle fragments, which is manifested as AB spin system in phosphorus NMR.

Table S1. Crystal data and structure refinement parameters for **1**, **2**, **4** and **5**.

	1	**2**	**4**	**5**
Empirical formula	$C_{28}H_{51}BP_2PdRu$	$C_{68}H_{102}B_2F_{24}O_4P_4Pd_2Ru_2$	$C_{32}H_{51}O_2P_2PdRu$	$C_{41}H_{60}O_3P_2PdRu$
Formula weight	667.90	1999.93	737.13	870.30
Crystal system	Monoclinic	Triclinic	Triclinic	Monoclinic
Space group	$P2_1/c$	P-1	P-1	$P2_1/n$
Z	4	2	2	4
a, Å	10.9154(4)	14.6724(11)	9.8920(5)	14.0995(9)
b, Å	18.1161(6)	15.4144(11)	12.0215(6)	19.7160(13)
c, Å	15.8325(6)	20.2741(15)	15.1339(7)	15.7422(10)
α, °	90	99.8970(10)	109.1100(10)	90
β, °	106.5607(7)	99.7330(10)	105.3890(10)	110.4874(12)
γ, °	90	99.8720(10)	96.9360(10)	90
V, Å^3	3000.92(19)	4356.1(6)	1596.37(14)	4099.3(5)
D_{calc} (g cm^{-1})	1.478	1.525	1.534	1.410
Linear absorption, μ (cm^{-1})	12.24	9.12	11.63	9.2
F(000)	1376	2016	758	1800
$2\Theta_{max}$, °	60	54	60	60
Reflections measured	38541	73348	21508	52539
Independent reflections	8753	18998	9295	11939
Observed reflections [$I > 2\sigma(I)$]	8016	16889	7335	10242
Parameters	326	1009	355	449
R1	0.0309	0.0465	0.0352	0.0317
wR2	0.0591	0.1634	0.0764	0.0763
GOF	1.195	1.147	1.002	1.056
$\Delta\rho_{max}$/ $\Delta\rho_{min}$ (e Å^{-3})	0.550/−0.850	3.587/−1.870	0.638/-0.831	2.145/−1.008

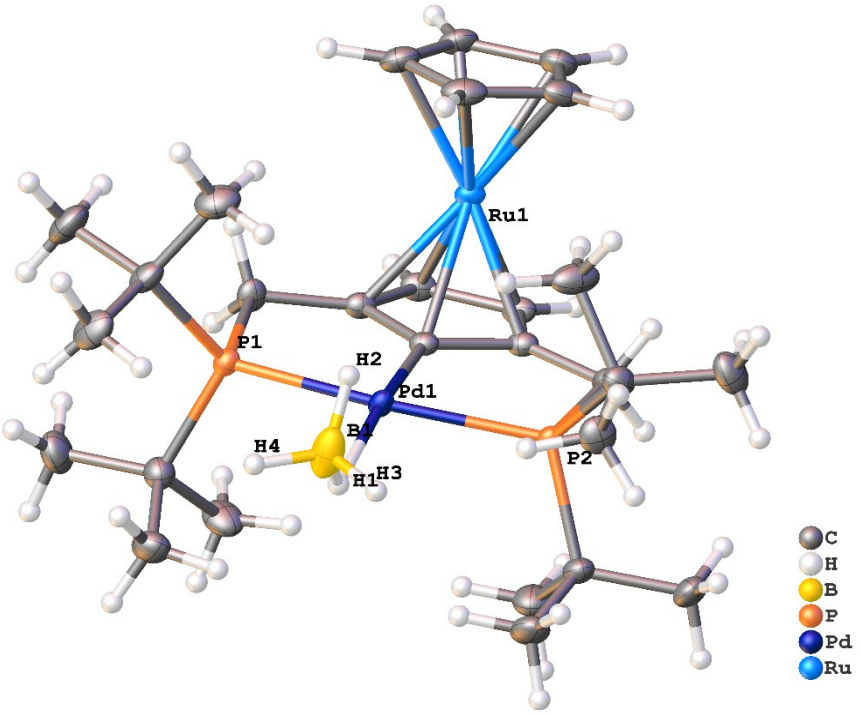
Table S2. The distances (in Å) between two ^{t}Bu groups in **syn-** and **anti**-position in complexes **1**, **4** and **5**.

Complex	**syn**-position		**anti**-position	
1	H18C···H26B	3.40	H14B···H22C	2.61
			H16C···H24B	3.53
4	H19C···H26A	3.39	H15A···H22C	2.38
			H16C···H24A	3.71
5	H19B···H26C	3.50	H16B···H24C	2.33
			H15C···H22B	3.16

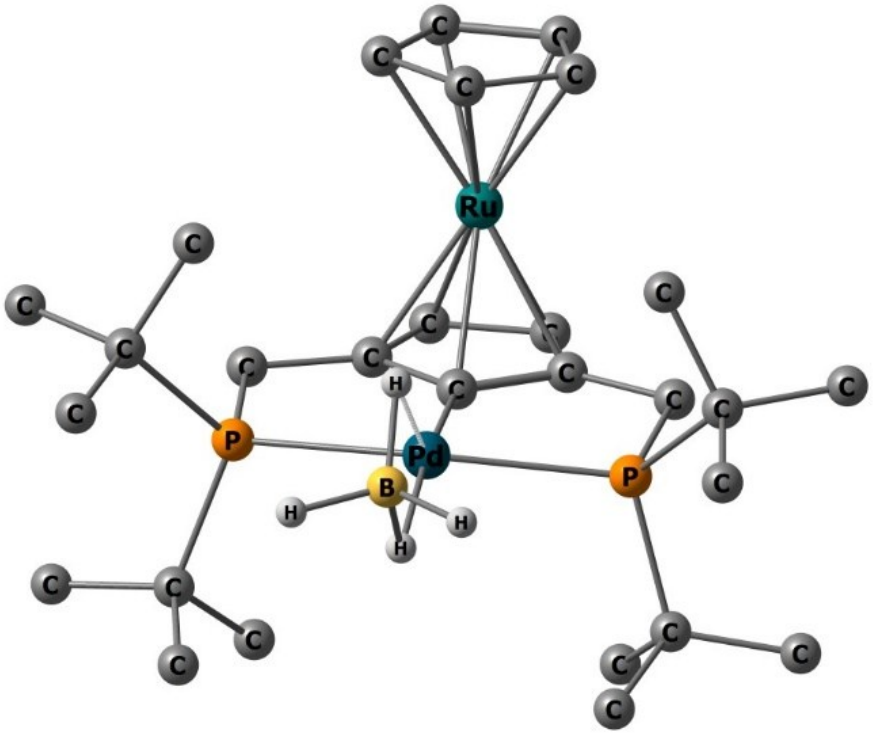
Table S3. Geometry parameters of crystal and DFT-optimized structures of **1**.

Distances	**1**	**M06**	**BP86**	**B3LYP**
Pd–C	1.980(2)	1.999	1.996	1.997
Pd–P_1	2.3443(7)	2.390	2.388	2.405
Pd–P_2	2.3454(7)	2.397	2.390	2.407
Pd···B	2.587(3)	2.563	2.546	2.662
Pd–H_1(B)	**1.87(2)**	**1.816**	**1.779**	**1.771**
Pd···H_2(B)	**2.54(3)**	**2.482**	**2.491**	**2.696**
B–H_1	1.11(2)	1.284	1.301	1.292
B–H_2	1.10(3)	1.221	1.227	1.214
B–H_3	1.06(3)	1.213	1.219	1.211
B–H_4	1.04(4)	1.213	1.219	1.211
C–Pd–B	170.3(1)	166.37	166.69	166.92
P_1–Pd–P_2	160.58(2)	158.27	159.68	159.71
Pd–H_1–B	118(2)	110.32	110.54	119.90
Pd–H_2–B	80(2)	79.68	78.41	75.37

Figure S1. (a) General view of molecular structure of **1** (thermal ellipsoids of all non-hydrogen atoms are drawn at the 50% probability level. (b) M06-optimized geometry of ***syn*-1** configuration. Hydrogen atoms of the ligand are omitted for clarity.

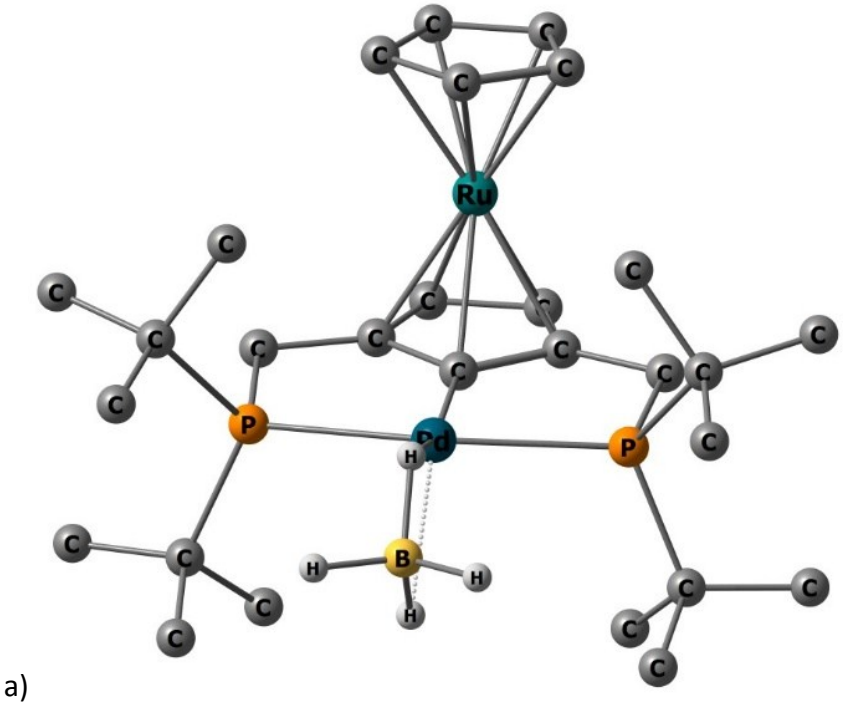


a)

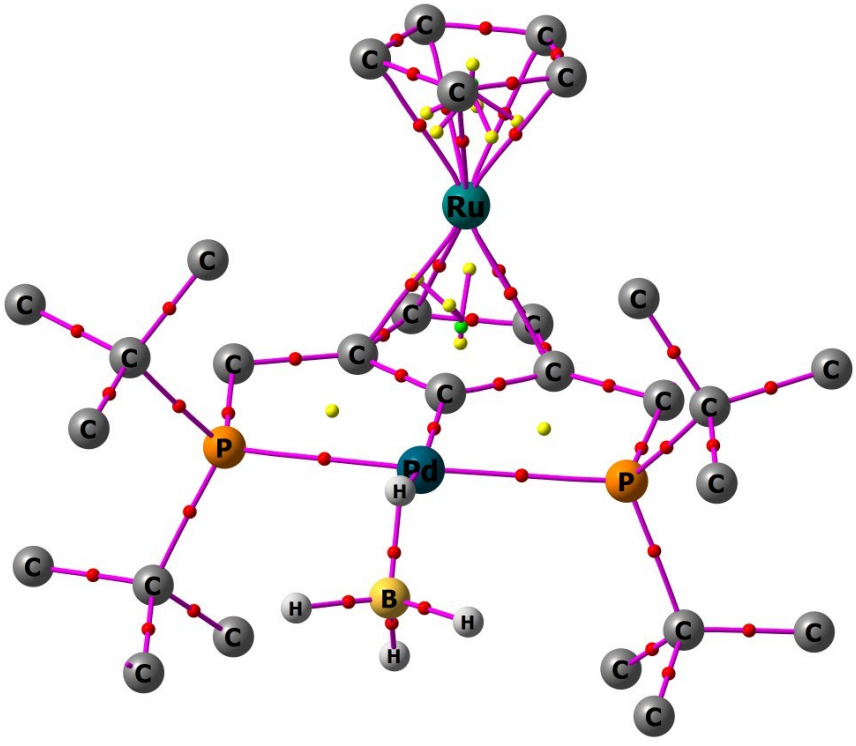


b)

Figure S2. (a) M06-optimized geometry of ***anti*-1** configuration. (b) QTAIM molecular graph of M06-optimized geometry of ***anti*-1** configuration. Hydrogen atoms of the ligand are omitted for clarity. Red spheres denote critical points (+3;−1), yellow spheres denote ring critical points (+3;+1) and green spheres denote cage critical points (+3;+3).



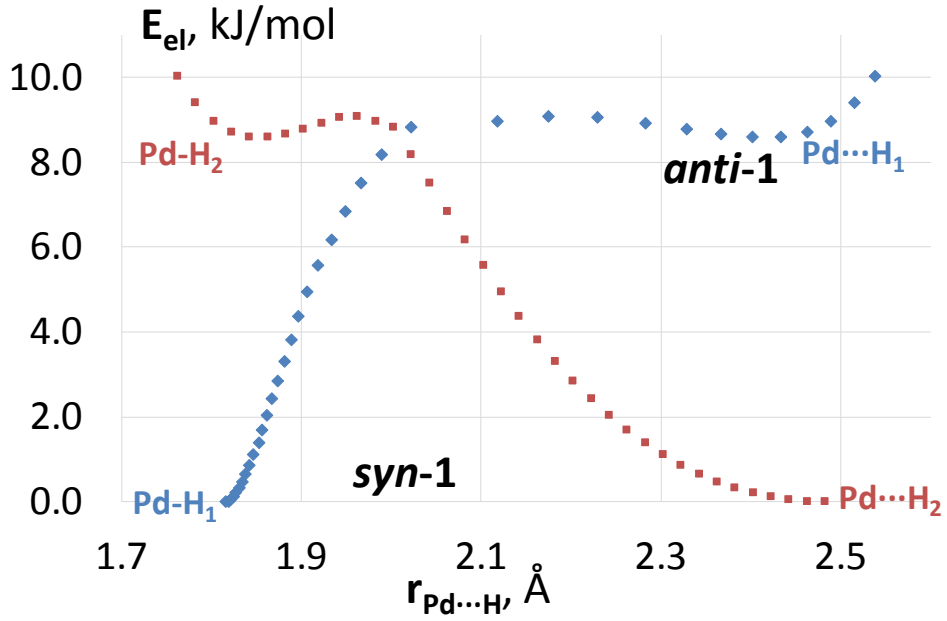
a)

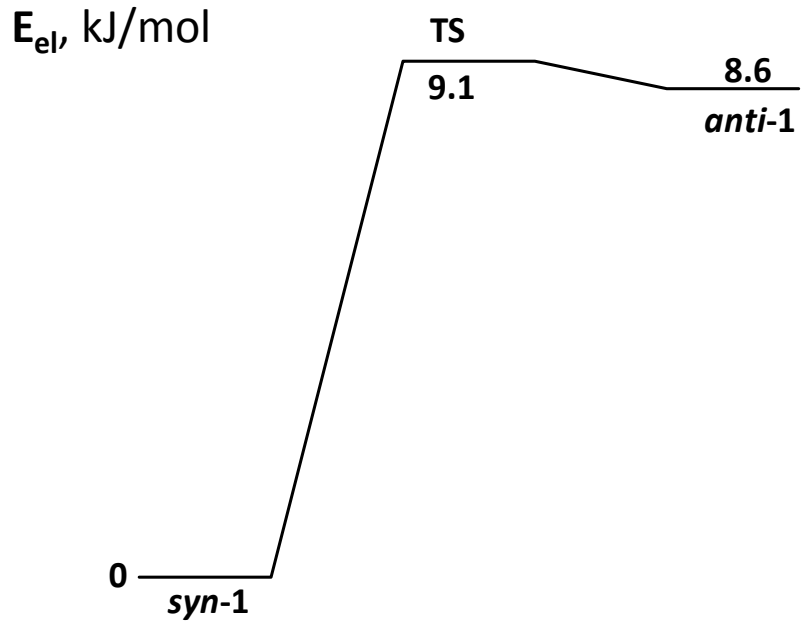


b)

Figure S3. (a) Energy scan of shortening Pd···H_2 coordinate (step size = 0.02 Å). (b) Energy profile of the BH_{br}/BH_{term} exchange for **1**.

a)





b)

Table S4. The main donor-acceptor orbital interactions and donation energy (E^2 and their sum ΣE^2 in kJ/mol) estimated from second-order perturbative analysis of donor-acceptor interactions for isomeric ***syn*-1** and ***anti*-1** configurations and ***syn,syn*-2**.

Compound	Donor orbital	Acceptor orbital	E^2	ΣE^2
***syn*-1**	$y_{B–H1}$	$d_{z^2(Pd)}^*$	137.7	195.0
		y^*_{Pd-C}	57.3	
	$y_{B–H2}$	$d_{z^2(Pd)}^*$	38.9	71.5
		$d_{xz(Pd)}^*$	30.1	
		y^*_{Pd-C}	2.5	
***anti*-1**	$y_{B–H2}$	$d_{z^2(Pd)}^*$	124.3	184.1
		y^*_{Pd-C}	52.3	
		$d_{xz(Pd)}^*$	7.5	
	$y_{B–H1}$	$d_{z^2(Pd)}^*$	70.3	94.6
		$d_{xz(Pd)}^*$	21.3	
		y^*_{Pd-C}	2.9	
***syn,syn*-2**	$y_{B–H1}$	$d_{z^2(Pd)}^*$	63.6	107.5
		y^*_{Pd-C}	43.9	
	$y_{B–H2}$	$d_{z^2(Pd)}^*$	20.9	41.4
		$d_{xz(Pd)}^*$	16.3	
		y^*_{Pd-C}	4.2	
	$y_{B–H3}$	$d_{z^2(Pd)}^*$	62.8	111.3
		y^*_{Pd-C}	49.0	
	$y_{B–H4}$	$d_{z^2(Pd)}^*$	15.5	36.4
		$d_{xz(Pd)}^*$	16.3	
		y^*_{Pd-C}	4.2	

Table S5. QTAIM delocalization indices (DI), sum of donation energy (sum ΣE^2 in kJ/mol) estimated from second-order perturbative analysis of donor-acceptor interactions and Wiberg bond indices (WIB) for **1** isomeric ***syn*-1** and ***anti*-1** configurations and ***syn,syn*-2**.

Compound	DI_1	DI_2	DI_1/DI_2	Σ_1E^2	Σ_2E^2	Σ_1E^2/Σ_2E^2	WIB_1	WIB_2	WIB_1/WIB_2
***syn*-1**	0.45	0.14	3.1	195.0	71.5	2.7	0.36	0.11	3.2
***anti*-1**	0.43	0.16	2.6	184.1	94.6	1.9	0.31	0.11	2.8
***syn,syn*-2**	0.38	0.14	2.7	107.5	41.4	2.6	0.20	0.06	3.5
	0.39	0.13	2.9	111.3	36.4	3.1	0.21	0.05	3.8

Figure S4. ^{1}H NMR spectrum (400 MHz) of **1** in C_6D_6.

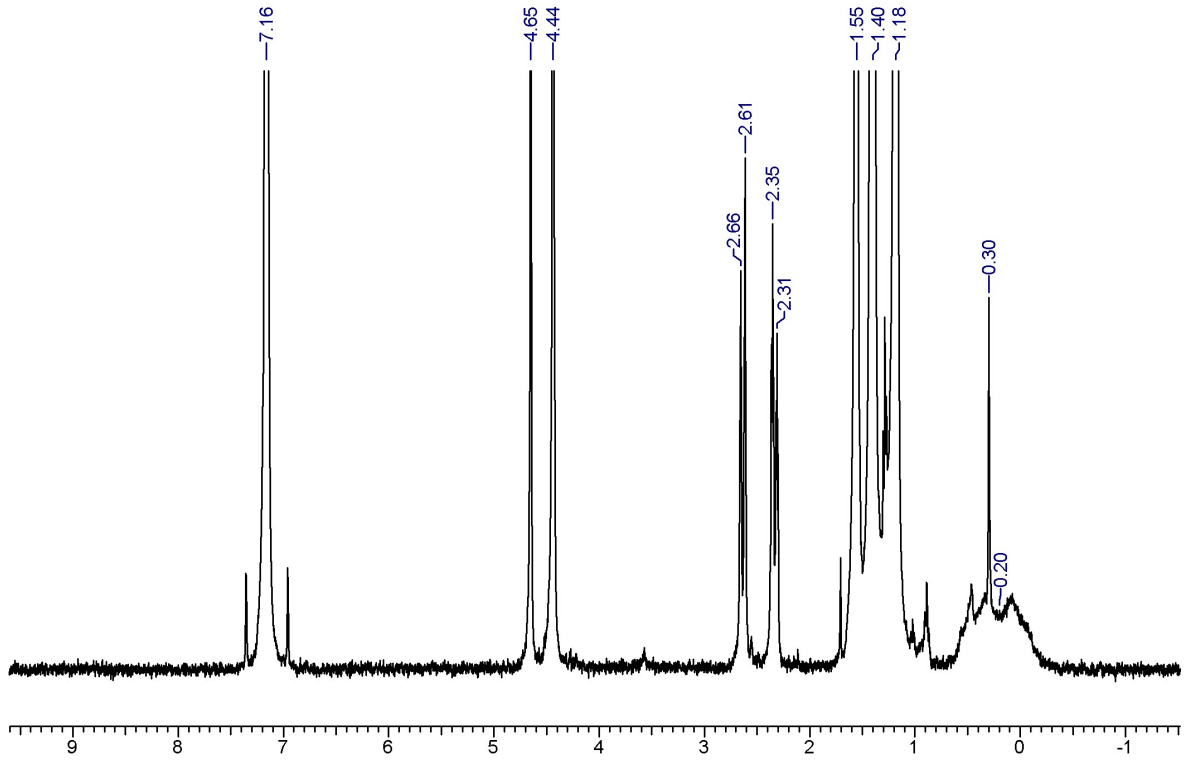


Figure S5. $^{11}B\{^{1}H\}$ NMR spectrum (128.4 MHz) of **1** in C_6D_6.

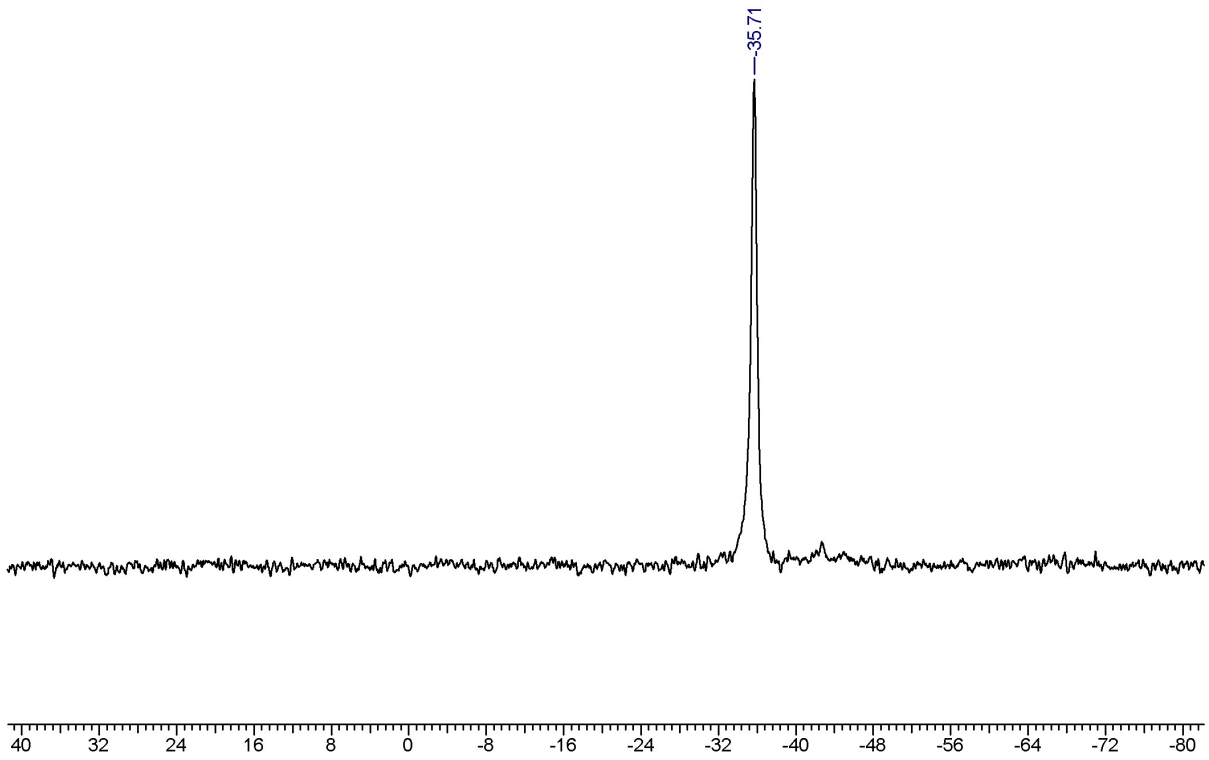


Figure S6. $^{31}P\{^{1}H\}$ NMR spectrum (162.0 MHz) of **1** in C_6D_6.

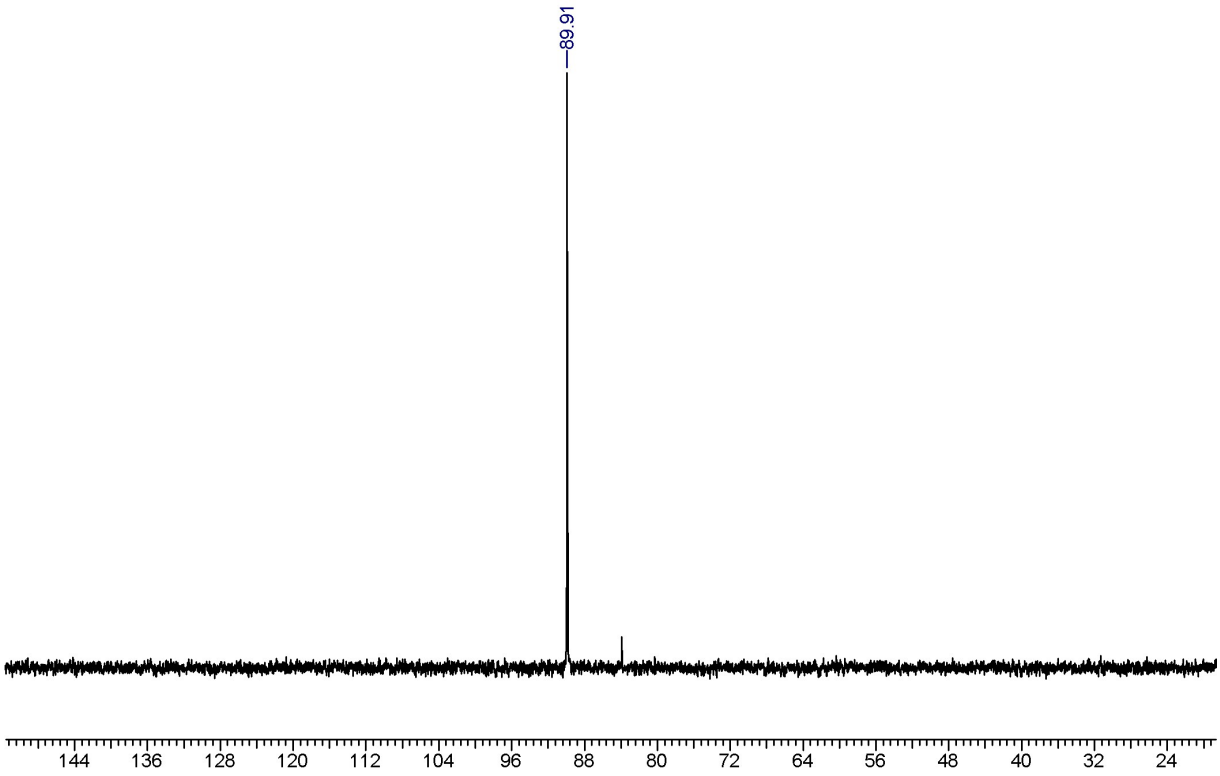


Figure S7. ^{1}H NMR spectrum (500 MHz) of **1** in toluene-d_8.

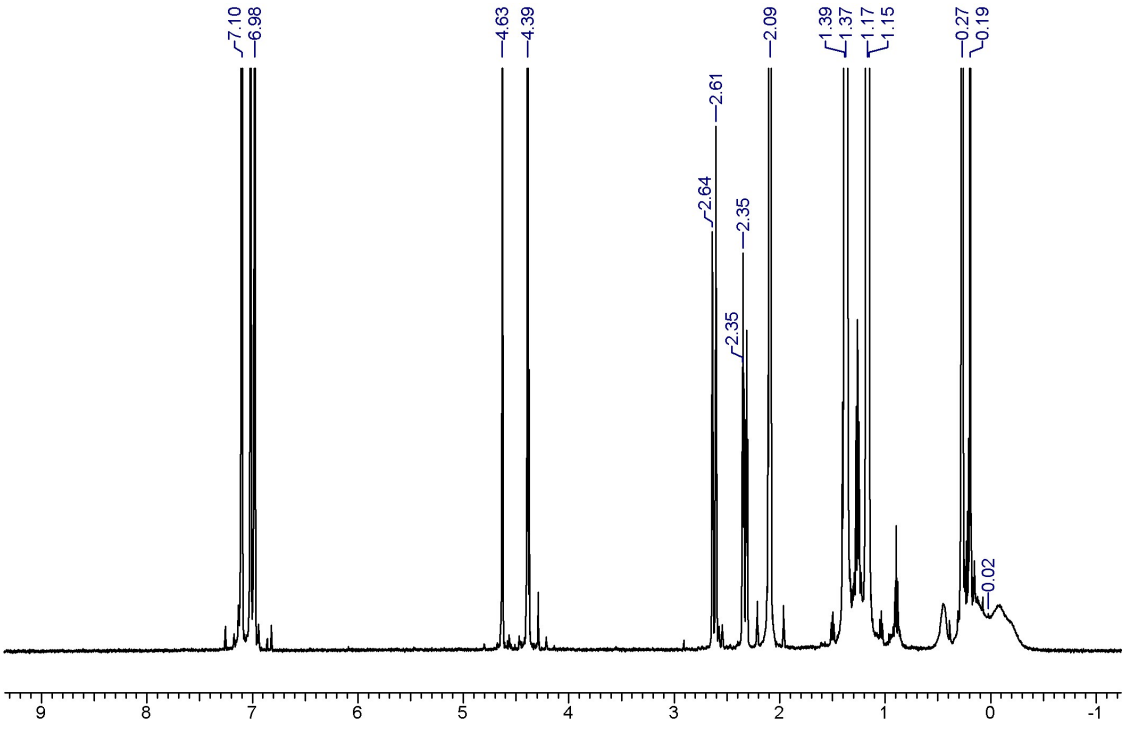


Figure S8. $^{11}B\{^{1}H\}$ NMR spectrum (160.5 MHz) of **1** in toluene-d_8.

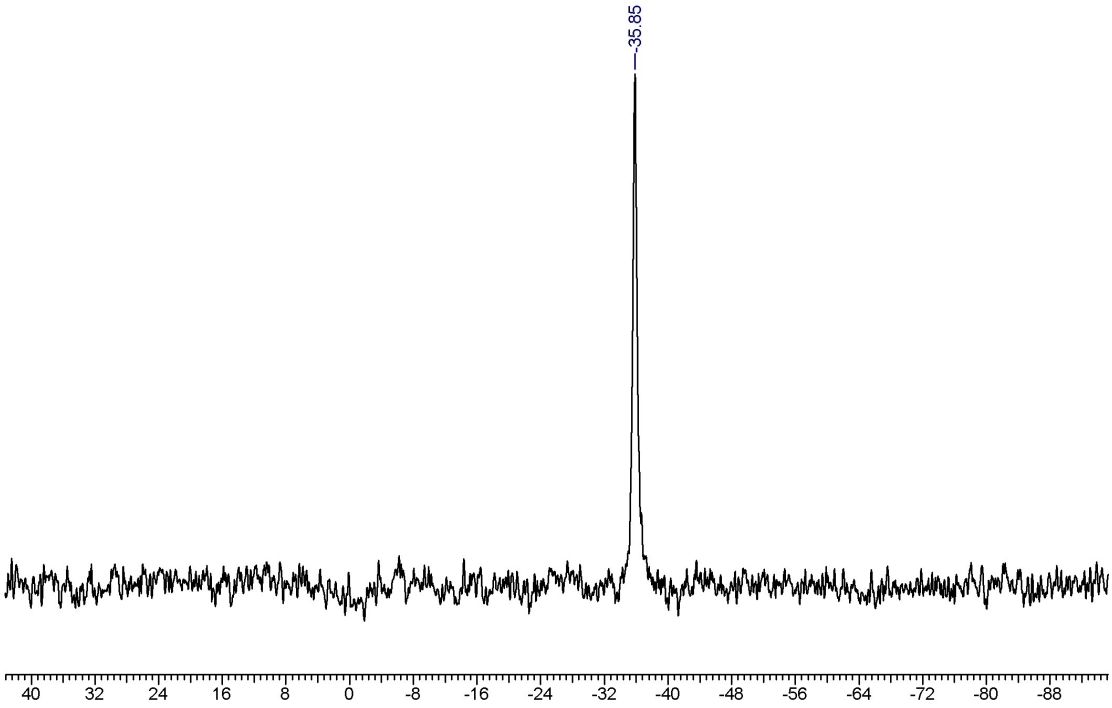


Figure S9. $^{31}P\{^{1}H\}$ NMR spectrum (202.5 MHz) of **1** in toluene-d_8.

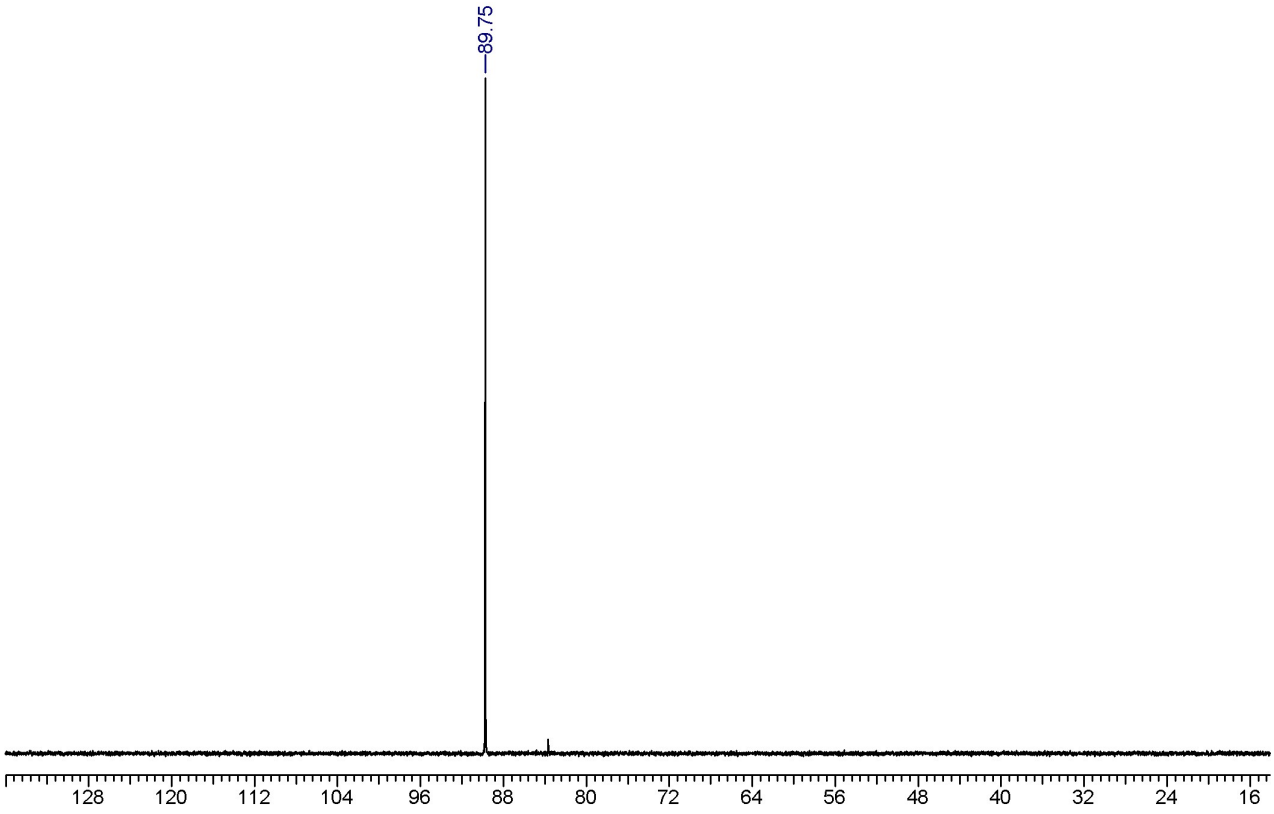


Figure S10. FTIR spectrum of **1** in KBr pellet.

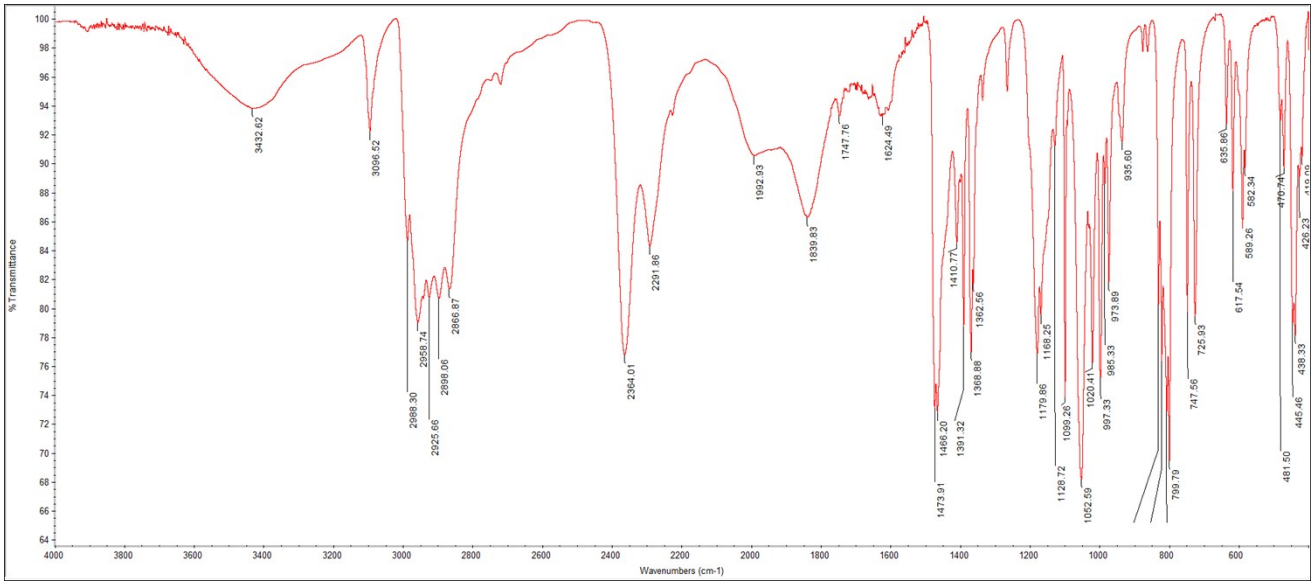


Figure S11. FTIR spectrum of **1-d_4** in KBr pellet.

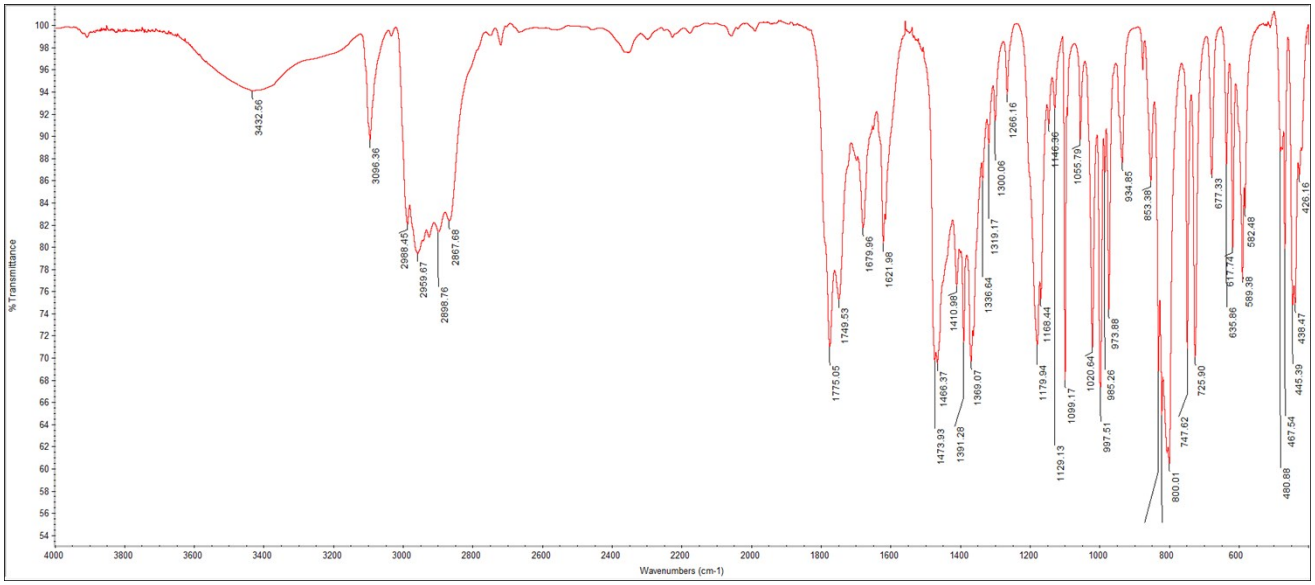


Figure S12. ^{1}H NMR spectrum (400 MHz) of **1-d_4** in C_6D_6.

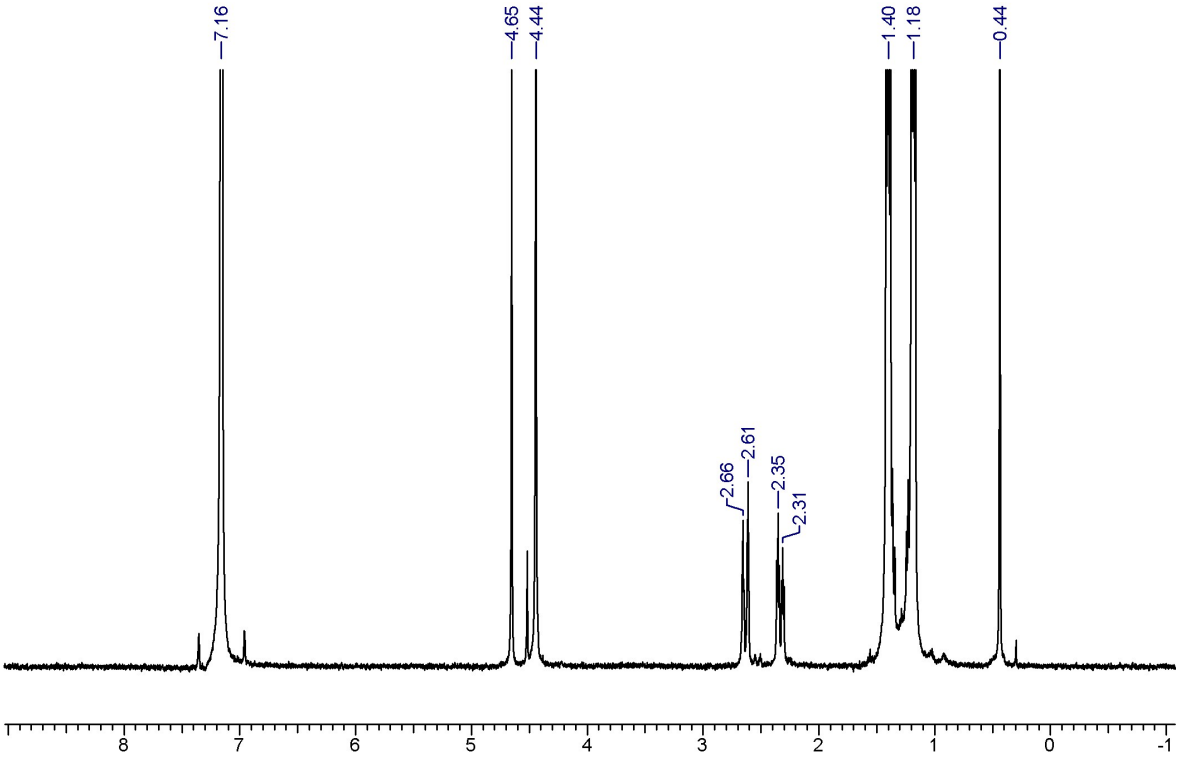


Figure S13. ^{2}H NMR spectrum (61.4 MHz) of **1-d_4** in C_6D_6.

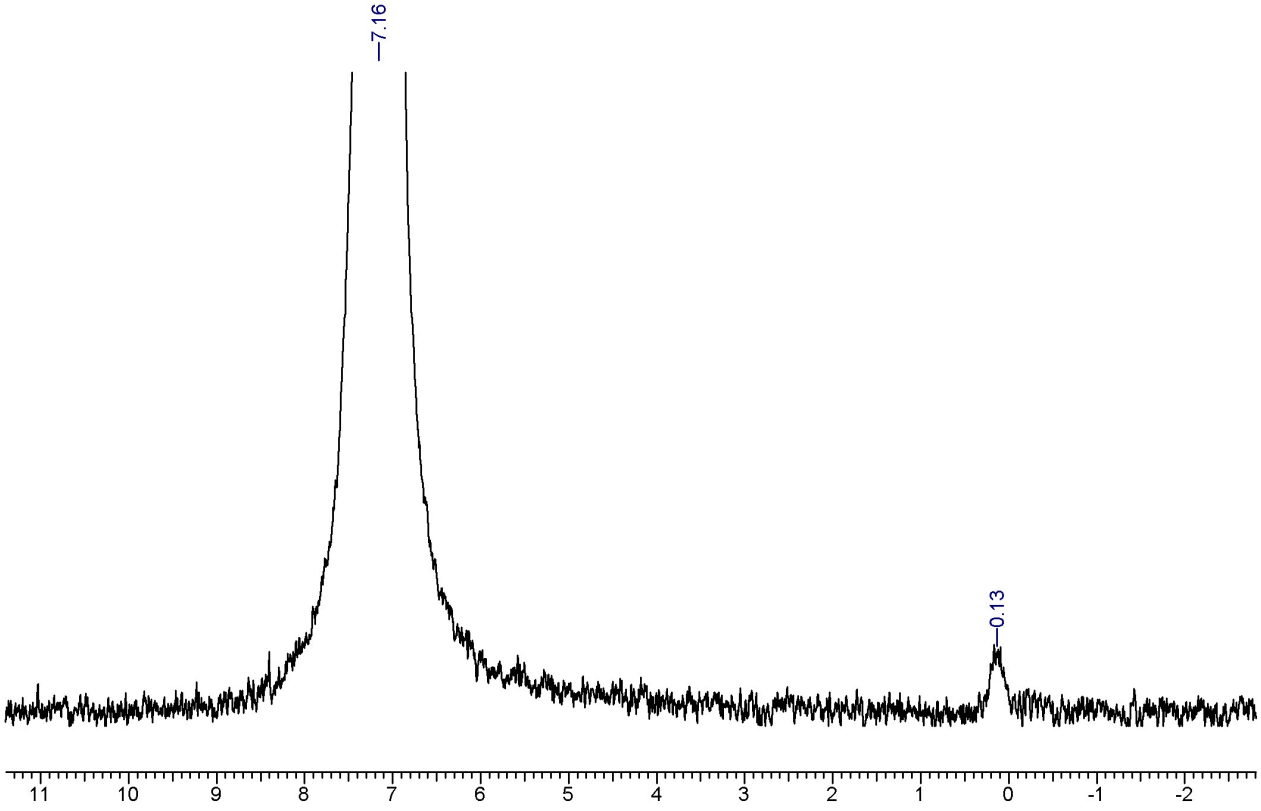


Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum (162.0 MHz) of **1-d_4** in C_6D_6.

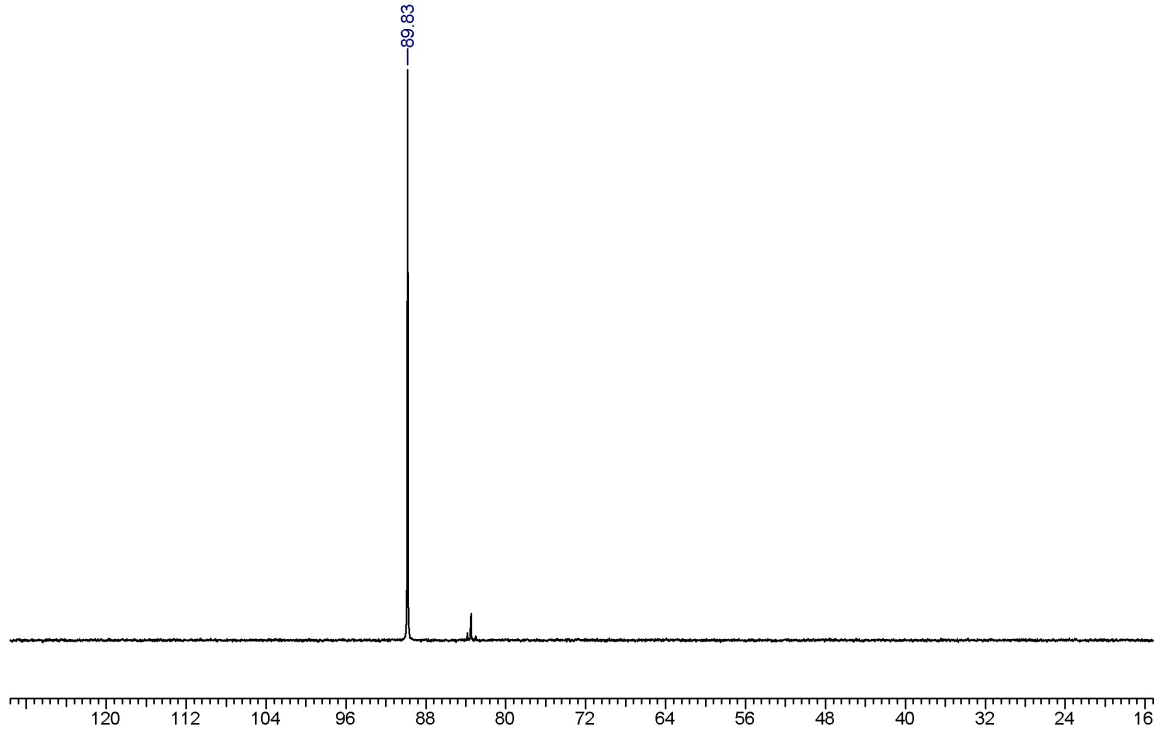


Figure S15. $^{11}B\{^{1}H\}$ NMR spectrum (128.4 MHz) of **1-d_4** in C_6D_6.

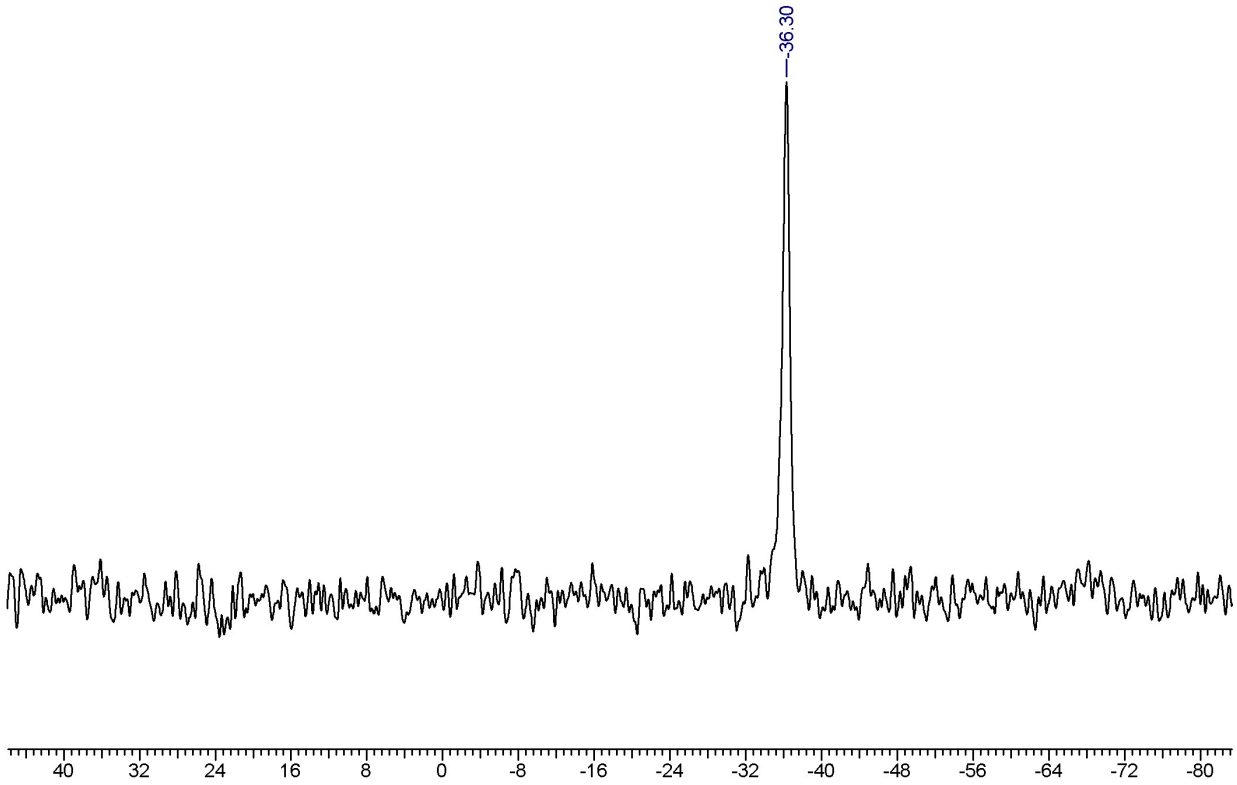


Table S6. CCDC analysis of the structures of Pd(II) tetrahydroborates.

№	Compound	$r_{(M\cdots B)}$	$r_{(M-H^{A}_{br})}$	$r_{(M\cdots H^{B}_{br})}$	$r_{(B-H^{A}_{br})}$	$r_{(B-H^{B}_{br})}$	$\angle_{(M-H^{A}-B)}$	$\angle_{(M-H^{B}-B)}$	CSD refcode	CSD №	Ref
1.	**Pd**(2,6-($^{i}Pr_2PO$)$_2C_6H_3$)($\eta^{1,2}$-BH_4)	2.420(2)	1.78(2)	2.21(2)	1.27(2)	1.14(2)	103(1)	86(1)	FIRCUH	1872776	[40]
2.	**Pd**(2,6-($^{t}Bu_2PO$)$_2C_6H_3$)($\eta^{1,2}$-BH_4)	2.464(4)	1.91(3)	2.11(3)	1.18(3)	1.25(4)	103(2)	91(2)	FIRCOB	1872775	[40]
3.	**Pd**[{2,5-($^{t}Bu_2PCH_2$)$_2C_5H_2$}Ru(C_5H_5)]($\eta^{1,2}$-BH_4)	2.587(3)	1.87(2)	2.54(3)	1.11(2)	1.10(3)	118(2)	80(2)	–	1882669	This work
4.	**Pd**[{2,5-($^{t}Bu_2PCH_2$)$_2C_5H_2$}Fe(C_5H_5)]($\eta^{1,2}$-BH_4)	2.613(9)	2.00(4)	2.56(6)	0.91(4)	1.13(5)	123(4)	80(3)	EYUJEN	248899	[41, 42]

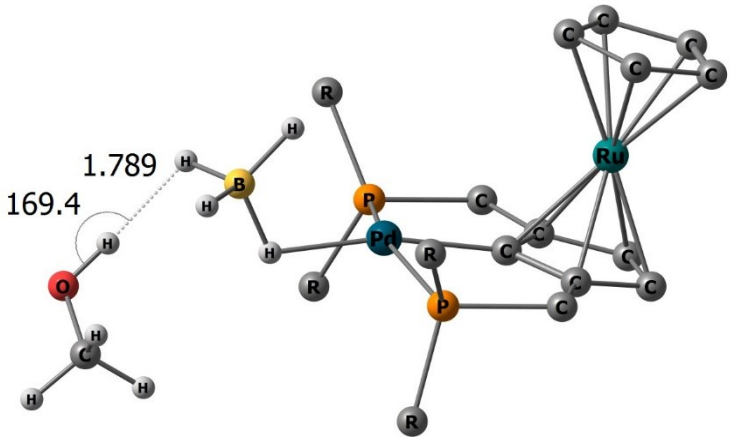
Table S7. ^{11}B and ^{1}H NMR characteristics of Pd(II) tetrahydroborates.

№	Compound	Solvent	^{11}B, δ_{BH4} (ppm)	^{1}H, δ_{BH4} (ppm)	Ref
1.	Pd[{2,5-($^{t}Bu_2PCH_2$)$_2C_5H_2$}Ru(C_5H_5)]($\eta^{1,2}$-BH_4)	C_6D_6	−35.8	+0.2	This work
		toluene-d_8	−35.9	0.0	This work
2.	Pd[{2,5-($^{t}Bu_2PCH_2$)$_2C_5H_2$}Fe(C_5H_5)]($\eta^{1,2}$-BH_4)	$CDCl_3$	−37.3 (83.1 Hz)	−0.5 (98 Hz)	[41, 42]
3.	Pd[{2,5-($^{i}Pr_2PCH_2$)$_2C_5H_2$}Fe(C_5H_5)]($\eta^{1,2}$-BH_4)	C_6D_6	−37.7 (81.3 Hz)	+0.3 (97/55 Hz)	[41, 42]
4.	Pd(2,6-($^{i}Pr_2PO$)$_2C_6H_3$)($\eta^{1,2}$-BH_4)	C_6D_6	−39.5 (81.0 Hz)	+0.2 (77 Hz)	[40]
5.	Pd(2,6-($^{t}Bu_2PO$)$_2C_6H_3$)($\eta^{1,2}$-BH_4)	C_6D_6	−39.8 (82.4 Hz)	+0.4 (75 Hz)	[40]

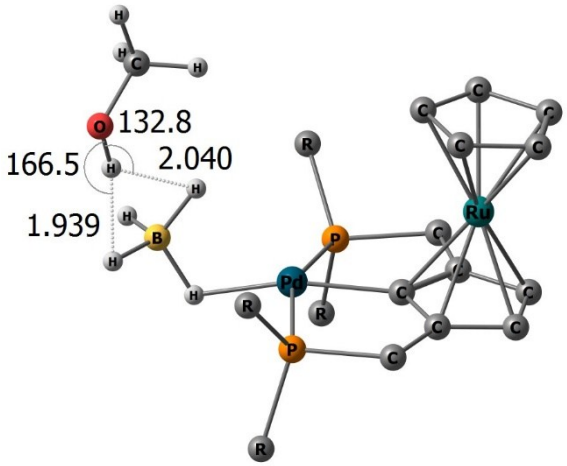
Table S8. Chemical shifts (δ_H in ppm) of selected ^{1}H NMR signals of **1** in the presence of fluorinated alcohols [CH_2FCH_2OH (MFE), CF_3CH_2OH (TFE) and $(CF_3)_2CHOH$ (HFIP)] in toluene-d_8.

	BH_4^-	–CH_2–				–C_5H_2–	C_5H_5 (Cp)	^{t}Bu–	
free **1**	0.06	2.68	2.64	2.38	2.35	4.67	4.43	1.41	1.20
MFE									
1.4 eqv	0.05	2.67	2.64	2.38	2.35	4.67	4.43	1.41	1.20
3.5 eqv	0.04	2.67	2.64	2.38	2.35	4.66	4.42	1.41	1.20
17.0 eqv	0.00	2.67	2.63	2.38	2.35	4.66	4.42	1.40	1.20
TFE									
1.65 eqv	0.03	2.67	2.64	2.38	2.35	4.66	4.42	1.40	1.20
4.65 eqv	0.01	2.66	2.63	2.38	2.34	4.66	4.42	1.39	1.19
14.0 eqv	−0.05	2.65	2.62	2.36	2.33	4.65	4.41	1.37	1.18
HFIP									
0.7 eqv	0.05	2.67	2.63	2.38	2.33	4.67	4.43	1.40	1.20
1.8 eqv	−0.01	2.65	2.61	2.36	2.32	4.66	4.42	1.38	1.18
7.0 eqv	−0.11	2.62	2.58	2.34	2.29	4.64	4.40	1.33	1.15
13.85 eqv	−0.18	2.60	2.56	2.32	2.28	4.63	4.39	1.32	1.14

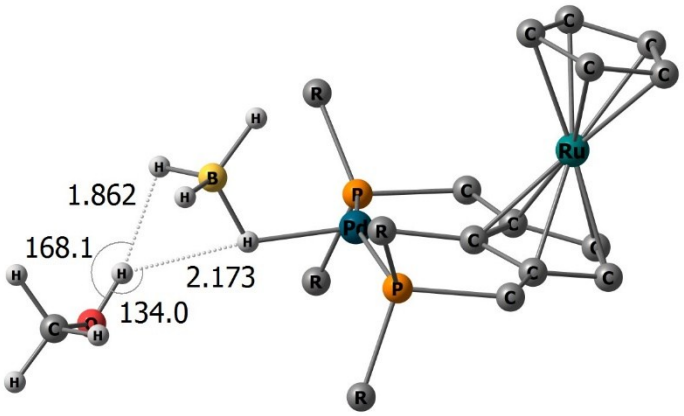
Figure S16. M06-optimized geometries of DHB complexes of **1** with MeOH in toluene. Hydrogen atoms of the ligand are omitted for clarity.



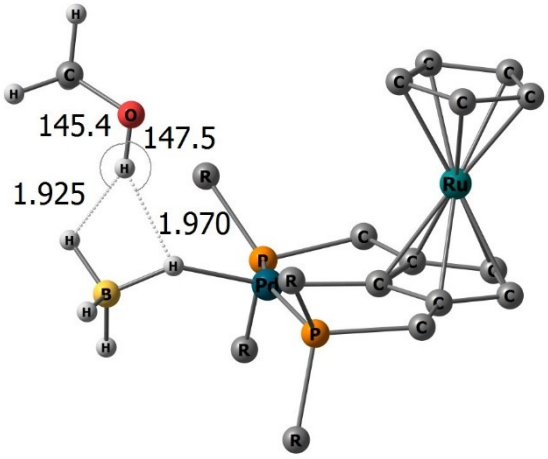
***syn*-1_Ia**



***syn*-1_IIa**

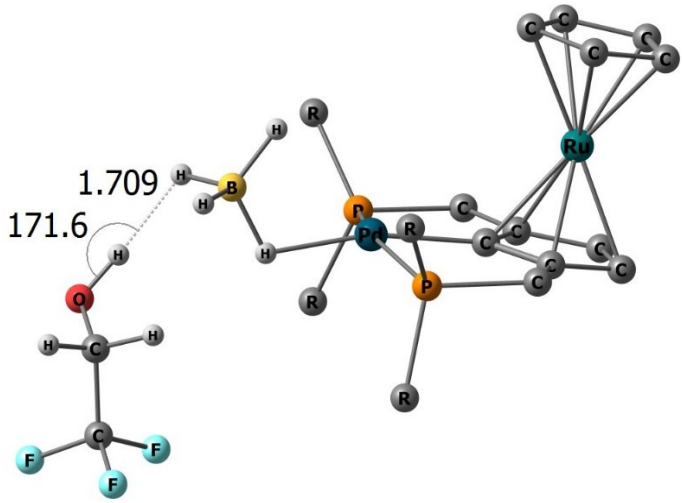


***syn*-1_IIab**

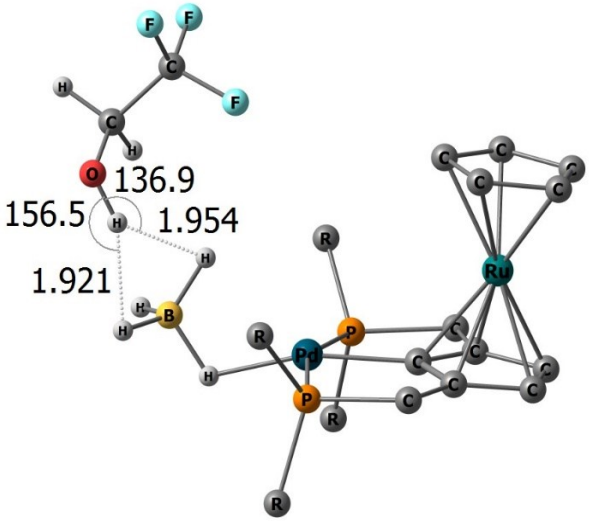


***anti*-1_IIab**

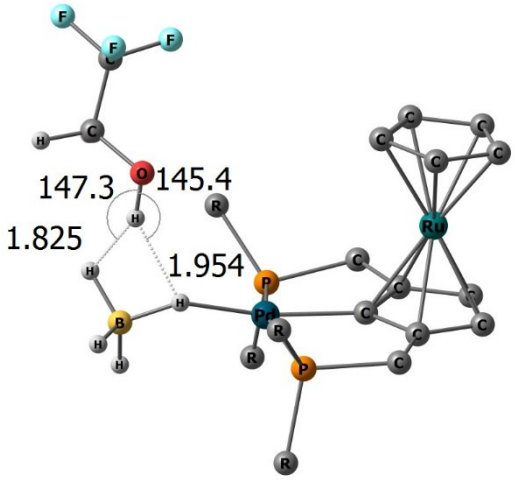
Figure S17. M06-optimized geometries of DHB complexes of **1** with TFE in toluene. Hydrogen atoms of the ligand are omitted for clarity.



***syn*-1_Ia**

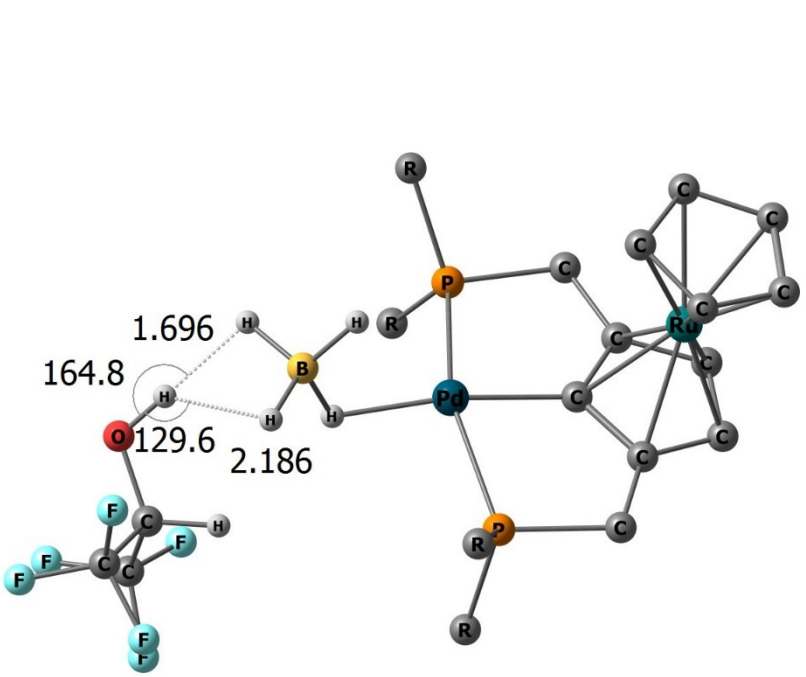


***syn*-1_IIa**

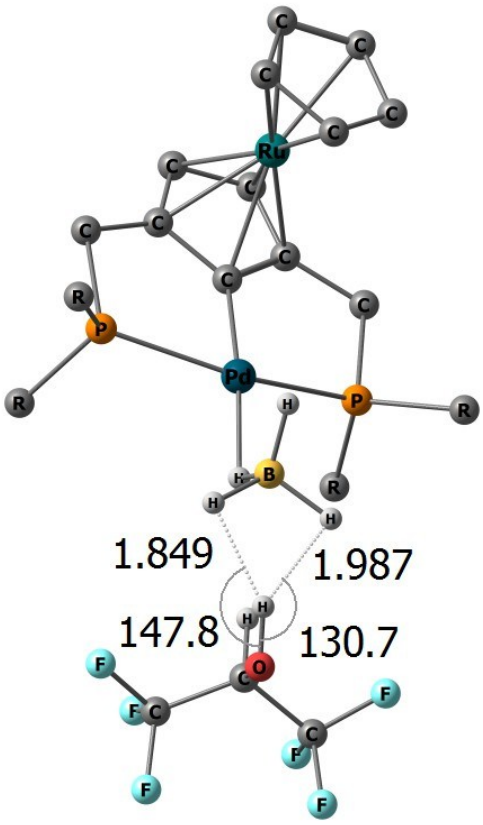


***anti*-1_IIab**

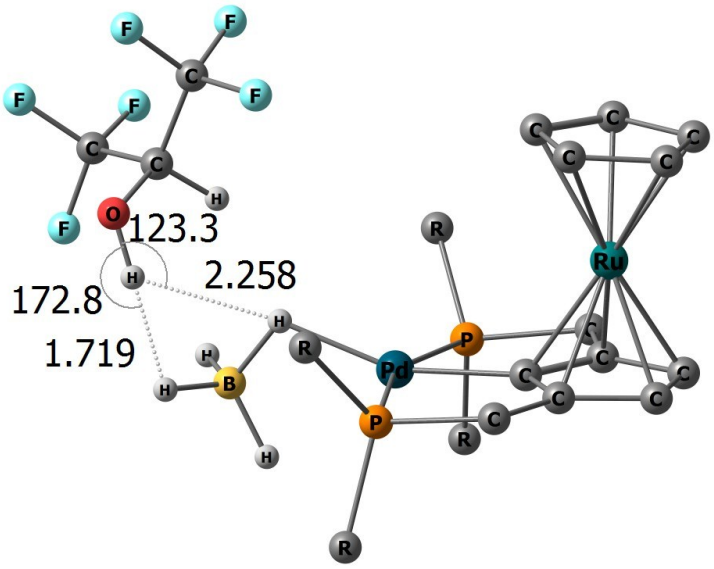
Figure S18. M06-optimized geometries of DHB complexes of **1** with HFIP in toluene. Hydrogen atoms of the ligand are omitted for clarity.



***syn*-1_Ia**

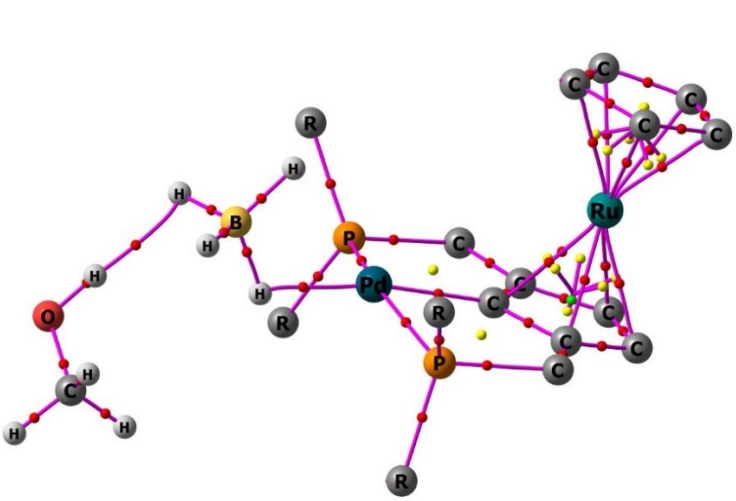


***syn*-1_IIa**

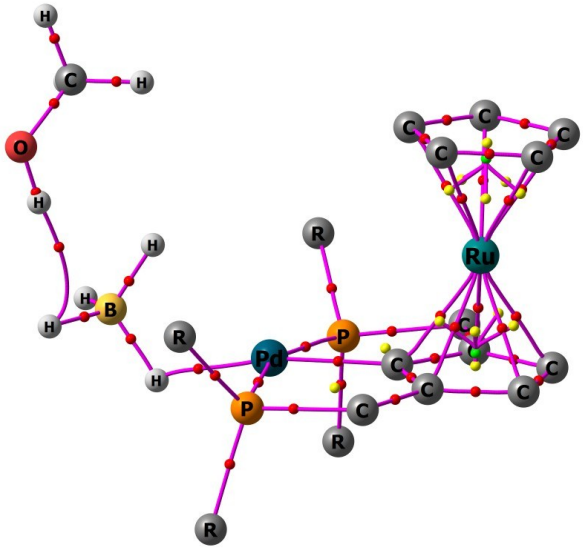


***anti*-1_IIab**

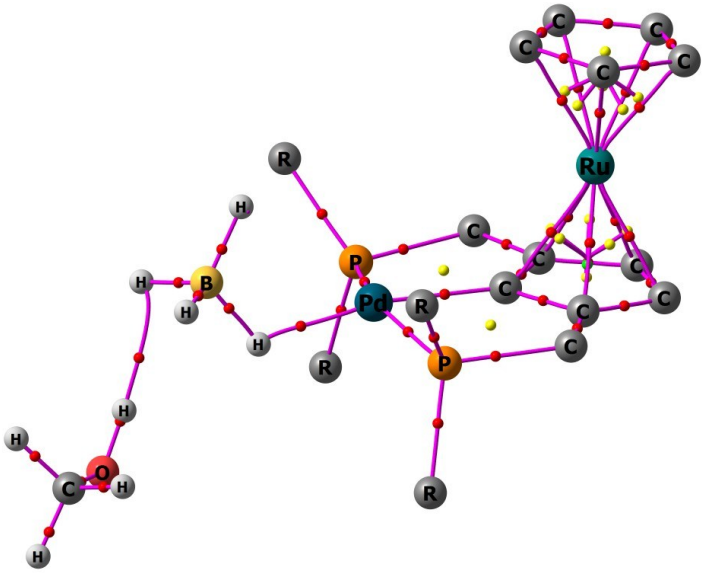
Figure S19. QTAIM molecular graph of M06-optimized geometries of DHB complexes of **1** with MeOH in toluene. Hydrogen atoms of the ligand are omitted for clarity. Red spheres denote critical points (+3;−1), yellow spheres denote ring critical points (+3;+1) and green spheres denote cage critical points (+3;+3).



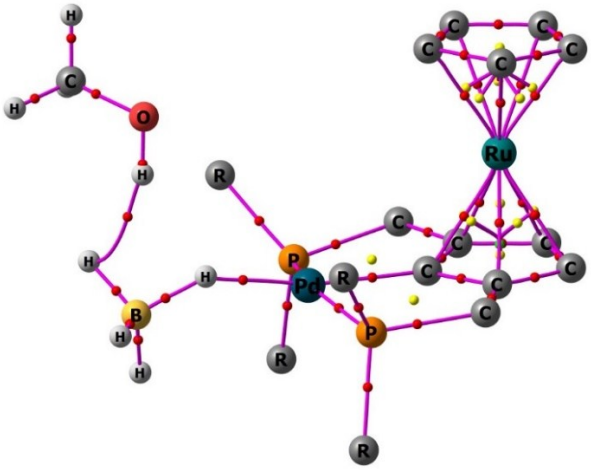
***syn*-1_Ia**



***syn*-1_IIa**

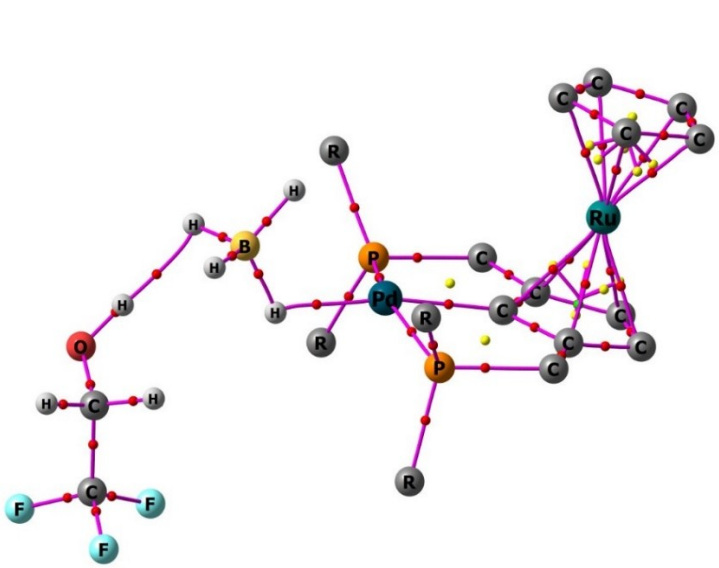


***syn*-1_IIab**

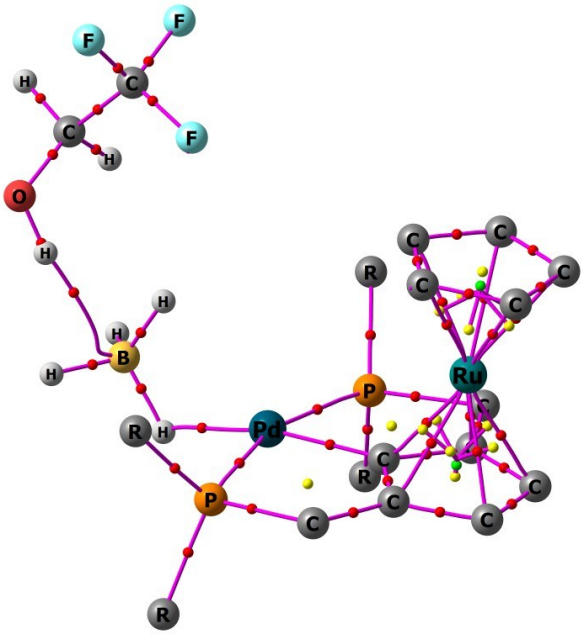


***anti*-1_IIab**

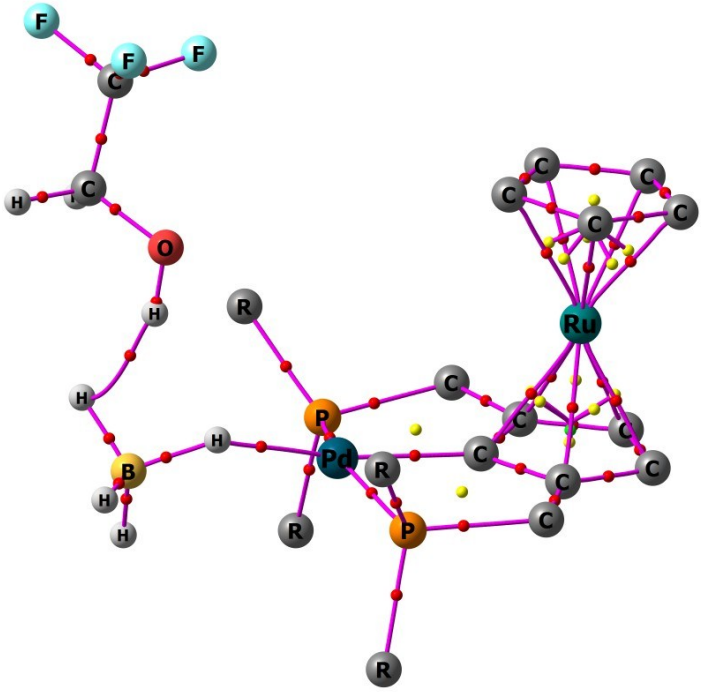
Figure S20. QTAIM molecular graph of M06-optimized geometries of DHB complexes of **1** with TFE in toluene. Hydrogen atoms of the ligand are omitted for clarity. Red spheres denote critical points (+3;−1), yellow spheres denote ring critical points (+3;+1) and green spheres denote cage critical points (+3;+3).



***syn*-1_Ia**

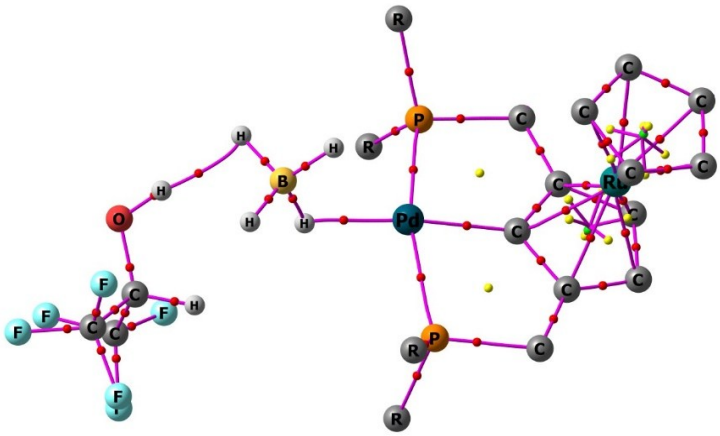


***syn*-1_IIa**

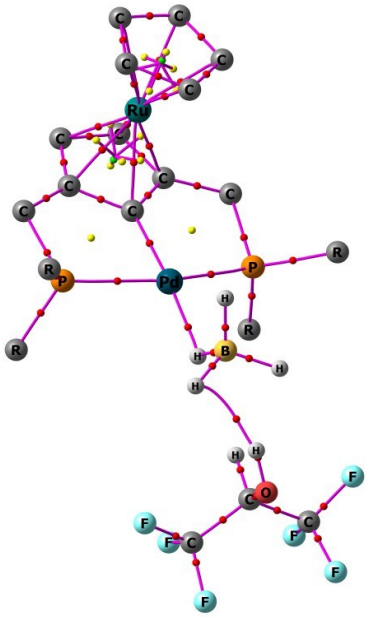


***anti*-1_IIab**

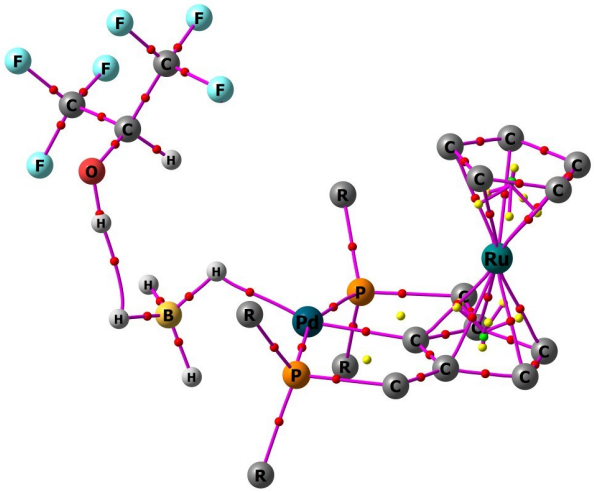
Figure S21. QTAIM molecular graph of M06-optimized geometries of DHB complexes of **1** with HFIP in toluene. Hydrogen atoms of the ligand are omitted for clarity. Red spheres denote critical points (+3;−1), yellow spheres denote ring critical points (+3;+1) and green spheres denote cage critical points (+3;+3).



syn*-1_Ia



***syn*-1_IIa**



***anti*-1_IIab**

	$r_{(H_B\cdots H_O)}$	∠OH···H	$r_{(O-H)}$	$\Delta r_{(O-H)}$	$\Delta r_{(B-H)}$
MeOH					
***syn*-1_Ia**	1.789	169	0.970	0.010	0.003
***syn*-1_IIa**	1.939	166	0.969	0.010	0.004
	2.040	133			0.000
***syn*-1_IIab**	1.862	168	0.969	0.010	0.007
	2.173	134			−0.005
***anti*-1_IIab**	1.925	145	0.969	0.010	0.006
	1.970	147			0.004
TFE					
	$r_{(H_B\cdots H_O)}$	∠OH···H	$r_{(O-H)}$	$\Delta r_{(O-H)}$	$\Delta r_{(B-H)}$
***syn*-1_Ia**	1.709	172	0.973	0.010	0.006
***syn*-1_IIa**	1.921	157	0.973	0.010	0.004
	1.954	137			0.001
***anti*-1_IIab**	1.825	147	0.972	0.010	0.008
	1.954	145			0.001
HFIP					
	$r_{(H_B\cdots H_O)}$	∠OH···H	$r_{(O-H)}$	$\Delta r_{(O-H)}$	$\Delta r_{(B-H)}$
syn*-1_Ia	1.696	165	0.978	0.015	0.007
	2.186	130			
***syn*-1_IIa**	1.849	148	0.975	0.013	0.007
	1.987	131			0.002
***anti*-1_IIab**	1.719	173	0.978	0.015	0.008
	2.258	123			

Table S9. Computed geometric parameters (distances $r_{(X-Y)}$ in Å, angles in degrees) for DHB complexes **1**·ROH in toluene.

* coordination on BH_{br} ligand generally leads to switching ***syn*-1** configuration to ***anti*-1**.

Table S10. Changes of NPA charges (Δq), Wiberg bond indexes (WBI) and its changes (ΔWBI) and energetic characteristics (in kJ/mol) for DHB complexes **1**·ROH in toluene.

	Δq[(O)H]	Δq[H(B)]	ΔWBI[OH]	ΔWBI[HB]	WBI[H···H]	ΔWBI[PdH(B)]	E²[a]
MeOH							
***syn*-1_Ia**	0.032	−0.010	−0.097	−0.022	0.022	−0.025	16.7
***syn*-1_IIa**	0.036	−0.003 0.000	−0.103	−0.011 0.000	0.009 0.003	−0.030	10.0 3.8
***syn*-1_IIab**	0.034	−0.002 −0.005	−0.113	−0.021 0.035	0.013 0.001	−0.024	13.4
***anti*-1_IIab**	0.039	−0.014 −0.076	−0.100	−0.018 −0.027	0.010 0.003	−0.007	10.0 3.3
TFE							
	Δq[(O)H]	**Δq[H(B)]**	**ΔWBI[OH]**	**ΔWBI[HB]**	**WBI[H···H]**	**ΔWBI[PdH(B)]**	**E²[a]**
***syn*-1_Ia**	0.041	−0.011	−0.132	−0.035	0.016	−0.035	26.4
***syn*-1_IIa**	0.039	−0.004 0.005	−0.119	−0.015 0.002	0.011 0.007	−0.041	13.0 7.9
***anti*-1_IIab**	0.047	−0.022 −0.081	−0.147	−0.031 −0.013	0.019 0.004	−0.017	18.4 5.0
HFIP							
	Δq[(O)H]	**Δq[H(B)]**	**ΔWBI[OH]**	**ΔWBI[HB]**	**WBI[H···H]**	**ΔWBI[PdH(B)]**	**E²[a]**
syn*-1_Ia	0.037	−0.007 0.005	−0.147	−0.040 −0.008	0.030 0.002	−0.038	31.0 3.8
***syn*-1_IIa**	0.035	0.001 0.003	−0.123	−0.021 −0.012	0.015 0.007	−0.039	13.0 7.9
***anti*-1_IIab**	0.037	−0.003 −0.001	−0.147	−0.043 0.060	0.030 0.000	−0.041	29.7

* coordination on BH_{br} ligand generally leads to switching ***syn*-1** configuration to ***anti*-1**.

[a] E^2 – donation energy from σ(B–H) of **1** to σ*(O–H) estimated from second-order perturbative analysis of donor –acceptor interactions within natural-bond orbital (NBO) analysis.

Table S11. Electron density at (3;−1) critical point of H···H bond (ρ_c in a.u.), Laplacian of electron density ($\nabla^2\rho_c$) and bond ellipticity (ε) for DHB complexes **1**·ROH in toluene.

MeOH			
	ρ_c	$\nabla^2\rho_c$	$\varepsilon_{H\cdots H}$
***syn*-1_Ia**	0.02	0.053	0.20
***syn*-1_IIa**	0.02	0.046	2.03
***syn*-1_IIab**	0.02	0.050	0.37
***anti*-1_IIab**	0.02	0.048	0.78
TFE			
	ρ_c	$\nabla^2\rho_c$	$\varepsilon_{H\cdots H}$
***syn*-1_Ia**	0.02	0.060	0.17
***syn*-1_IIa**	0.02	0.050	8.31
***anti*-1_IIab**	0.02	0.055	0.51
HFIP			
	ρ_c	$\nabla^2\rho_c$	$\varepsilon_{H\cdots H}$
syn*-1_Ia	0.02	0.061	0.26
***syn*-1_IIa**	0.02	0.052	1.17
***anti*-1_IIab**	0.02	0.060	0.23

* coordination on BH_{br} ligand generally leads to switching ***syn*-1** configuration to ***anti*-1**.

Table S12. Computed formation energy for DHB complexes **1**·ROH (ΔE_{el}, ΔE_{ZPVE}, $\Delta H°$ in kJ/mol), energy of DHB formation ($\Delta H^{theor}(\Delta\nu)$ and $\Delta H^{theor}(\Delta A)$ in kJ/mol) and energy of H···H interaction ($E_{H\cdots H}$ in kJ/mol).

MeOH						
	ΔE_{el}	**ΔE_{ZPVE}**	**$\Delta H°$**	**$\Delta H°_{theor}(\Delta\nu)$[a]**	**$\Delta H°_{theor}(\Delta A)$[b]**	**$E_{H\cdots H}$[c]**
***syn*-1_Ia**	−31.0	−26.4	−25.5	−14.3	−16.7	−13.8
***syn*-1_IIa**	−32.2	−28.0	−26.8	−13.8	−13.0	−10.9
***syn*-1_IIab**	−31.4	−27.2	−25.9	−12.1	−14.6	−12.1
***anti*-1_IIab**	−19.2	−17.6	−15.5	−12.6	−10.9	−12.6
TFE						
	ΔE_{el}	**ΔE_{ZPVE}**	**$\Delta H°$**	**$\Delta H°_{theor}(\Delta\nu)$[a]**	**$\Delta H°_{theor}(\Delta A)$[b]**	**$E_{H\cdots H}$[c]**
***syn*-1_Ia**	−42.3	−38.1	−36.4	−16.7	−26.8	−17.2
***syn*-1_IIa**	−44.8	−41.0	−39.2	−14.6	−22.2	−13.4
***anti*-1_IIab**	−25.9	−25.0	−22.2	−14.6	−19.7	−15.5
HFIP						
	ΔE_{el}	**ΔE_{ZPVE}**	**$\Delta H°$**	**$\Delta H°_{theor}(\Delta\nu)$[a]**	**$\Delta H°_{theor}(\Delta A)$[b]**	**$E_{H\cdots H}$[c]**
syn*-1_Ia	−59.8	−54.0	−52.7	−21.3	−29.3	−18.8
***syn*-1_IIa**	−61.5	−54.8	−54.0	−21.8	−23.4	−14.2
***anti*-1_IIab**	−52.7	−47.7	−46.4	−21.3	−21.3	−18.0

* coordination on BH_{br} ligand generally leads to switching ***syn*-1** configuration to ***anti*-1**. [a] DHB formation enthalpy in gas phase calculated from $\Delta\nu_{OH}$ by formula $-\Delta H°_{HB}(\Delta\nu) = 75\cdot|\Delta\nu_{XH}|/(720+|\Delta\nu_{XH}|)$, see refs. [31-36]; [b] DHB formation enthalpy in gas phase calculated from ΔA_{OH} by formula $-\Delta H°_{HB}(\Delta A) = 12.1\cdot(\sqrt{A_{bonded}}-\sqrt{A_{free}})$, see refs. [31-36]; [c] $E_{H\cdots H} = 0.5\cdot V(r)$ in kJ/mol, see refs. [43, 44]

Figure S22. General view of molecular structure of **2** (thermal ellipsoids of all non-hydrogen atoms are drawn at the 50% probability level.

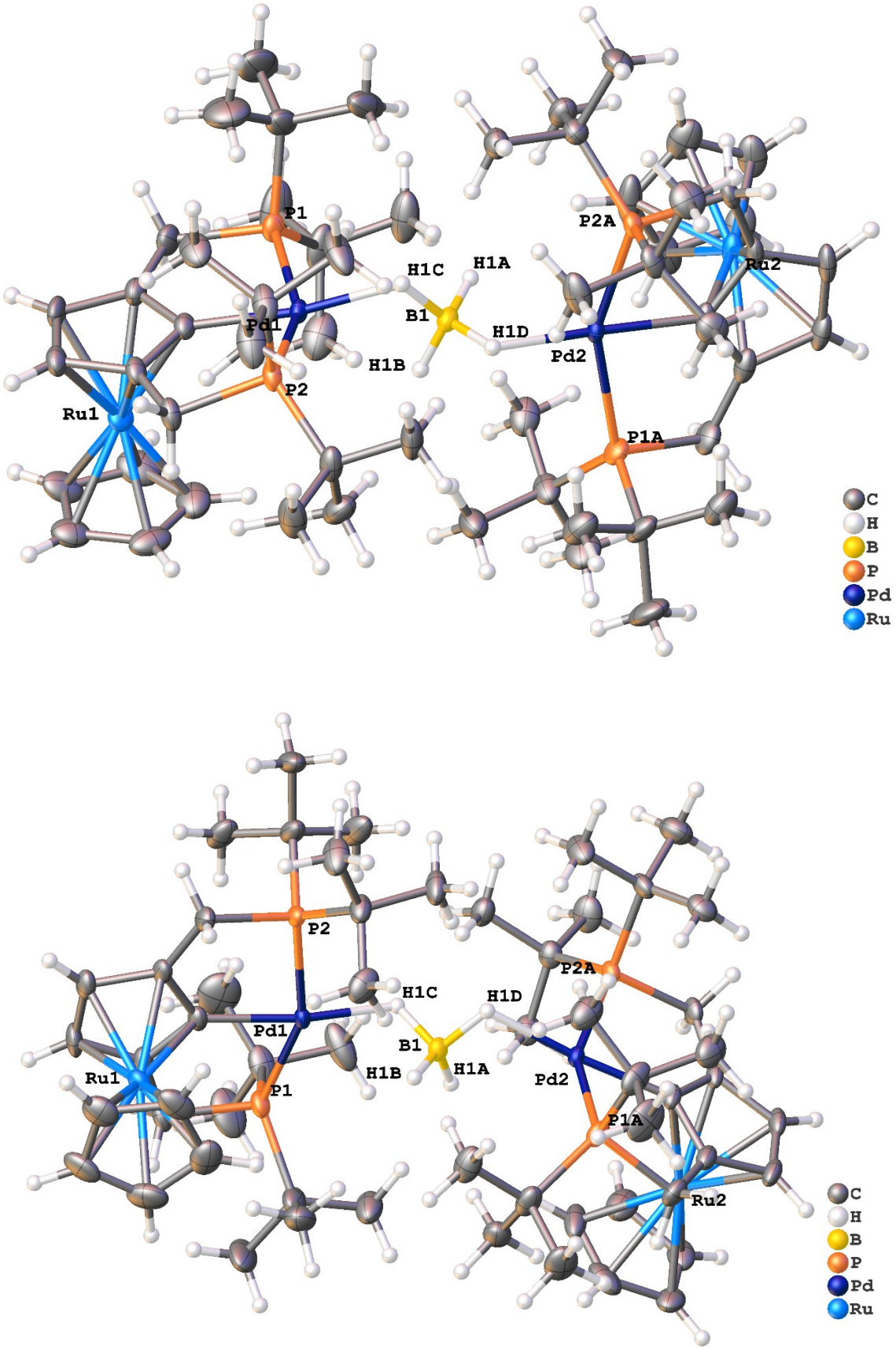


Table S13. Geometry parameters of crystal and M06-optimized structure of **2**.

Distances	**2**	**M06**
Pd_1–C	1.980(3)	1.996
Pd_2–C	1.981(4)	1.994
Pd_1–P_1	2.349(1)	2.390
Pd_1–P_2	2.3913(9)	2.436
Pd_2–P_3	2.380(1)	2.410
Pd_2–P_4	2.382(1)	2.421
Pd_1···B	2.577(5)	2.585
Pd_2···B	2.555(5)	2.577
Pd_1–H_1(B)	**1.866**	**1.901**
Pd_1···H_2(B)	**2.434**	**2.452**
Pd_2–H_3(B)	**1.926**	**1.895**
Pd_2···H_4(B)	**2.490**	**2.481**
B–H_1	1.190	1.267
B–H_2	1.073	1.208
B–H_3	1.256	1.272
B–H_4	1.070	1.207
C–Pd_1–B	164.4(1)	162.41
C–Pd_2–B	156.3(1)	158.14
P_1–Pd_1–P_2	156.66(4)	156.50
P_3–Pd_2–P_4	154.24(4)	154.80
Pd_1–H_1–B	113.2	107.13
Pd_1–H_2–B	85.3	81.93
Pd_2–H_3–B	104.9	107.85
Pd_2–H_4–B	81.2	81.09

Figure S23. QTAIM molecular graph of M06-optimized geometry of **2**. Hydrogen atoms of the ligand are omitted for clarity. Red spheres denote critical points (+3;−1), yellow spheres denote ring critical points (+3;+1) and green spheres denote cage critical points (+3;+3).

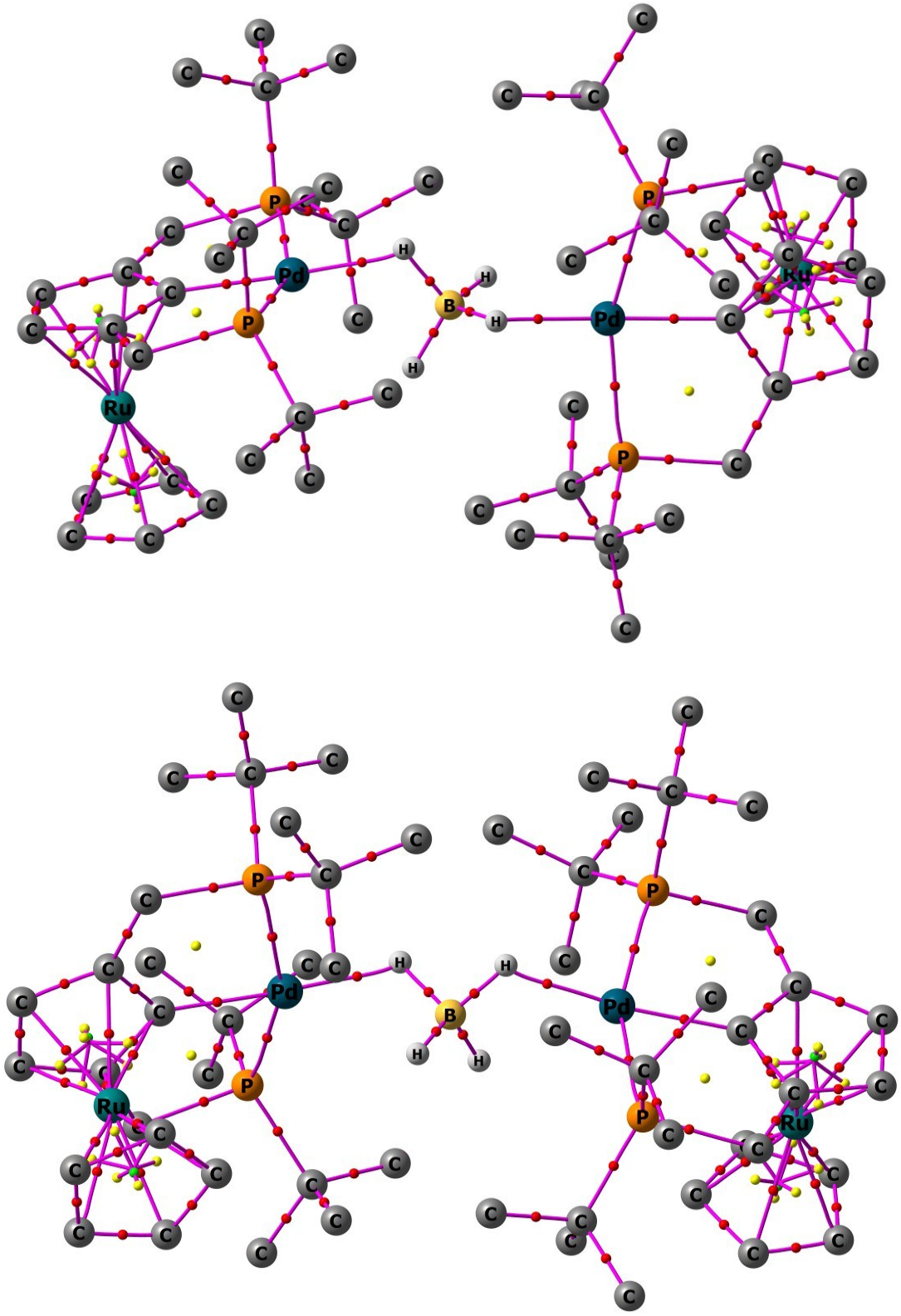


Figure S24. FTIR spectra of **2** and **2-d$_4$** in KBr pellet.

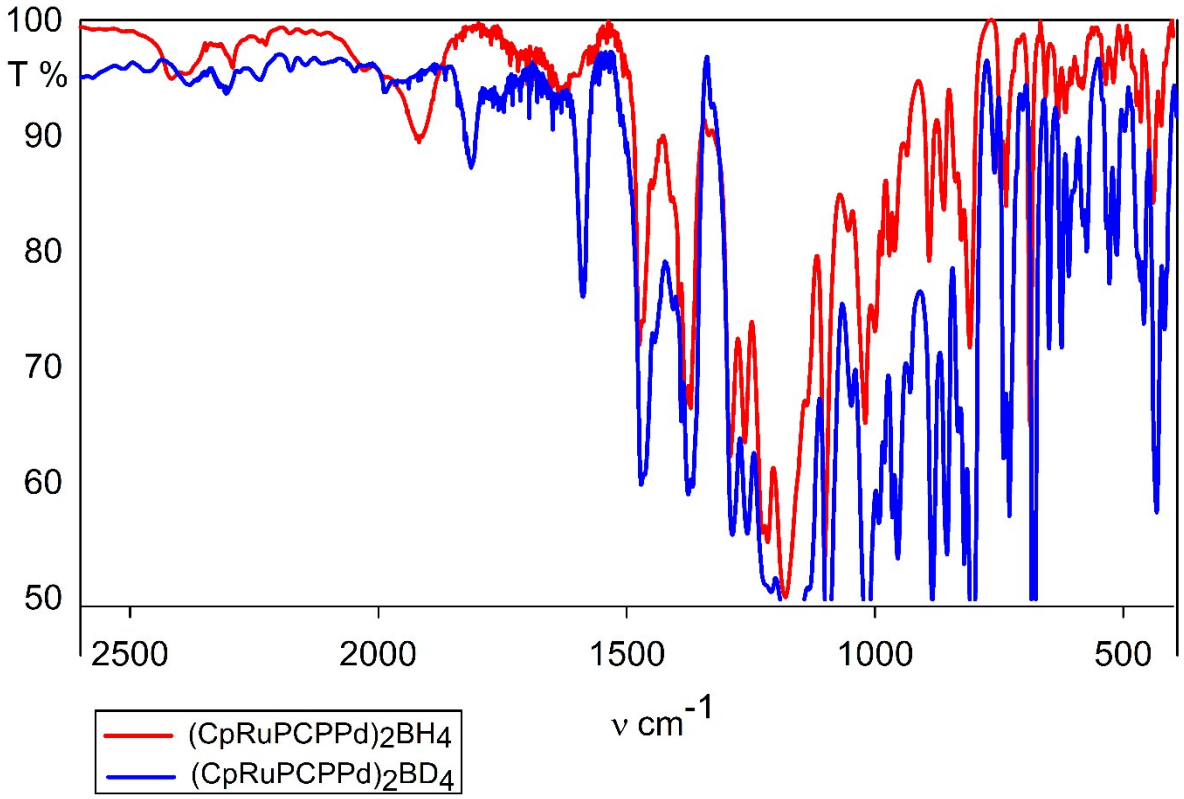


Figure S25. The $^{31}P\{^1H\}$ monitoring of the reaction of **1-d$_4$** (spectrum 1) with 20-fold excess of HFIP (spectrum 2). Spectra (3–5) are measured at 0.5 h, 18 h and 40 h after mixing.

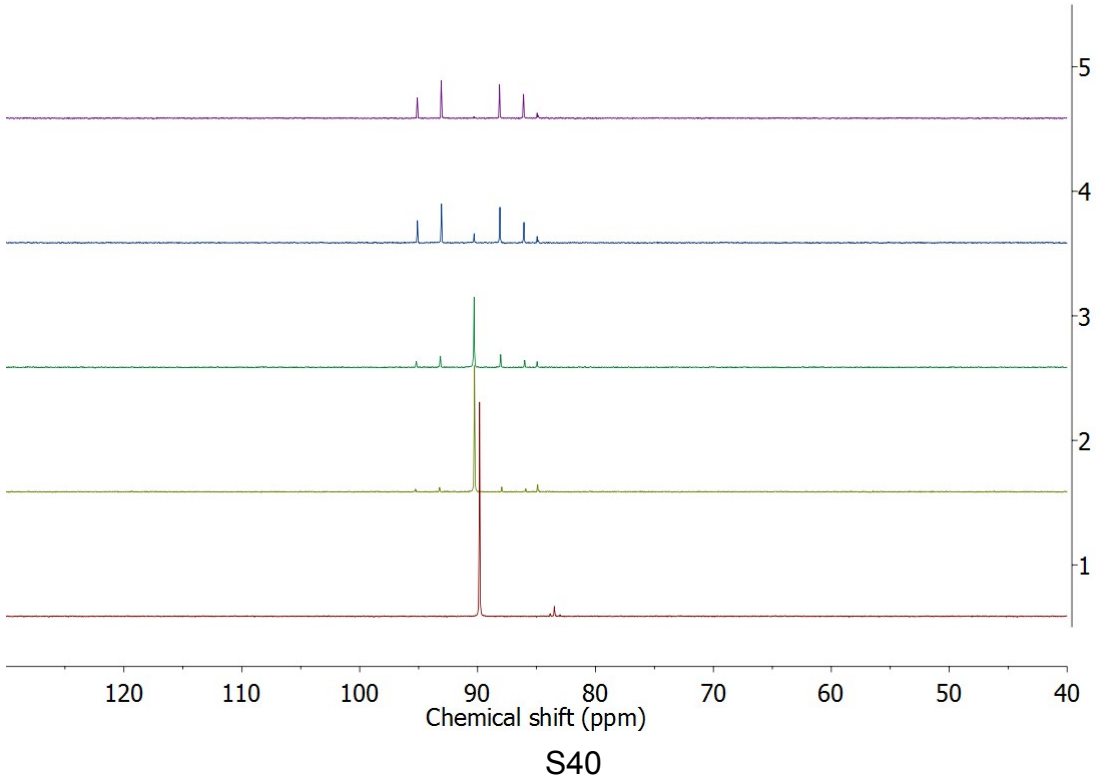


Figure S26. M06-optimized geometry of **3**. Hydrogen atoms of the ligand are omitted for clarity.

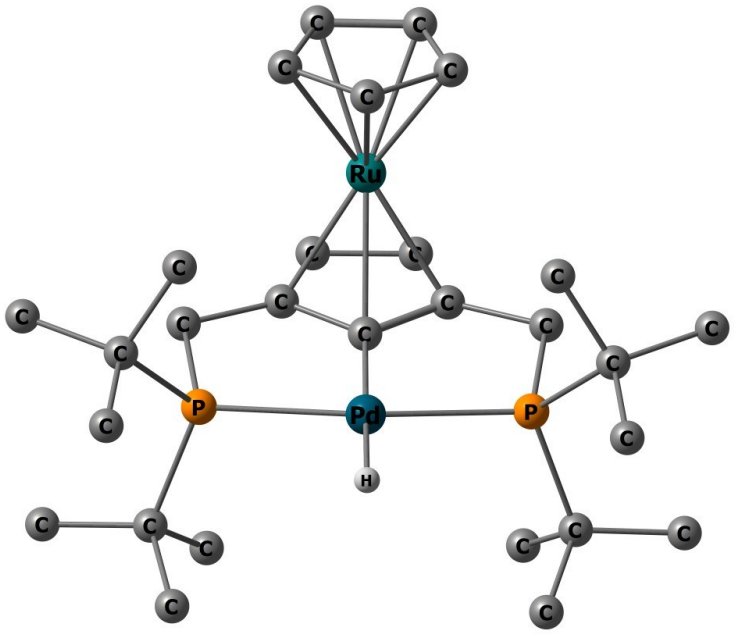


Figure S27. ^{1}H NMR monitoring of BH_3 abstraction from **1** by pyridine excess (15 mol. equiv.) in toluene-d_8.

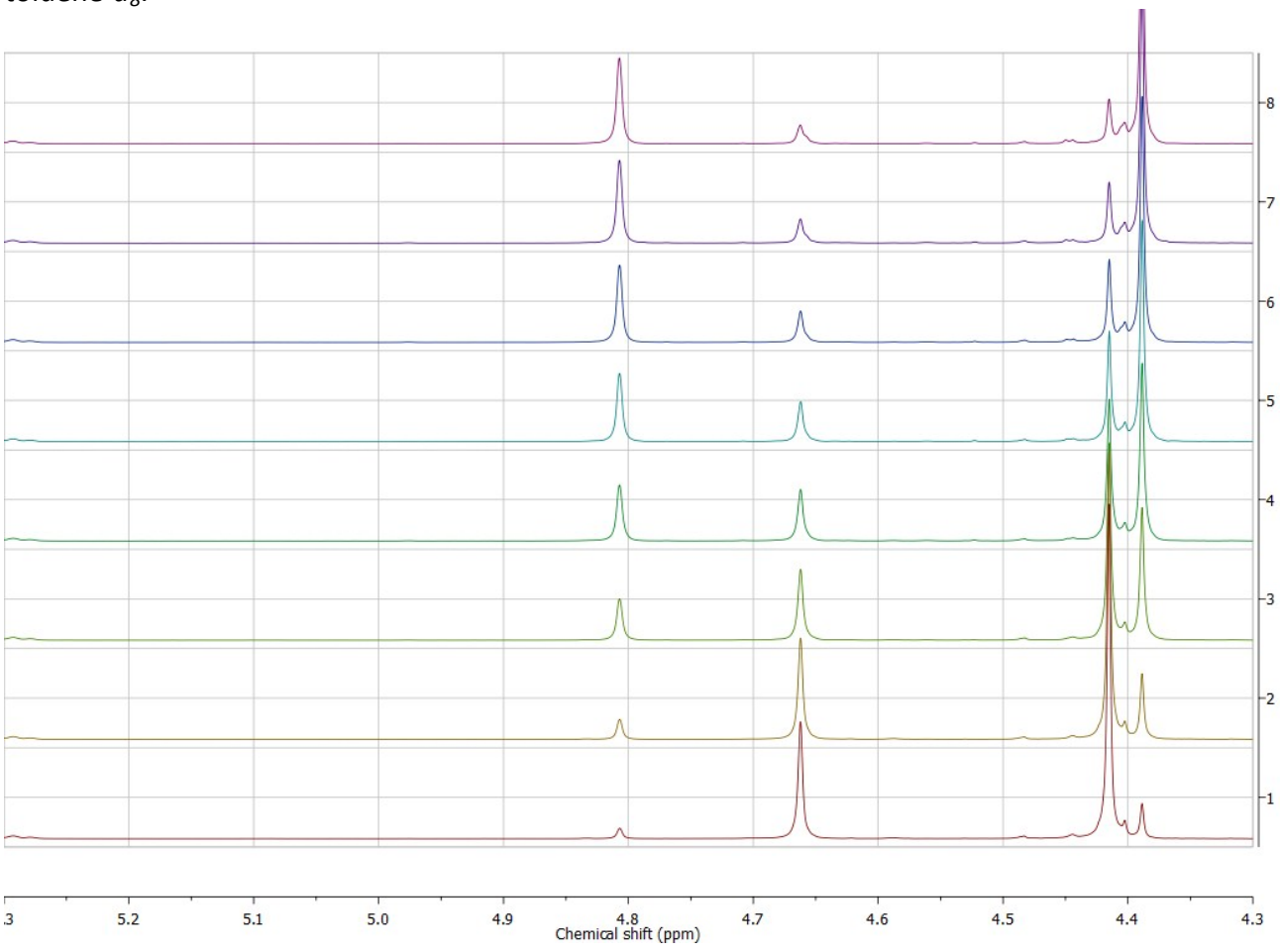


Figure S28. The linear dependence of ln(1/K) *vs* time (s) of BH_3 abstraction from **1** by pyridine excess (15 mol. equiv.) in toluene-d_8.

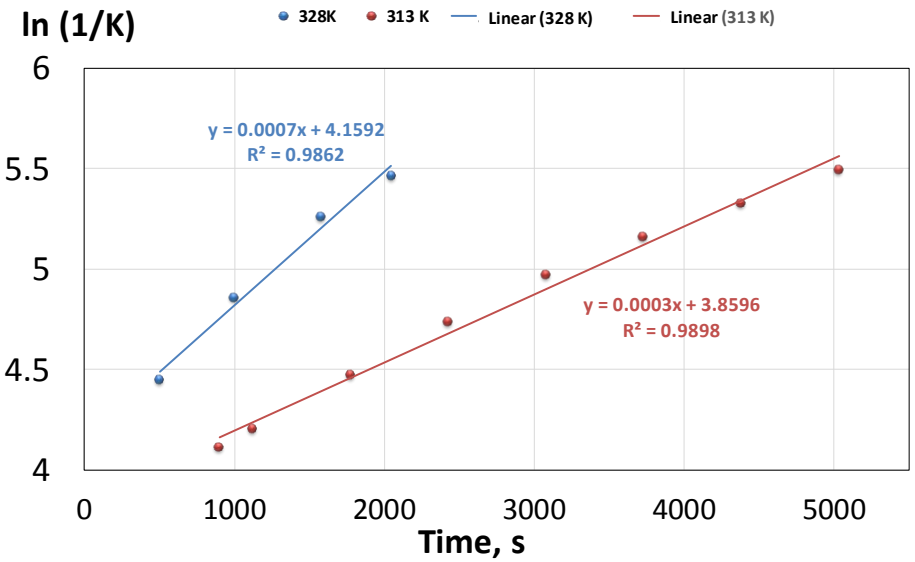
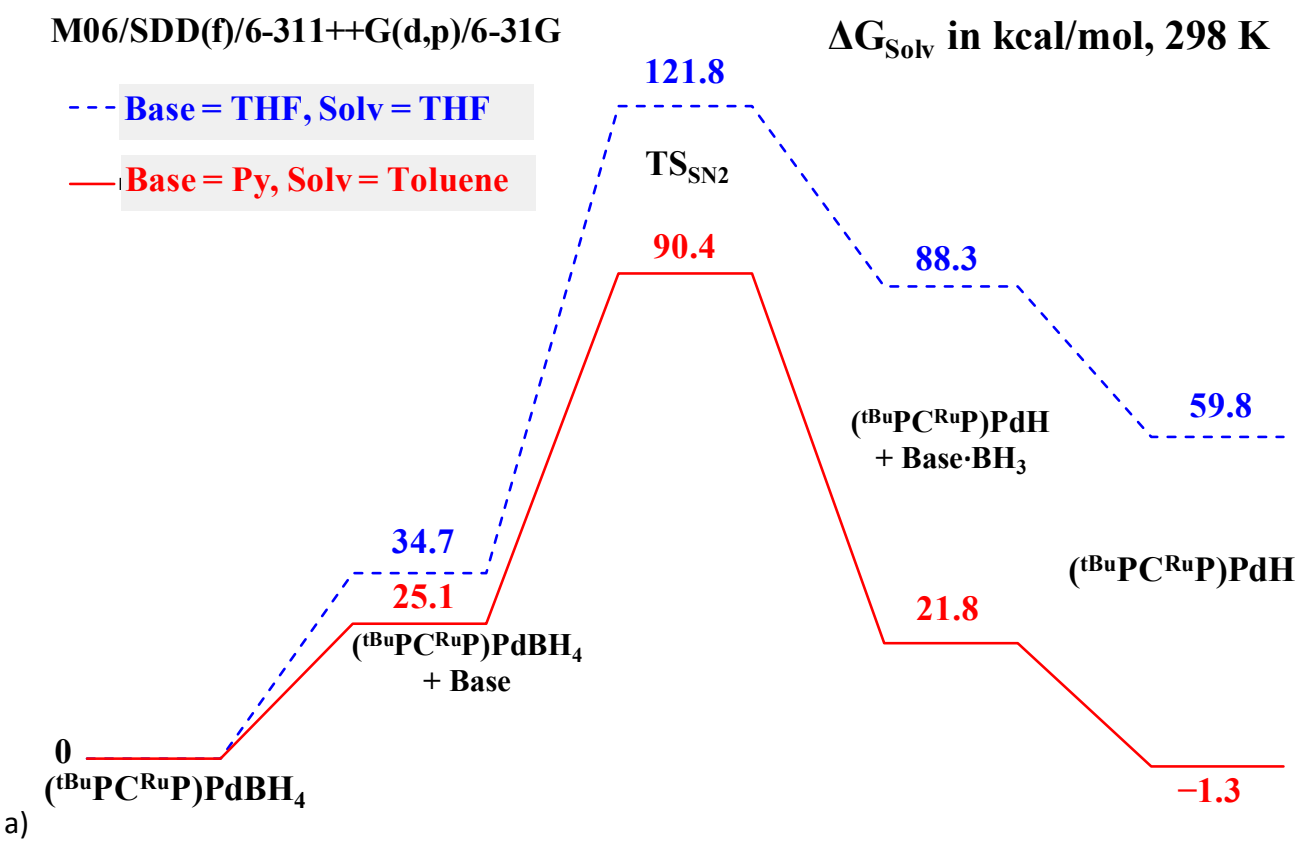
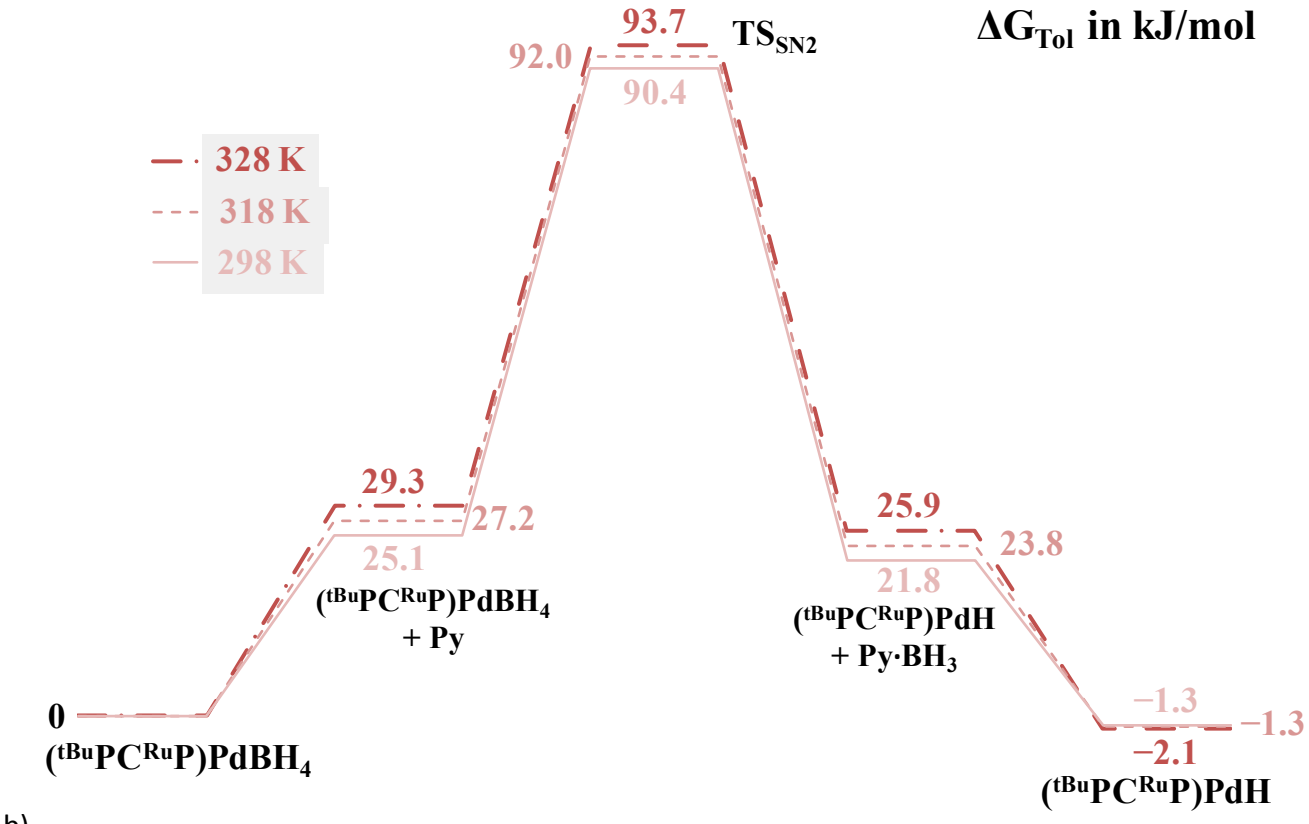


Figure S29. Computed energy profiles of BH_3 abstraction from **1**: (a) by THF in THF and Py in toluene at 298 K and (b) by Py in toluene at 298–328 K .



a)



b)

Figure S30. ^{1}H NMR spectrum (500 MHz) of **3** in toluene-d_8.

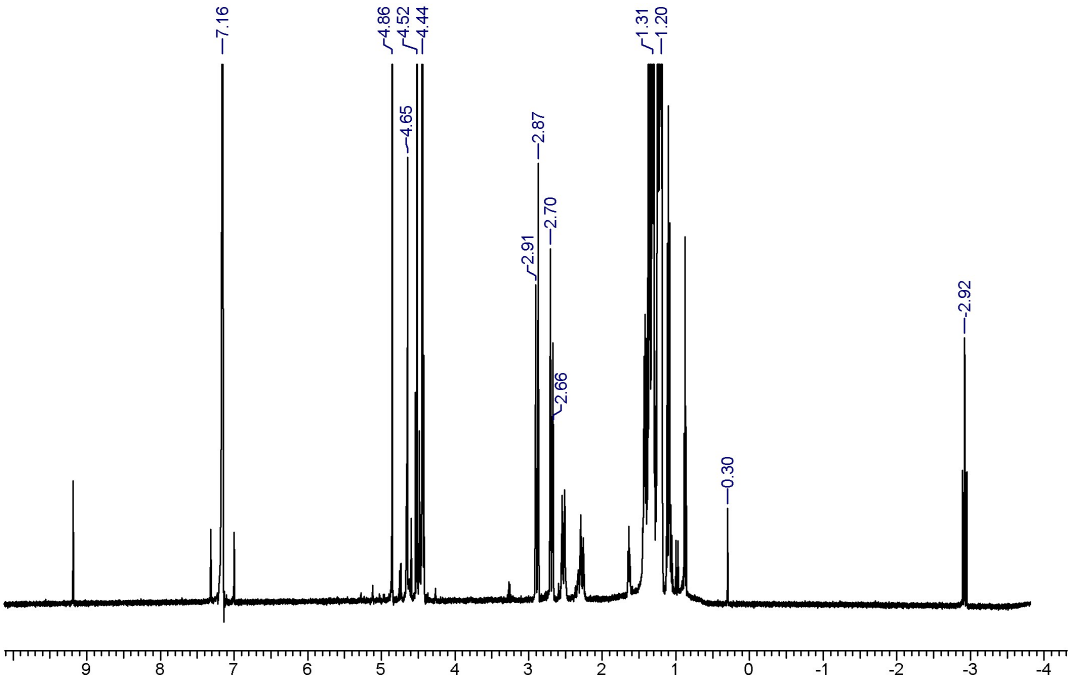


Figure S31. ^{31}P NMR spectrum (202.5 MHz) of **3** in toluene-d_8.

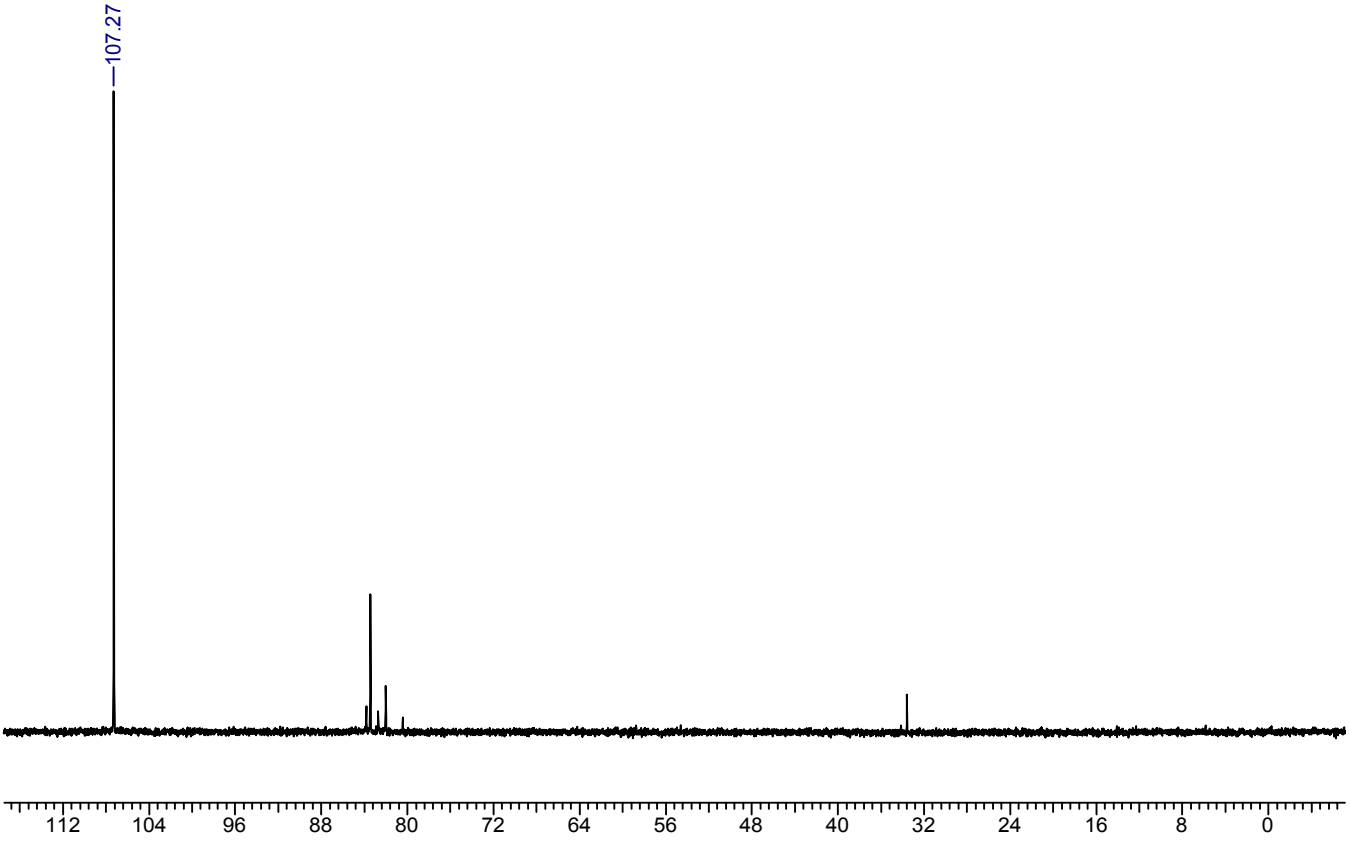


Figure S32. General view of molecular structure of **4** (thermal ellipsoids of all non-hydrogen atoms are drawn at the 50% probability level.

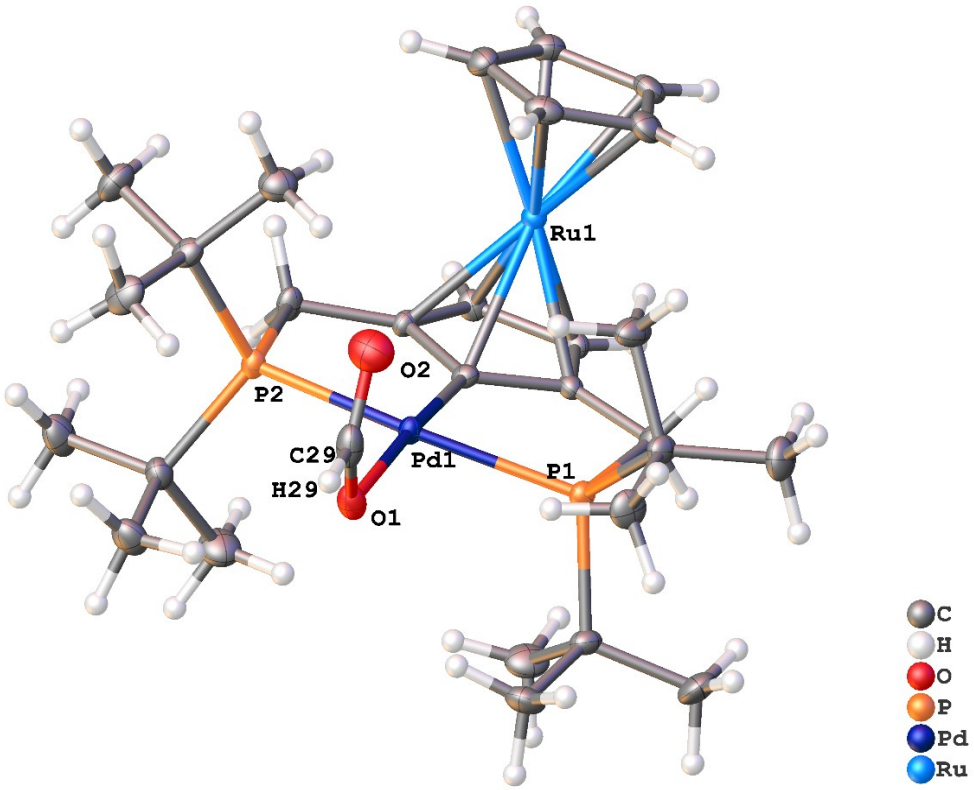


Figure S33. QTAIM molecular graph of M06-optimized geometry of **4**. Hydrogen atoms of the ligand are omitted for clarity. Red spheres denote critical points (+3;−1), yellow spheres denote ring critical points (+3;+1) and green spheres denote cage critical points (+3;+3).

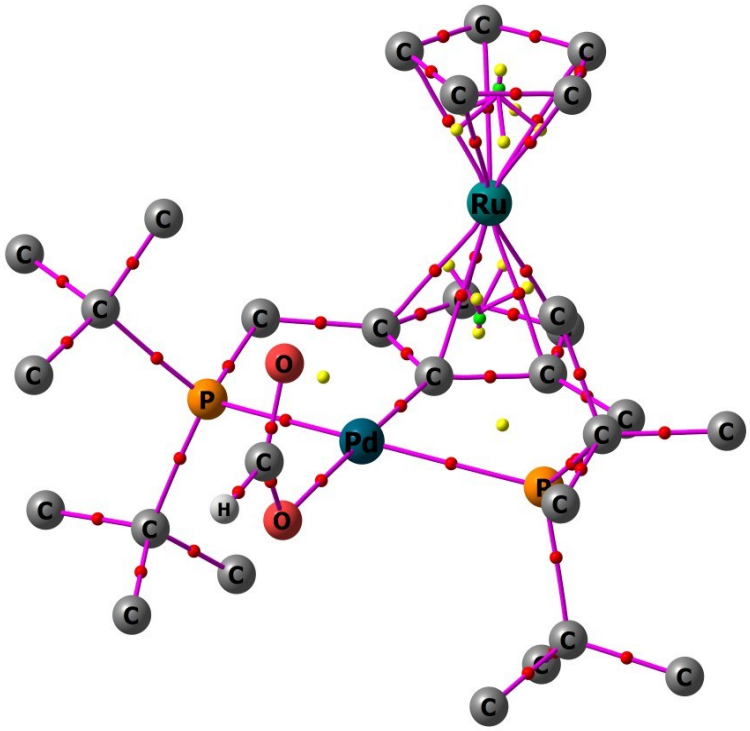


Table S14. Geometry parameters of crystal and M06-optimized structure of **4**.

Distances	**4**	**M06**
Pd–C	1.966(3)	1.979
Pd–P_1	2.3401(8)	2.372
Pd–P_2	2.3463(9)	2.376
Pd–O_1	2.167(2)	2.166
Pd···O_2	3.184(2)	3.192
Pd···C(H)	2.962(3)	2.978
C–Pd–C(H)	162.0(1)	160.54
P_1–Pd–P_2	160.90(3)	159.36
Pd–O_1–C(H)	117.7(2)	117.81
Pd–O_2–C(H)	68.4(2)	68.88

Figure S34. Crystal packing of **4** (thermal ellipsoids of all non-hydrogen atoms are drawn at the 50% probability level).

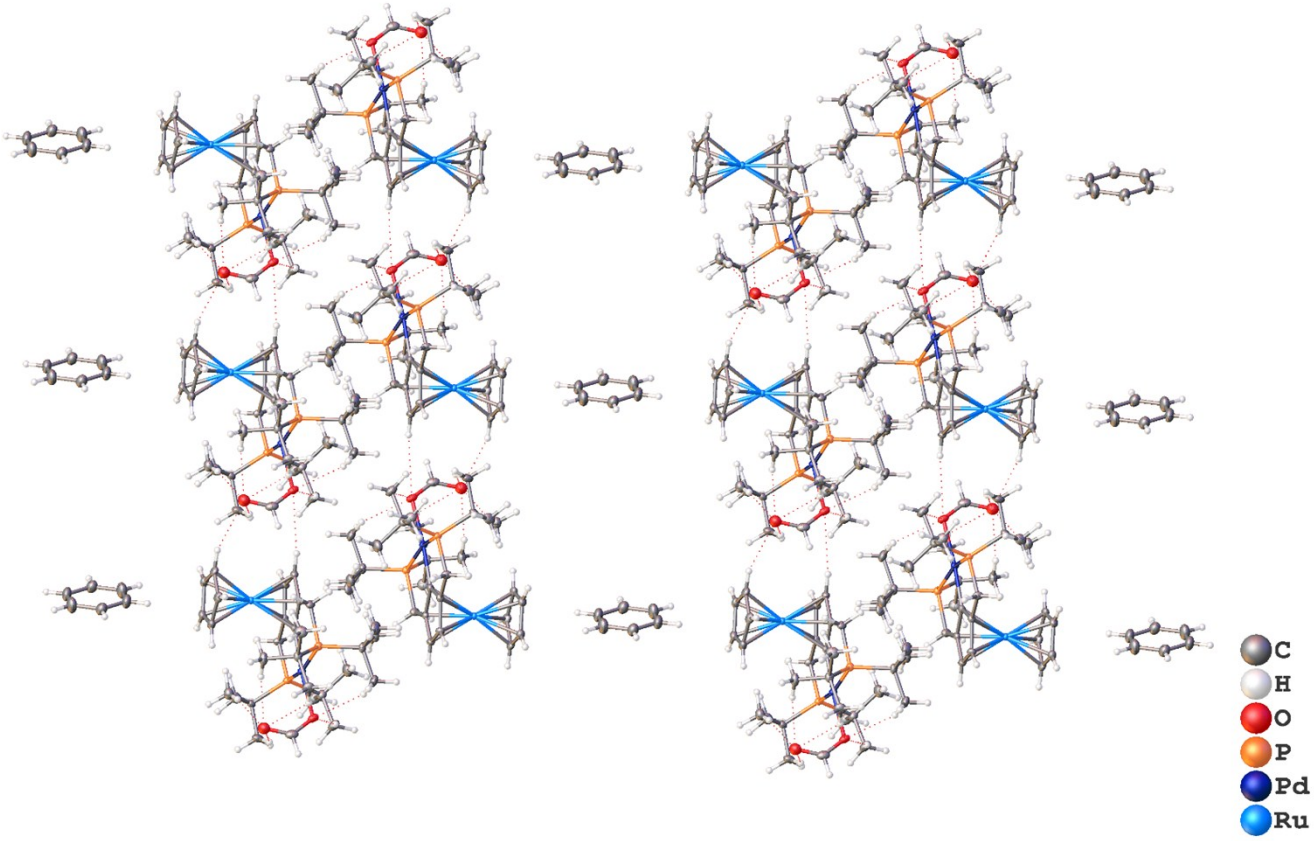


Figure S35. ^{1}H NMR spectrum (400 MHz) of **4** in C_6D_6.

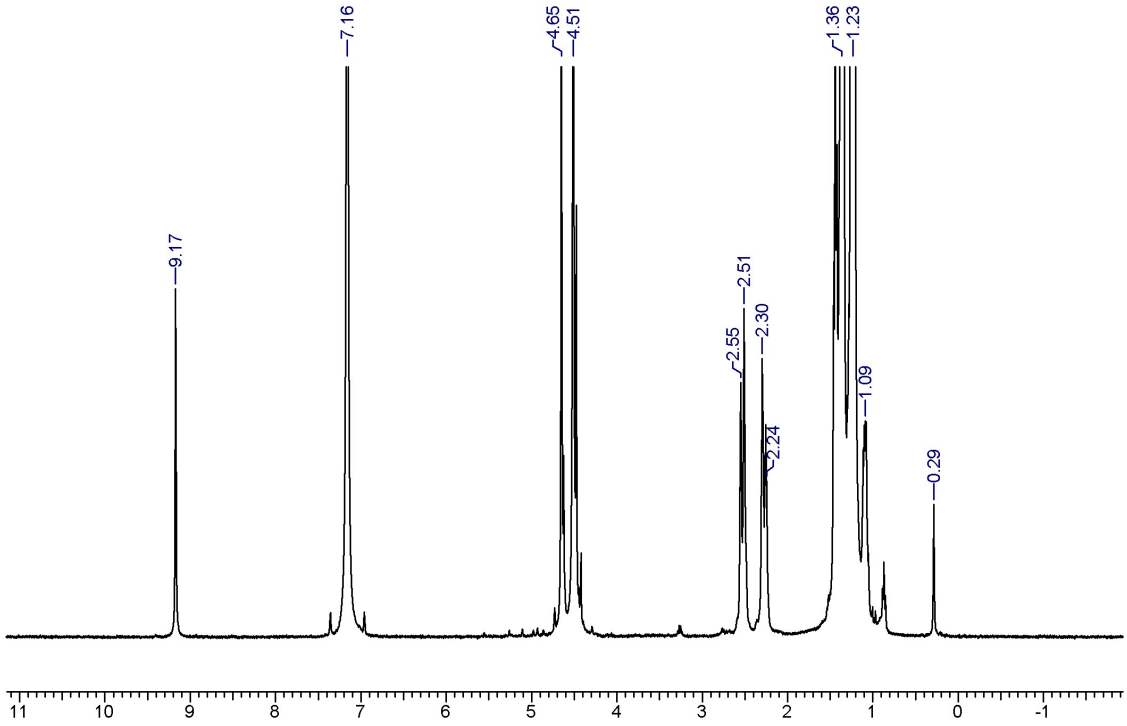


Figure S36. ^{13}C NMR spectrum (100.6 MHz) of **4** in C_6D_6.

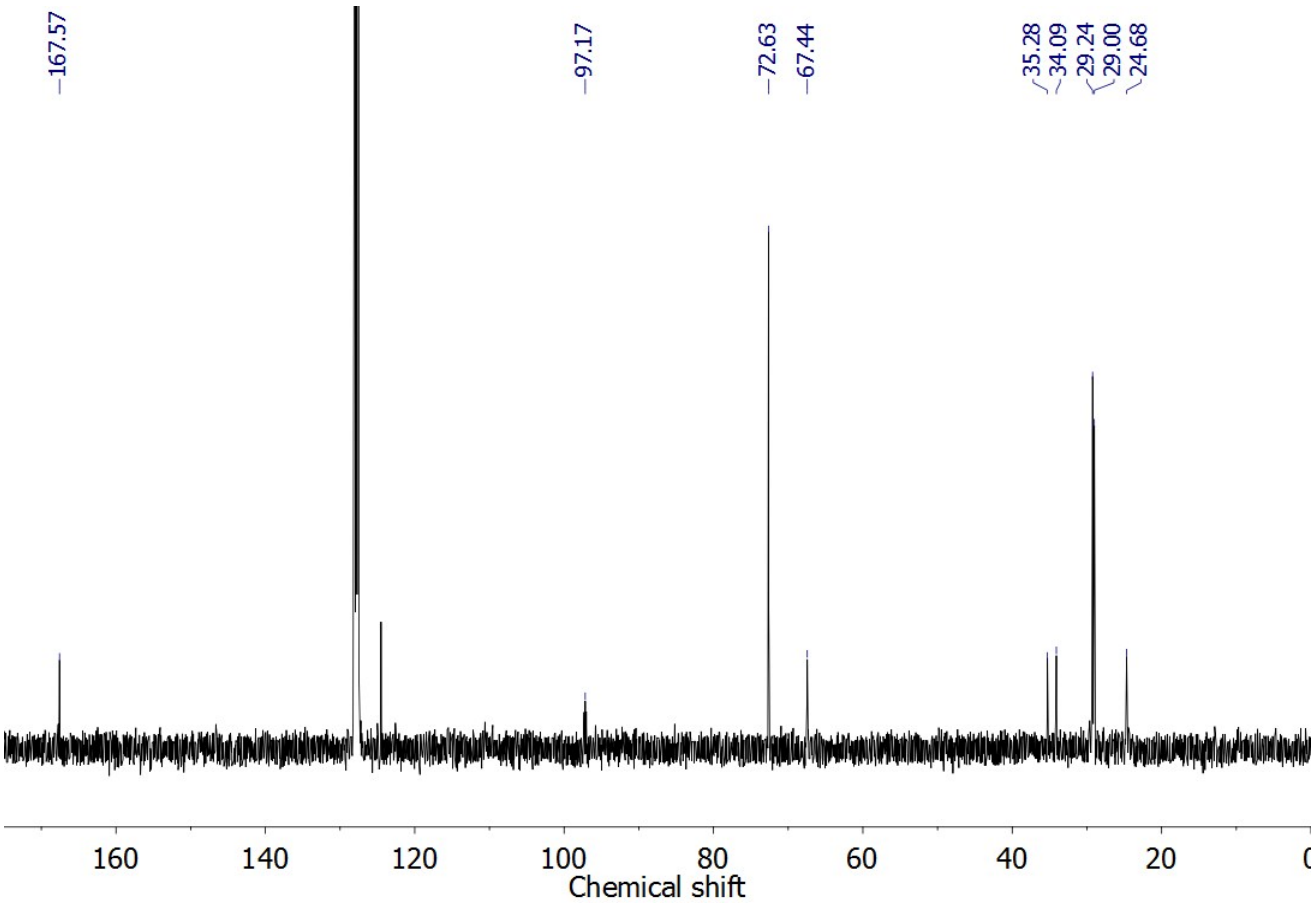


Figure S37. $^{31}P\{^{1}H\}$ NMR spectrum (162.0 MHz) of **4** in C_6D_6.

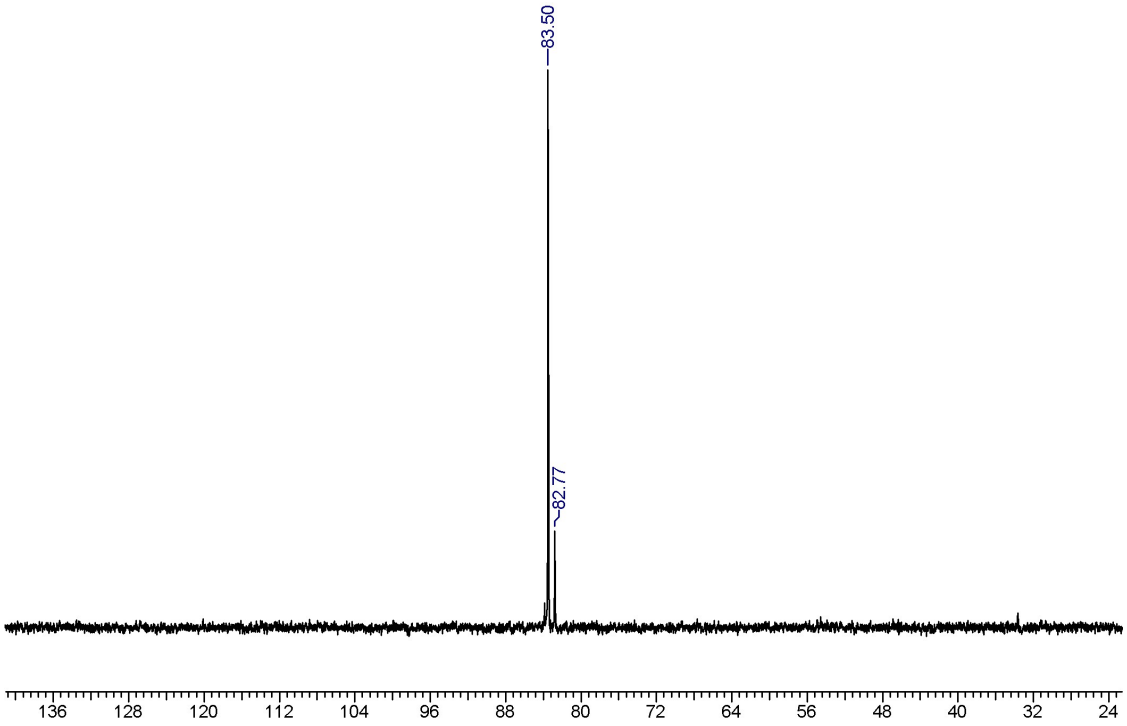


Figure S38. FTIR spectrum of **4** in KBr pellet.

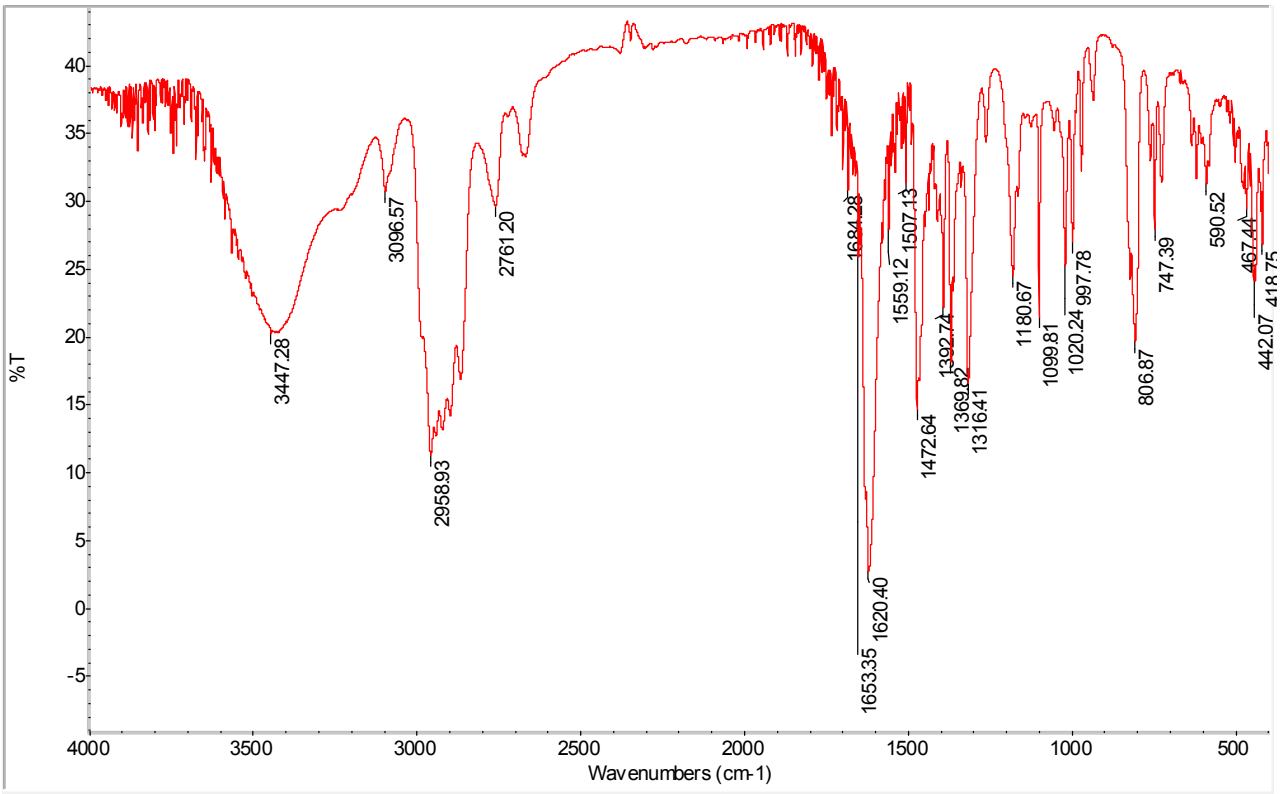


Figure S39. General view of molecular structure of **5** (thermal ellipsoids of all non-hydrogen atoms are drawn at the 50% probability level.

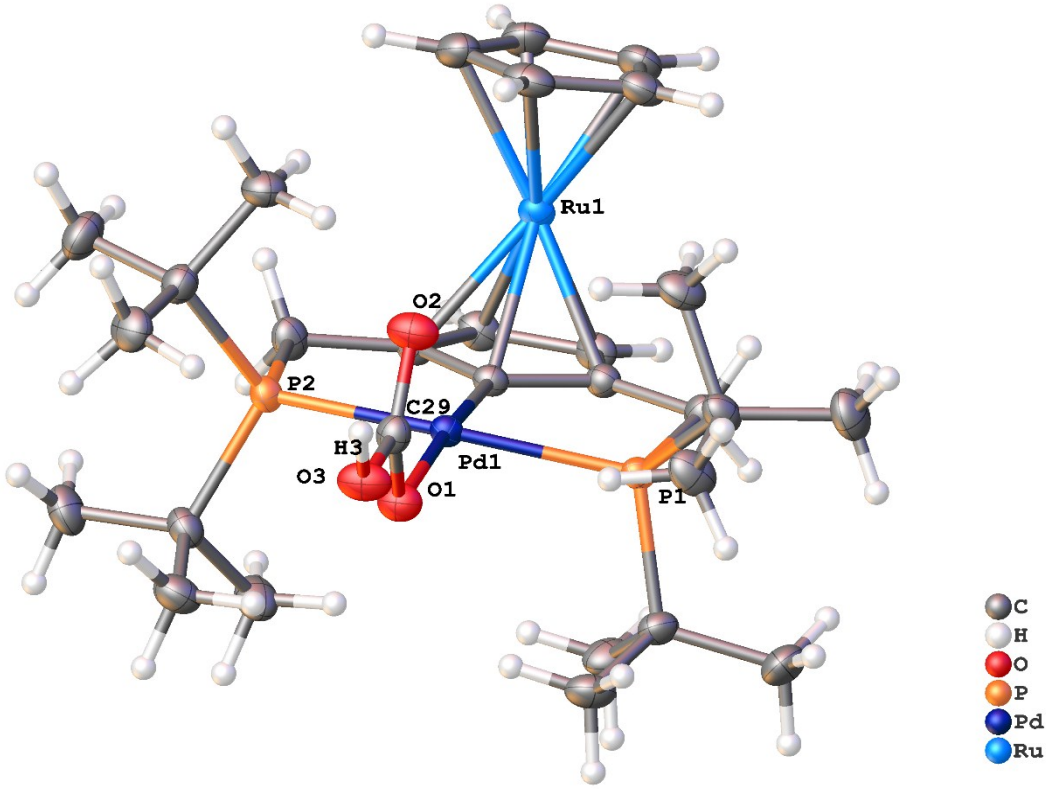


Figure S40. QTAIM molecular graph of M06-optimized geometry of **5**. Hydrogen atoms of the ligand are omitted for clarity. Red spheres denote critical points (+3;−1), yellow spheres denote ring critical points (+3;+1) and green spheres denote cage critical points (+3;+3).

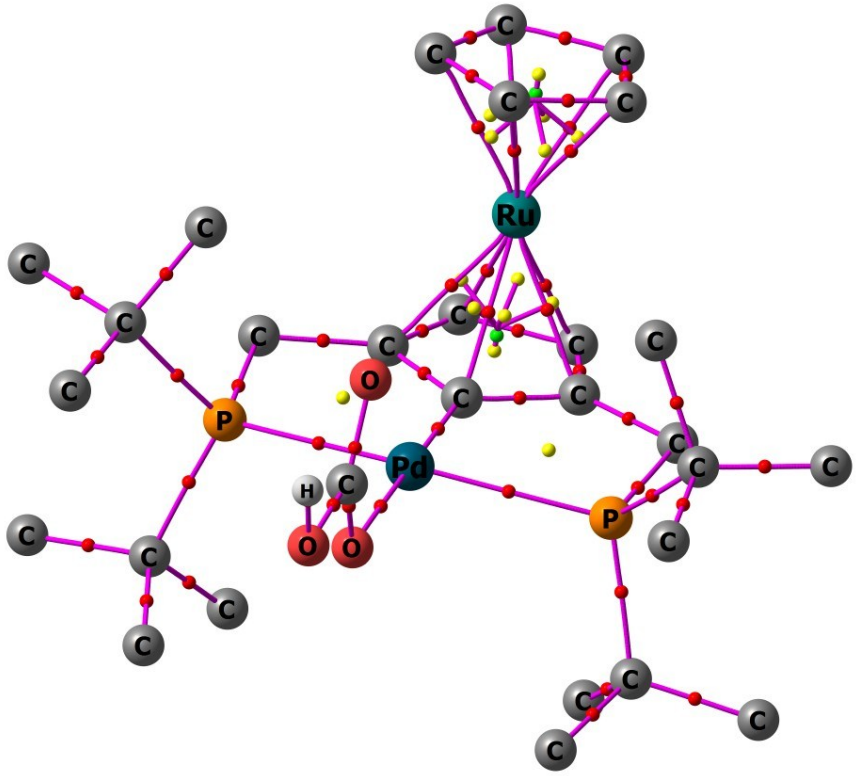


Table S15. Geometry parameters of crystal and M06-optimized structures of **5**.

Distances	**5**	**M06**
Pd–C	1.955(2)	1.975
Pd–P_1	2.3207(6)	2.372
Pd–P_2	2.3321(7)	2.374
Pd–O_1	2.128(2)	2.166
Pd···O_2	3.004(1)	3.204
Pd···C(OH)	2.905(2)	2.973
C–Pd–C(OH)	162.49(7)	159.75
P_1–Pd–P_2	161.03(2)	159.42
Pd–O_1–C(OH)	115.7(1)	117.92
Pd–O_2–C(OH)	71.7(1)	68.07

Figure S41. Crystal packing of **5** (thermal ellipsoids of all non-hydrogen atoms are drawn at the 50% probability level).

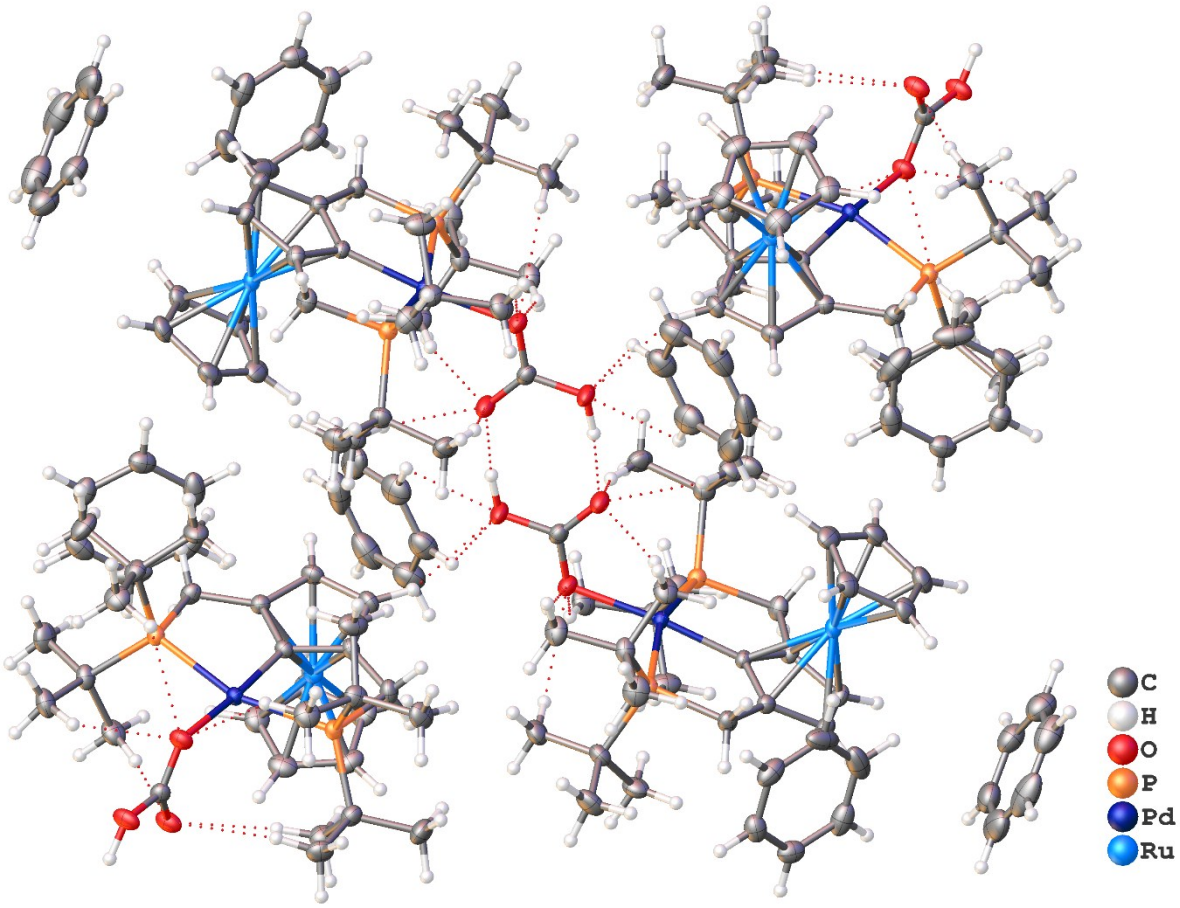


Figure S42. ^{1}H NMR spectrum (500 MHz) of **5** in C_6D_6.

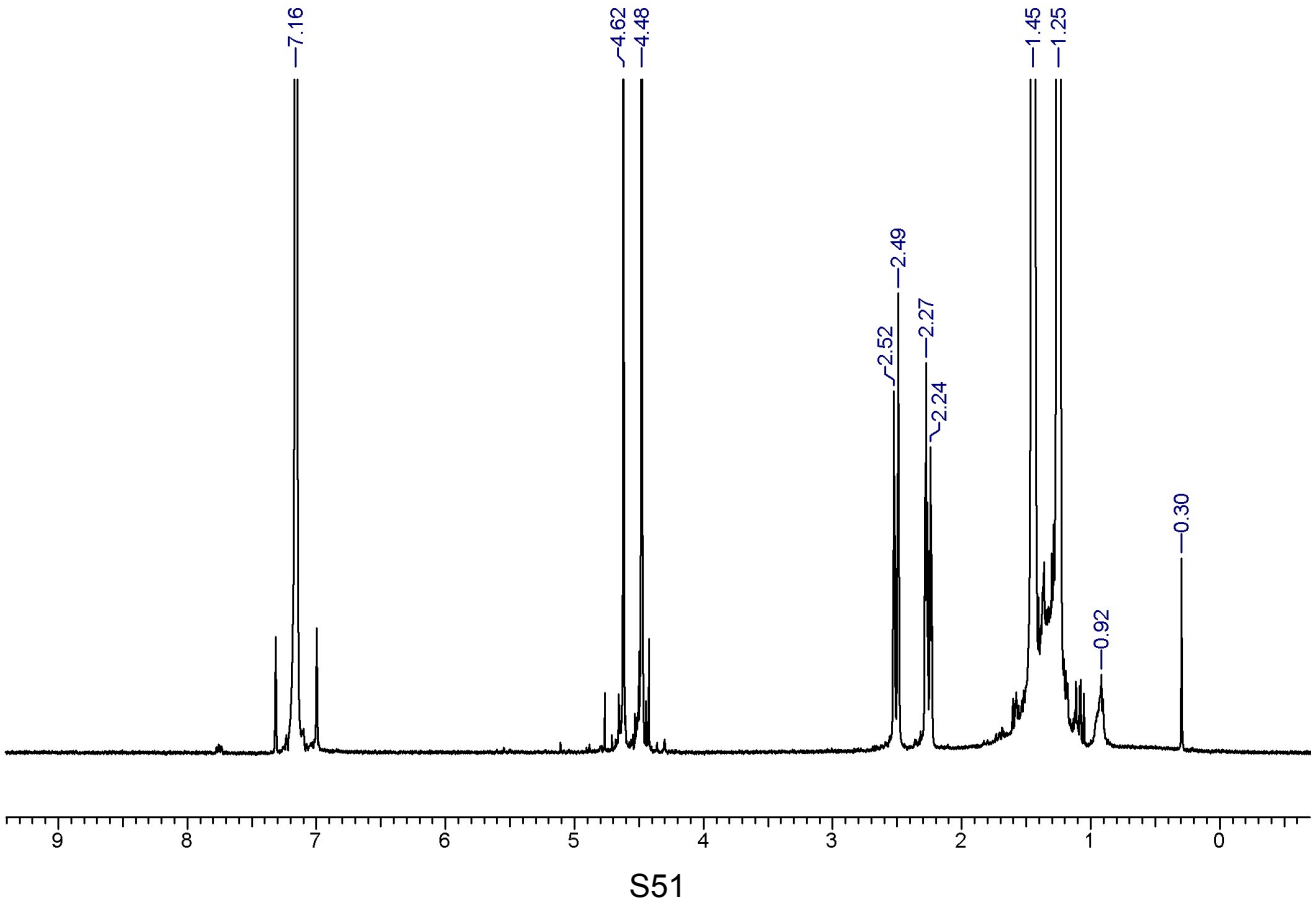


Figure S43. ^{13}C NMR spectrum (125.8 MHz) of **5** in C_6D_6.

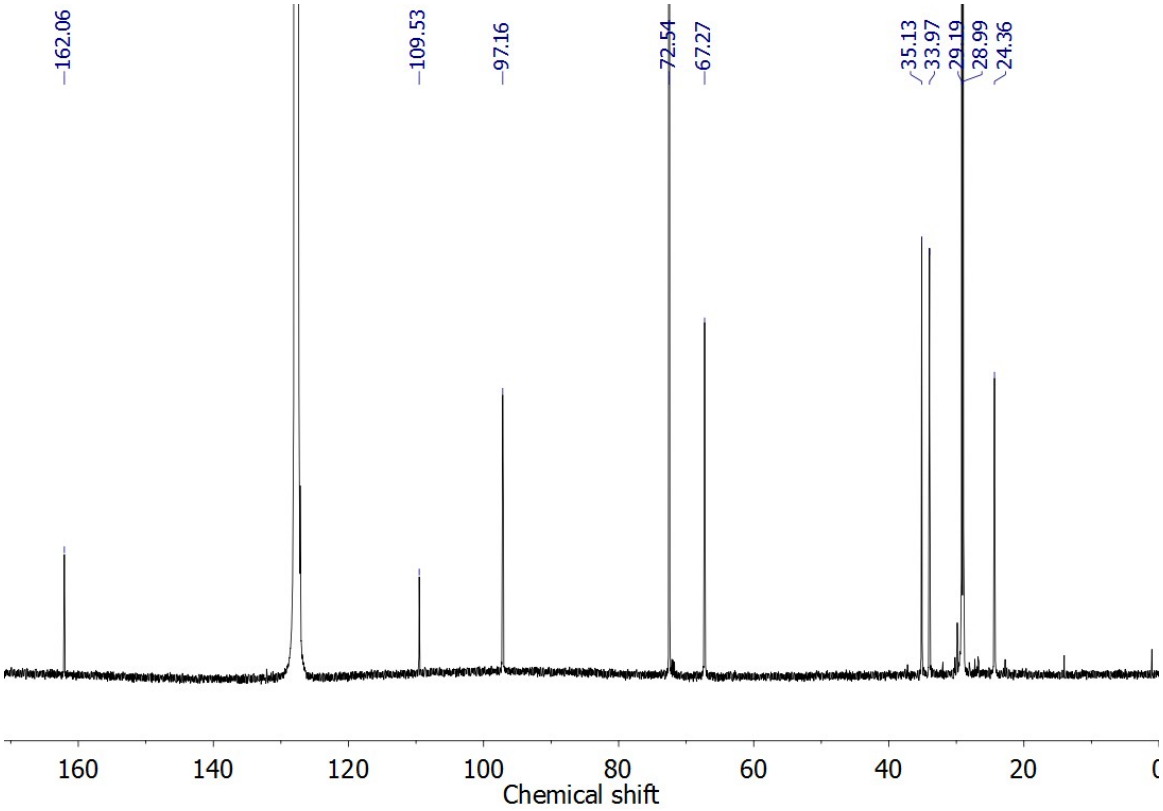


Figure S44. ^{31}P NMR spectrum (202.5 MHz) of **5** in C_6D_6.

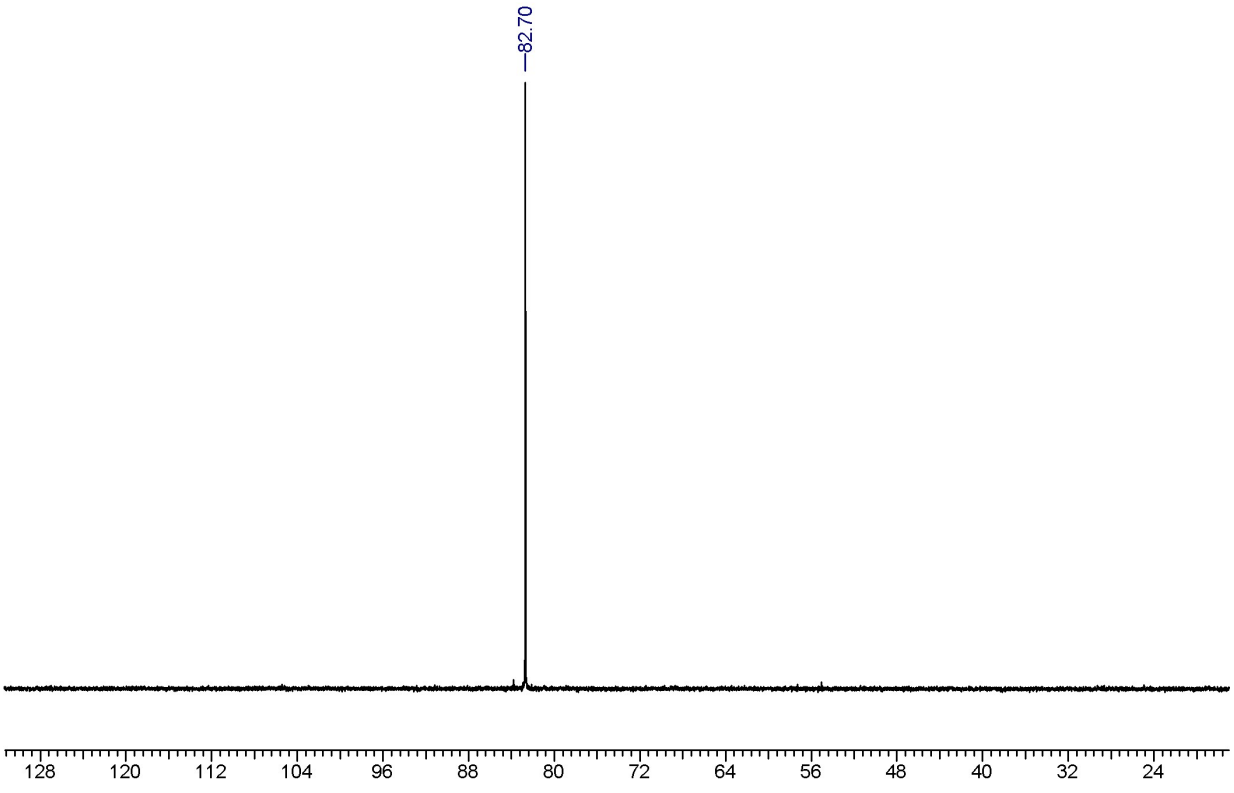


Figure S45. FTIR spectrum of **5** in KBr pellet.

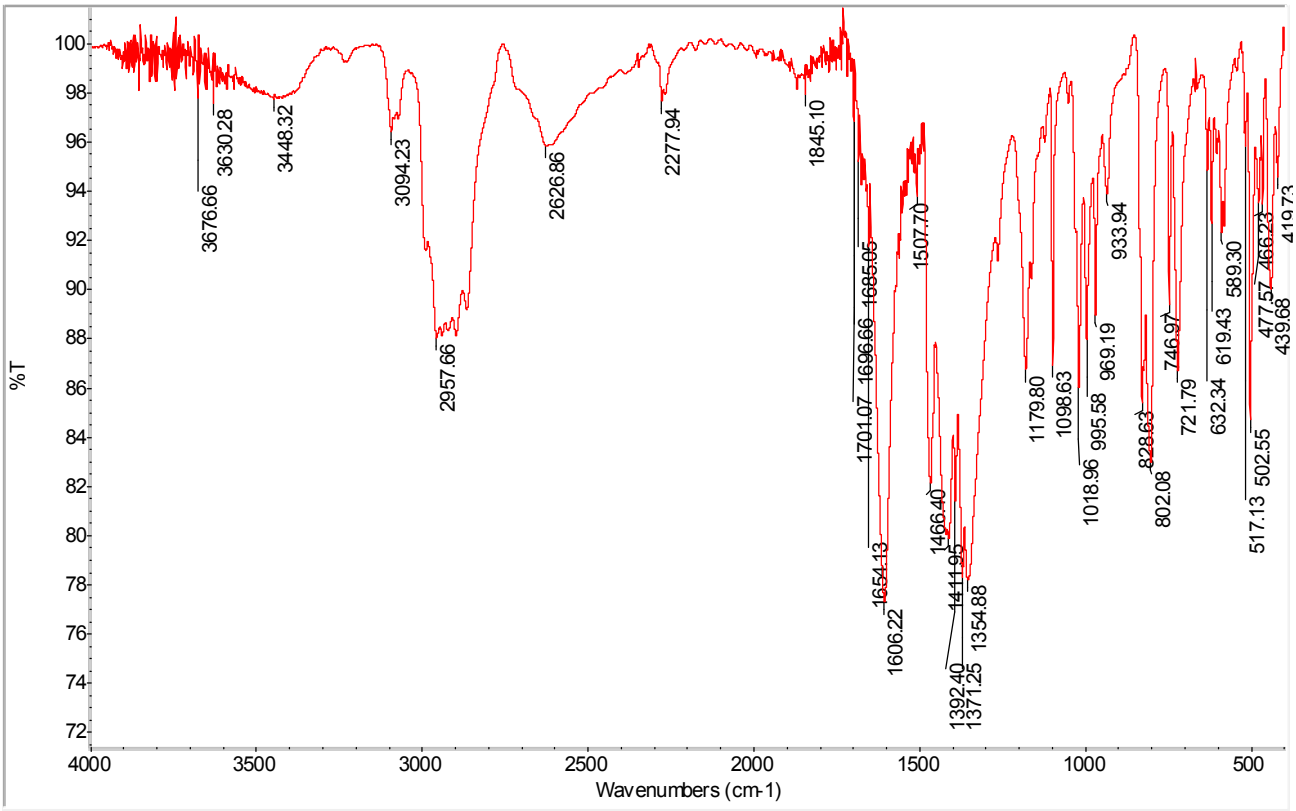


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Table S16. DFT-optimized geometries (Cartesian coordinates) and electronic energies in toluene or in tetrahydrofuran.

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B3LYP_*syn*-Pd(^{tBu}PC^{Ru}P)(η^{1,2}-BH$_4$) (*syn*-1) toluene

E= -2028.24312206 Ha

46	0.113127000	-1.048335000	-0.175060000
44	-0.081111000	2.820015000	-0.676694000
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15	2.462666000	-0.733059000	-0.578866000
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1	-0.746842000	-3.623374000	1.890257000

84

PBE0_*syn*-Pd(^{tBu}PC^{Ru}P)(η^{1,2}-BH$_4$) (*syn*-1) toluene

E= -2026.51554356 Ha

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1	1.185758000	2.887316000	-2.769211000
6	-0.839221000	2.118063000	-2.180584000
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6	-0.156889000	2.961203000	1.956880000
1	-0.120724000	2.181375000	2.704684000
6	0.967580000	3.624124000	1.378283000
1	2.006081000	3.443571000	1.619073000
6	0.482308000	4.590513000	0.447247000
1	1.087214000	5.262621000	-0.145589000
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6	-2.562797000	0.489608000	-0.963947000
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1	-3.144554000	1.167316000	-0.339492000
6	2.487960000	0.768106000	-0.968145000
1	2.977123000	1.489811000	-0.313713000
1	3.116684000	0.674383000	-1.858854000
6	-2.844688000	-2.447928000	-1.251913000
6	-2.081379000	-2.200690000	-2.568169000
1	-2.297918000	-3.026509000	-3.258712000
1	-0.999255000	-2.171012000	-2.405220000
1	-2.379452000	-1.270082000	-3.062201000
6	-4.353966000	-2.419719000	-1.537793000
1	-4.572780000	-3.127311000	-2.349020000
1	-4.701351000	-1.431998000	-1.862807000
1	-4.941675000	-2.728185000	-0.668387000
6	-2.442925000	-3.837092000	-0.725177000
1	-2.718839000	-4.590355000	-1.475418000
1	-2.944400000	-4.096901000	0.209802000
1	-1.364773000	-3.904024000	-0.554042000
6	-3.436377000	-0.968088000	1.460596000
6	-2.695349000	-0.048113000	2.450414000
1	-3.341189000	0.134659000	3.319908000
1	-2.447497000	0.920538000	2.001730000
1	-1.767007000	-0.509353000	2.800372000
6	-4.806539000	-0.343131000	1.138486000
1	-5.390994000	-0.310295000	2.067903000
1	-5.379655000	-0.922732000	0.411143000
1	-4.728519000	0.686277000	0.774000000
6	-3.657166000	-2.338068000	2.121507000
1	-4.158570000	-2.183190000	3.086475000
1	-2.713718000	-2.856192000	2.315510000
1	-4.302874000	-2.984132000	1.517859000
6	3.026274000	-2.121622000	-1.355957000
6	2.227346000	-1.887587000	-2.653460000
1	2.480234000	-2.681548000	-3.368475000
1	2.462827000	-0.928753000	-3.127031000
1	1.148105000	-1.924267000	-2.474585000
6	4.523837000	-1.970881000	-1.663177000
1	4.779642000	-2.635196000	-2.499803000
1	5.149950000	-2.259918000	-0.814165000
1	4.789314000	-0.950426000	-1.963101000
6	2.737983000	-3.553371000	-0.870959000
1	3.078952000	-4.260353000	-1.639261000
1	1.667589000	-3.712581000	-0.710668000
1	3.252759000	-3.797038000	0.061400000
6	3.560766000	-0.669371000	1.383366000
6	2.772895000	0.158044000	2.417992000
1	3.422278000	0.363920000	3.279597000
1	1.890867000	-0.383758000	2.772355000
1	2.441695000	1.119090000	2.007398000
6	4.860792000	0.080959000	1.038759000
1	5.462249000	0.156523000	1.954743000
1	4.680593000	1.102456000	0.688600000
1	5.465678000	-0.436753000	0.290916000
6	3.917469000	-2.030829000	2.000386000
1	4.444581000	-1.857395000	2.948328000
1	4.586027000	-2.611433000	1.356608000
1	3.026421000	-2.626268000	2.218719000
5	0.158872000	-2.930052000	2.139536000
1	0.165022000	-2.876023000	0.849395000
1	0.095767000	-1.842208000	2.692223000
1	1.195871000	-3.504331000	2.398229000
1	-0.811435000	-3.615862000	2.386211000

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BP86_*syn*-Pd(^{tBu}PC^{Ru}P)(η^{1,2}-BH$_4$) (*syn*-1) toluene

E= -2028.44414588 Ha

46	0.061299000	-1.199567000	0.310575000
44	-0.131157000	2.661451000	-0.198750000
15	-2.300834000	-1.116588000	-0.039306000
15	2.396099000	-0.892897000	-0.085893000
6	-0.028026000	0.488744000	-0.751261000
6	1.103176000	1.204979000	-1.298239000
6	0.602386000	2.218052000	-2.201199000
1	1.199956000	2.902975000	-2.803670000
6	-0.843341000	2.146326000	-2.192549000
1	-1.512902000	2.768231000	-2.787640000
6	-1.230913000	1.089138000	-1.284126000
6	-0.122415000	3.067710000	1.975174000
1	-0.070936000	2.302562000	2.747522000
6	0.999901000	3.730861000	1.362093000
1	2.049664000	3.567931000	1.600981000
6	0.490798000	4.682285000	0.408591000
1	1.087107000	5.353137000	-0.208143000
6	-0.947331000	4.607378000	0.430482000
1	-1.628666000	5.211647000	-0.166705000
6	-1.325255000	3.610333000	1.397437000
1	-2.344850000	3.339081000	1.666489000
6	-2.582188000	0.506267000	-0.968150000
1	-3.172127000	0.313867000	-1.880004000
1	-3.185656000	1.177816000	-0.343086000
6	2.508844000	0.759820000	-0.995805000
1	3.043497000	1.480401000	-0.362455000
1	3.111758000	0.639411000	-1.911150000
6	-2.886064000	-2.466100000	-1.280992000
6	-2.113877000	-2.215810000	-2.607218000
1	-2.348038000	-3.036654000	-3.312885000
1	-1.021970000	-2.207089000	-2.442911000
1	-2.397667000	-1.266301000	-3.094559000
6	-4.409514000	-2.414506000	-1.562269000
1	-4.645795000	-3.122903000	-2.380834000
1	-4.746169000	-1.412320000	-1.886029000
1	-5.002367000	-2.718112000	-0.682850000
6	-2.494563000	-3.872358000	-0.752600000
1	-2.772982000	-4.627460000	-1.513910000
1	-3.009575000	-4.133480000	0.185517000
1	-1.409212000	-3.948006000	-0.572543000
6	-3.468688000	-0.977478000	1.487960000
6	-2.712458000	-0.057650000	2.487201000
1	-3.352867000	0.111134000	3.375356000
1	-2.475504000	0.926966000	2.044320000
1	-1.767797000	-0.519823000	2.820759000
6	-4.849085000	-0.341213000	1.166799000
1	-5.431989000	-0.293622000	2.107832000
1	-5.435650000	-0.930382000	0.443579000
1	-4.766311000	0.692515000	0.786848000
6	-3.689293000	-2.366153000	2.141938000
1	-4.195057000	-2.221076000	3.116968000
1	-2.736356000	-2.889176000	2.331113000
1	-4.339540000	-3.012909000	1.526668000
6	3.066555000	-2.167784000	-1.362825000
6	2.256654000	-1.952112000	-2.672778000
1	2.520703000	-2.754862000	-3.388467000
1	2.479701000	-0.985825000	-3.158818000
1	1.169161000	-2.001823000	-2.488093000
6	4.576608000	-1.995838000	-1.666191000
1	4.850922000	-2.669303000	-2.502231000
1	5.206489000	-2.269974000	-0.802853000
6	4.830581000	-0.965379000	-1.976118000
1	2.791906000	-3.608818000	-0.855568000
1	3.132193000	-4.327531000	-1.626918000
1	1.715967000	-3.775806000	-0.679026000
1	3.325048000	-3.839940000	0.080500000
6	3.582154000	-0.667286000	1.415130000
6	2.778104000	0.184756000	2.437431000
1	3.420437000	0.392600000	3.315838000
1	1.875722000	-0.347396000	2.783308000
1	2.462812000	1.153824000	2.008867000
6	4.898799000	0.079952000	1.066238000
1	5.495534000	0.176156000	1.994769000
1	4.722701000	1.102704000	0.688393000
1	5.515942000	-0.459621000	0.330131000
6	3.926506000	-2.037876000	2.052552000
1	4.450117000	-1.860362000	3.012697000
1	4.603189000	-2.632507000	1.413733000
1	3.021150000	-2.631158000	2.266615000
5	0.158852000	-2.983613000	2.124339000
1	0.147275000	-2.900027000	0.825583000
1	0.118854000	-1.901038000	2.700061000
1	1.198682000	-3.578119000	2.351206000
1	-0.824517000	-3.662056000	2.367643000

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M06_*syn*-Pd(^{tBu}PC^{Ru}P)(η^{1,2}-BH$_4$) (*syn*-1) toluene

E= -2027.28058420 Ha

46	0.124488000	-1.033407000	-0.150510000
44	-0.091843000	2.721563000	-0.676020000
15	-2.243185000	-0.944651000	-0.513390000
15	2.450716000	-0.701910000	-0.584802000
6	0.027028000	0.595658000	-1.304078000
6	1.142104000	1.324837000	-1.825553000
6	0.638998000	2.346377000	-2.691332000
1	1.229648000	3.052393000	-3.262552000
6	-0.790918000	2.262016000	-2.688315000
1	-1.462715000	2.893054000	-3.257649000
6	-1.167539000	1.187882000	-1.821452000
6	-0.105013000	2.987746000	1.507075000
1	-0.070402000	2.163446000	2.208792000
6	1.018609000	3.674677000	0.961603000
1	2.058660000	3.474368000	1.185953000
6	0.536628000	4.686737000	0.082912000
1	1.143966000	5.385011000	-0.477259000
6	-0.886545000	4.626960000	0.082628000
1	-1.550107000	5.272020000	-0.477521000
6	-1.282440000	3.578344000	0.961315000
1	-2.302460000	3.294356000	1.187290000
6	-2.511955000	0.636187000	-1.476315000
1	-3.120386000	0.431349000	-2.365440000
1	-3.086443000	1.335906000	-0.864570000
6	2.541708000	0.937655000	-1.474238000
1	3.003747000	1.674411000	-0.812130000
1	3.194163000	0.855460000	-2.351616000
6	-2.780674000	-2.308645000	-1.705079000
6	-1.997545000	-2.095273000	-3.012501000
1	-2.220152000	-2.929546000	-3.693757000
1	-0.914138000	-2.086443000	-2.833644000
1	-2.269148000	-1.165385000	-3.527979000
6	-4.282489000	-2.297920000	-2.016081000
1	-4.485349000	-3.036502000	-2.806193000
1	-4.629206000	-1.322142000	-2.383100000
1	-4.885272000	-2.578619000	-1.144359000
6	-2.379068000	-3.679875000	-1.138522000
1	-2.643612000	-4.455304000	-1.872810000
1	-2.889784000	-3.919127000	-0.200011000
1	-1.298911000	-3.739004000	-0.954142000
6	-3.419554000	-0.784138000	0.957284000
6	-2.700386000	0.146390000	1.949767000
1	-3.368769000	0.346091000	2.800461000
1	-2.435006000	1.109640000	1.491837000
1	-1.781342000	-0.314631000	2.333462000
6	-4.781817000	-0.167204000	0.601262000
1	-5.393071000	-0.140158000	1.515844000
1	-5.333339000	-0.748553000	-0.145335000
1	-4.698117000	0.865944000	0.241738000
6	-3.647264000	-2.142509000	1.634170000
1	-4.167354000	-1.973017000	2.588724000
1	-2.702648000	-2.654321000	1.857384000
1	-4.280253000	-2.804000000	1.029355000
6	3.069524000	-1.952626000	-1.858112000
6	2.287399000	-1.703924000	-3.160391000
1	2.526149000	-2.509981000	-3.869481000
1	2.553084000	-0.752880000	-3.638937000
1	1.202640000	-1.711787000	-2.993754000
6	4.569065000	-1.839626000	-2.160340000
1	4.810818000	-2.514083000	-2.995604000
1	5.188564000	-2.141703000	-1.307880000
1	4.859816000	-0.824822000	-2.464511000
6	2.742554000	-3.373905000	-1.372805000
1	3.103058000	-4.095182000	-2.121198000
1	1.660440000	-3.516854000	-1.254539000
1	3.215680000	-3.616950000	-0.414848000
6	3.645007000	-0.501766000	0.863099000
6	2.877304000	0.330247000	1.906402000
1	3.540354000	0.530146000	2.761110000
1	1.993989000	-0.207532000	2.274397000
1	2.546090000	1.297647000	1.502204000
6	4.945164000	0.233521000	0.500911000
1	5.554083000	0.319766000	1.413351000
1	4.769140000	1.252380000	0.134037000
1	5.543355000	-0.302478000	-0.243187000
6	3.991373000	-1.862477000	1.481808000
1	4.545071000	-1.689701000	2.416658000
1	4.633278000	-2.465597000	0.827693000
1	3.092041000	-2.439321000	1.731703000
5	0.203198000	-2.690804000	1.802425000
1	0.243897000	-2.717358000	0.519261000
1	0.121755000	-1.566895000	2.273781000
1	1.236940000	-3.231908000	2.132788000
1	-0.771648000	-3.357758000	2.077088000

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M06_*anti*-Pd(^{tBu}PC^{Ru}P)(η^{1,2}-BH$_4$) (*anti*-1) toluene

E= -2027.27731267 Ha

46	0.054923000	-1.237276000	0.279079000
44	-0.116843000	2.540729000	-0.251056000
15	-2.319072000	-1.093857000	-0.027070000
15	2.399021000	-0.878332000	-0.080917000
6	-0.031459000	0.388185000	-0.879155000
6	1.086841000	1.111795000	-1.397558000
6	0.590452000	2.138214000	-2.263151000
1	1.185629000	2.835254000	-2.840731000
6	-0.840548000	2.074972000	-2.244732000

1	-1.509549000	2.716011000	-2.806224000
6	-1.222476000	1.010136000	-1.367170000
6	-0.110760000	2.885089000	1.925315000
1	-0.077490000	2.093061000	2.662828000
6	1.014203000	3.543068000	1.347258000
1	2.055028000	3.347924000	1.573934000
6	0.531764000	4.524303000	0.435025000
1	1.139255000	5.195873000	-0.156792000
6	-0.891861000	4.474423000	0.447276000
1	-1.554856000	5.101332000	-0.133837000
6	-1.288618000	3.462547000	1.367102000
1	-2.309016000	3.194973000	1.611508000
6	-2.570547000	0.495054000	-0.983805000
1	-3.200648000	0.299680000	-1.858554000
1	-3.115410000	1.213112000	-0.365512000
6	2.484349000	0.723906000	-1.043648000
1	2.972940000	1.490849000	-0.437571000
1	3.112339000	0.585201000	-1.930622000
6	-3.029292000	-2.391445000	-1.208617000
6	-2.202387000	-2.273572000	-2.503419000
1	-2.538074000	-3.051560000	-3.204270000
1	-1.133310000	-2.433764000	-2.309252000
1	-2.320994000	-1.304343000	-3.004306000
6	-4.515039000	-2.171554000	-1.527277000
1	-4.798406000	-2.844103000	-2.350813000
1	-4.745146000	-1.146514000	-1.847587000
1	-5.154516000	-2.420425000	-0.671920000
6	-2.843286000	-3.815784000	-0.666932000
1	-3.183871000	-4.524219000	-1.436965000
1	-3.428972000	-4.004806000	0.238564000
1	-1.793787000	-4.034951000	-0.441717000
6	-3.351028000	-0.883011000	1.540556000
6	-2.517602000	0.037944000	2.449947000
1	-3.090111000	0.248739000	3.365432000
1	-2.284472000	0.995616000	1.965173000
1	-1.569398000	-0.436264000	2.737983000
6	-4.724973000	-0.237121000	1.309122000
1	-5.237981000	-0.158095000	2.279339000
1	-5.364773000	-0.830482000	0.647240000
1	-4.652126000	0.778729000	0.899779000
6	-3.537776000	-2.230394000	2.252338000
1	-3.912796000	-2.040496000	3.269008000
1	-2.596059000	-2.788577000	2.341439000
1	-4.276096000	-2.863165000	1.745125000
6	3.199738000	-2.107339000	-1.277655000
6	2.349872000	-2.055280000	-2.561716000
1	2.742832000	-2.797621000	-3.271425000
1	2.377361000	-1.076781000	-3.057772000
1	1.300957000	-2.308223000	-2.356443000
6	4.657011000	-1.759384000	-1.611256000
1	4.993906000	-2.413254000	-2.429679000
1	5.321693000	-1.939879000	-0.757666000
1	4.790268000	-0.721958000	-1.945732000
6	3.142227000	-3.544106000	-0.739869000
1	3.523950000	-4.220464000	-1.519379000
1	2.118980000	-3.847689000	-0.493785000
1	3.758983000	-3.686353000	0.153326000
6	3.445100000	-0.572301000	1.461229000
6	2.538926000	0.228240000	2.413550000
1	3.114999000	0.501424000	3.310293000
1	1.668117000	-0.361982000	2.729680000
1	2.171204000	1.152721000	1.948173000
6	4.724657000	0.237969000	1.204278000
1	5.276906000	0.319967000	2.152451000
1	4.513768000	1.260683000	0.866423000
1	5.390775000	-0.236198000	0.475368000
6	3.812117000	-1.899713000	2.138428000
1	4.199907000	-1.682667000	3.144776000
1	4.598605000	-2.435632000	1.592804000
1	2.943149000	-2.561964000	2.249867000
5	0.178354000	-3.523450000	1.405706000
1	0.162482000	-3.647799000	0.188871000
1	0.118794000	-2.307613000	1.792182000
1	1.223097000	-3.941992000	1.859624000
1	-0.799758000	-4.048655000	1.895773000

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M06_Pd(^{tBu}PC^{Ru}P)(η^2-BH$_4$) TS$_{exch}$_toluene

E= -2027.27712701 Ha

46	0.103371000	-1.086368000	-0.197537000
44	-0.053305000	2.702290000	-0.724959000
15	-2.266172000	-0.937112000	-0.508133000
15	2.445295000	-0.734524000	-0.560119000
6	0.017161000	0.549226000	-1.340057000
6	1.136477000	1.260627000	-1.873251000
6	0.640801000	2.285726000	-2.740726000
1	1.236973000	2.974428000	-3.327192000
6	-0.790180000	2.231519000	-2.713271000
1	-1.459026000	2.873021000	-3.274420000
6	-1.173158000	1.174371000	-1.827323000
6	-0.034186000	3.043758000	1.451093000
1	0.005313000	2.249783000	2.186189000
6	1.085565000	3.705679000	0.867051000
1	2.128204000	3.513128000	1.087298000
6	0.594961000	4.687347000	-0.040561000
1	1.196988000	5.362054000	-0.634347000
6	-0.828410000	4.633623000	-0.019643000
1	-1.496687000	5.259720000	-0.595579000
6	-1.216718000	3.618748000	0.900706000
1	-2.234730000	3.346691000	1.150152000
6	-2.521710000	0.668898000	-1.431739000
1	-3.175597000	0.505351000	-2.295782000
1	-3.039695000	1.379318000	-0.782597000
6	2.534321000	0.857101000	-1.540112000
1	3.046081000	1.623216000	-0.952480000
1	3.142511000	0.700164000	-2.437984000
6	-2.946869000	-2.229197000	-1.711444000
6	-2.172651000	-2.037108000	-3.028968000
1	-2.473878000	-2.829096000	-3.729842000
1	-1.088510000	-2.118813000	-2.874061000
1	-2.378795000	-1.073223000	-3.511108000
6	-4.450121000	-2.074959000	-1.979000000
1	-4.730116000	-2.750226000	-2.801460000
1	-4.733225000	-1.057400000	-2.279799000
1	-5.049774000	-2.360021000	-1.106156000
6	-2.671348000	-3.654449000	-1.211087000
1	-3.023352000	-4.363440000	-1.975290000
1	-3.193753000	-3.885670000	-0.276941000
1	-1.602233000	-3.829866000	-1.047432000
6	-3.323010000	-0.760130000	1.047364000
6	-2.506989000	0.144009000	1.989017000
1	-3.092990000	0.329653000	2.901349000
1	-2.274556000	1.114952000	1.529955000
1	-1.559695000	-0.330333000	2.278280000
6	-4.694055000	-0.110156000	0.806278000
1	-5.215687000	-0.039198000	1.772472000
1	-5.328350000	-0.697047000	0.133786000
1	-4.617149000	0.909151000	0.406897000
6	-3.522875000	-2.122141000	1.726246000
1	-3.948077000	-1.955876000	2.727239000
1	-2.577699000	-2.667483000	1.849868000
1	-4.227110000	-2.755545000	1.172621000
6	3.224658000	-1.989817000	-1.743282000
6	2.364930000	-1.952601000	-3.021033000
1	2.752091000	-2.702842000	-3.725687000
1	2.386815000	-0.979908000	-3.528674000
1	1.318262000	-2.204045000	-2.802547000
6	4.681875000	-1.659543000	-2.094356000
1	5.008433000	-2.330681000	-2.902884000
1	5.351915000	-1.827742000	-1.242486000
1	4.818618000	-0.629308000	-2.449190000
6	3.158434000	-3.417738000	-1.181909000
1	3.530369000	-4.109105000	-1.952912000
1	2.134099000	-3.710502000	-0.925968000
1	3.778638000	-3.551310000	-0.289918000
6	3.509095000	-0.415570000	0.968117000
6	2.616969000	0.399757000	1.920918000
1	3.204287000	0.680699000	2.807914000
1	1.747350000	-0.182955000	2.252965000
1	2.248571000	1.320422000	1.448654000
6	4.788820000	0.387083000	0.687367000
1	5.355009000	0.470446000	1.627151000
1	4.578388000	1.409461000	0.348549000
1	5.441873000	-0.093761000	-0.049044000
6	3.881276000	-1.735285000	1.657370000
1	4.284642000	-1.505601000	2.654756000
1	4.658085000	-2.281097000	1.107559000
1	3.011472000	-2.391894000	1.791057000
5	0.220214000	-3.224155000	1.084332000
1	0.224195000	-3.266985000	-0.151413000
1	0.155661000	-2.040330000	1.513605000
1	1.261578000	-3.689562000	1.496813000
1	-0.764775000	-3.799716000	1.494445000

6

M06_MeOH_toluene

E= -115.691311605 Ha

6	-0.047490000	0.655394000	0.000000000
1	-1.089787000	0.982864000	0.000000000
1	0.439144000	1.074398000	0.891626000
1	0.439144000	1.074398000	-0.891626000
8	-0.046654000	-0.752509000	0.000000000
1	0.863118000	-1.058656000	0.000000000

90

M06_*syn*-1·MeOH_DHB_Ia_toluene

E= -2142.98376288 Ha

46	-2.008536000	10.357410000	11.876123000
44	0.003704000	13.286363000	13.180365000
15	-3.866736000	11.833385000	12.235690000
15	0.097632000	9.608236000	11.027648000
6	-1.081496000	12.111317000	11.645066000
6	0.280728000	12.300060000	11.247262000
6	0.510019000	13.704678000	11.105226000
1	1.432910000	14.175404000	10.788689000
6	-0.705048000	14.385929000	11.438736000
1	-0.854983000	15.458545000	11.416281000
6	-1.684012000	13.400883000	11.782682000
6	-0.008456000	12.351690000	15.173237000
1	-0.511541000	11.417439000	15.389767000
6	1.340555000	12.495338000	14.737118000
1	2.048018000	11.691121000	14.580178000
6	1.606614000	13.883564000	14.564738000
1	2.546201000	14.316764000	14.248995000
6	0.421321000	14.601838000	14.892682000
1	0.302586000	15.676805000	14.871746000
6	-0.575805000	13.656379000	15.268112000
1	-1.582220000	13.894310000	15.588451000
6	-3.115823000	13.545284000	12.182733000
1	-3.683233000	14.179814000	11.491127000
1	-3.208568000	14.006821000	13.168619000
6	1.177263000	11.128799000	11.008382000
1	1.932710000	11.036180000	11.793267000
1	1.720791000	11.194071000	10.058340000
6	-5.029768000	11.785357000	10.747687000
6	-4.193212000	12.178506000	9.517071000
1	-4.821933000	12.081235000	8.619994000
1	-3.325813000	11.516283000	9.394424000
1	-3.831428000	13.213866000	9.557468000
6	-6.222510000	12.741981000	10.866838000
1	-6.776765000	12.734026000	9.916393000
1	-5.913027000	13.778753000	11.057095000
1	-6.921009000	12.434061000	11.653729000
6	-5.536460000	10.349812000	10.531744000
1	-6.141592000	10.322539000	9.613415000
1	-6.163639000	9.989294000	11.353652000
1	-4.706364000	9.641664000	10.410990000
6	-4.810091000	11.802886000	13.874241000
6	-3.746785000	11.526502000	14.951332000
1	-4.224553000	11.560038000	15.941710000
1	-2.943833000	12.276604000	14.936024000
1	-3.293418000	10.535427000	14.820313000
6	-5.517611000	13.126838000	14.207335000
1	-6.075375000	12.988555000	15.145582000
1	-6.236279000	13.433126000	13.439640000
1	-4.814532000	13.952525000	14.372920000
6	-5.842167000	10.667421000	13.900037000
1	-6.223515000	10.567925000	14.927040000
1	-5.401214000	9.704135000	13.616486000
1	-6.700971000	10.873322000	13.249165000
6	-0.057392000	9.127764000	9.207537000
6	-0.434669000	10.398735000	8.425259000
1	-0.680482000	10.111617000	7.392389000
1	0.385017000	11.126644000	8.378933000
1	-1.312685000	10.898234000	8.854226000
6	1.227535000	8.545615000	8.606047000
1	1.082879000	8.420586000	7.522439000
1	1.468708000	7.559145000	9.019097000
1	2.092520000	9.207665000	8.747926000
6	-1.209839000	8.122448000	9.057056000
1	-1.300919000	7.836231000	7.998567000
1	-2.161163000	8.571167000	9.372887000
1	-1.060926000	7.208064000	9.643538000
6	1.091446000	8.352909000	12.024171000
6	0.915706000	8.780140000	13.493159000
1	1.528112000	8.126164000	14.131264000
1	-0.130176000	8.690834000	13.813241000
1	1.237400000	9.817655000	13.664627000
6	2.591082000	8.336053000	11.688504000
1	3.083460000	7.617054000	12.360197000
1	3.074436000	9.308346000	11.847253000
1	2.792529000	8.014703000	10.661535000
6	0.515794000	6.941080000	11.850202000
1	1.005481000	6.271175000	12.572478000
1	0.703834000	6.537810000	10.847214000
1	-0.563132000	6.911623000	12.050298000
5	-3.008918000	8.191440000	12.794557000
1	-2.932286000	8.792555000	11.666731000
1	-2.384856000	8.719148000	13.697792000
1	-2.580084000	7.083082000	12.550501000
1	-4.195663000	8.174826000	13.059763000
1	-4.806638000	7.105086000	11.762608000
8	-5.288420000	6.622724000	11.073145000
6	-4.369999000	6.231849000	10.091398000
1	-3.531524000	5.651165000	10.503672000
1	-3.950870000	7.087069000	9.538628000
1	-4.896025000	5.597527000	9.370581000

90

M06_*syn*-1·MeOH_DHB_IIa_toluene

E= -2142.98414435 Ha

46	-2.011187000	10.448268000	11.814795000
44	0.085029000	13.238127000	13.284122000
15	-3.833177000	11.944102000	12.225223000
15	0.099865000	9.682371000	10.974895000
6	-1.055040000	12.197393000	11.689543000
6	0.300092000	12.383074000	11.272335000
6	0.561815000	13.789057000	11.231728000
1	1.488766000	14.260304000	10.928068000
6	-0.628511000	14.472902000	11.640286000
1	-0.751940000	15.547549000	11.698779000
6	-1.622595000	13.487873000	11.936763000
6	0.126673000	12.149290000	15.194413000
1	-0.349113000	11.188038000	15.345065000
6	1.466154000	12.366188000	14.756303000
1	2.197631000	11.600449000	14.531383000
6	1.688829000	13.771344000	14.691806000
1	2.611526000	14.256303000	14.402634000
6	0.488180000	14.426018000	15.089981000
1	0.338064000	15.495376000	15.154515000
6	-0.475803000	13.424623000	15.400077000
1	-1.484873000	13.605717000	15.747369000
6	-3.042890000	13.628556000	12.379090000
1	-3.602186000	14.363045000	11.787166000
1	-3.106841000	13.955383000	13.420460000
6	1.165097000	11.218539000	10.917661000
1	1.996126000	11.107349000	11.618084000
1	1.613304000	11.323072000	9.922219000
6	-4.922915000	12.083426000	10.688469000
6	-4.053874000	12.681144000	9.567359000
1	-4.615182000	12.624976000	8.623252000
1	-3.115343000	12.127654000	9.436423000
1	-3.807212000	13.735735000	9.742977000
6	-6.155345000	12.976343000	10.878253000
1	-6.649965000	13.102420000	9.903411000
1	-5.894205000	13.978305000	11.244912000
1	-6.889213000	12.532189000	11.560953000
6	-5.362759000	10.676978000	10.251615000
1	-6.003967000	10.766674000	9.362274000
1	-5.930377000	10.147372000	11.025277000
1	-4.499130000	10.052985000	9.986750000
6	-4.842569000	11.768429000	13.810898000
6	-3.818495000	11.423537000	14.908038000
1	-4.337916000	11.372667000	15.876407000
1	-3.025861000	12.181134000	14.988437000
1	-3.343831000	10.451519000	14.720817000
6	-5.588108000	13.049740000	14.216571000
1	-6.118887000	12.853234000	15.160138000
1	-6.335518000	13.357479000	13.478291000
1	-4.912056000	13.894823000	14.397429000
6	-5.846339000	10.613552000	13.697663000
1	-6.285524000	10.434034000	14.690348000
1	-5.364966000	9.681461000	13.375608000
1	-6.670963000	10.845199000	13.011982000
6	-0.049044000	9.151683000	9.168154000
6	-0.587776000	10.365703000	8.391136000
1	-0.742312000	10.070662000	7.343014000
1	0.101041000	11.219802000	8.396120000
1	-1.553981000	10.698979000	8.792554000
6	1.282030000	8.708331000	8.548621000
1	1.127481000	8.526854000	7.474313000
1	1.648425000	7.772838000	8.987624000
1	2.067240000	9.470980000	8.642340000
6	-1.081461000	8.020484000	9.034993000
1	-1.212226000	7.790014000	7.967196000
1	-0.773555000	7.099574000	9.540354000
6	1.110845000	8.455027000	11.997449000
6	0.857864000	8.851592000	13.462558000
1	1.454654000	8.203295000	14.121188000
1	-0.198751000	8.726050000	13.729768000
1	1.140418000	9.895508000	13.656801000
6	2.622366000	8.510189000	11.723769000
1	3.107307000	7.731514000	12.331143000
1	3.069645000	9.468406000	12.015712000
1	2.875427000	8.314822000	10.675788000
6	0.618134000	7.017536000	11.781664000
1	1.066736000	6.374838000	12.553145000
1	0.921539000	6.622637000	10.804047000
1	-0.471253000	6.933924000	11.878014000
5	-3.029953000	8.233710000	12.574888000
1	-2.978884000	8.923000000	11.502103000
1	-2.482527000	8.770627000	13.525478000
1	-2.485346000	7.185732000	12.284677000
1	-4.212958000	8.082754000	12.787221000
1	-1.854404000	6.915649000	14.097671000
8	-1.500294000	6.568176000	14.930585000
6	-1.924461000	7.414038000	15.962867000
1	-3.016675000	7.544234000	15.982094000
1	-1.465691000	8.415131000	15.907638000
1	-1.621477000	6.963436000	16.913361000

90

M06_*syn*-1·MeOH_DHB_IIab_toluene

E= -2142.98389593 Ha

46	-2.057292000	10.464334000	11.856754000
44	0.091092000	13.263489000	13.256894000
15	-3.854876000	11.995961000	12.240218000
15	0.033295000	9.645563000	11.029319000
6	-1.074112000	12.194932000	11.700562000
6	0.281151000	12.348025000	11.270972000
6	0.562764000	13.748087000	11.186782000
1	1.494834000	14.196396000	10.864559000
6	-0.615214000	14.460945000	11.580985000
1	-0.722371000	15.538563000	11.608296000
6	-1.622042000	13.500165000	11.911610000
6	0.115600000	12.238523000	15.203212000
1	-0.388398000	11.298644000	15.391229000
6	1.456689000	12.396442000	14.745472000
1	2.159751000	11.599162000	14.539915000
6	1.724591000	13.790655000	14.631726000
1	2.659546000	14.234719000	14.317348000
6	0.549662000	14.497432000	15.017602000
1	0.435152000	15.572686000	15.047157000
6	-0.443313000	13.539063000	15.370267000
1	-1.442969000	13.764002000	15.719308000
6	-3.041043000	13.673291000	12.347076000
1	-3.588224000	14.396835000	11.730869000
1	-3.103504000	14.033189000	13.377627000

6	1.127154000	11.160661000	10.945885000
1	1.951386000	11.050044000	11.654335000
1	1.583581000	11.236392000	9.951594000
6	-4.952729000	12.102776000	10.707753000
6	-4.086829000	12.664519000	9.565708000
1	-4.652738000	12.582116000	8.626404000
1	-3.151508000	12.103129000	9.445637000
1	-3.835300000	13.723002000	9.708562000
6	-6.178498000	13.007235000	10.883089000
1	-6.677652000	13.113757000	9.908281000
1	-5.910346000	14.015745000	11.226356000
1	-6.910785000	12.581438000	11.579138000
6	-5.401581000	10.686684000	10.312903000
1	-6.045142000	10.750637000	9.423247000
1	-5.972114000	10.184193000	11.102899000
1	-4.543706000	10.049769000	10.060406000
6	-4.850217000	11.876153000	13.838367000
6	-3.813830000	11.576994000	14.937136000
1	-4.326554000	11.543142000	15.909666000
1	-3.033146000	12.349109000	14.992262000
1	-3.325115000	10.608017000	14.773001000
6	-5.599857000	13.167260000	14.202962000
1	-6.093094000	13.014748000	15.174670000
1	-6.378810000	13.422554000	13.477519000
1	-4.932342000	14.031120000	14.312613000
6	-5.848459000	10.712855000	13.774167000
1	-6.286054000	10.571118000	14.773595000
1	-5.363501000	9.770936000	13.488082000
1	-6.674035000	10.913313000	13.079675000
6	-0.127908000	9.087147000	9.232014000
6	-0.643669000	10.298327000	8.435276000
1	-0.802387000	9.989356000	7.391929000
1	0.060435000	11.139875000	8.428242000
1	-1.604809000	10.654110000	8.829103000
6	1.194073000	8.607561000	8.619785000
1	1.034340000	8.407960000	7.549535000
1	1.544446000	7.674405000	9.076605000
1	1.992970000	9.357664000	8.697453000
6	-1.182615000	7.973577000	9.120173000
1	-1.322542000	7.726556000	8.057140000
1	-2.154163000	8.292192000	9.520805000
1	-0.883822000	7.057121000	9.639961000
6	1.021568000	8.417160000	12.072059000
6	0.770188000	8.835455000	13.531556000
1	1.381557000	8.206426000	14.195650000
1	-0.284455000	8.706299000	13.808036000
1	1.044007000	9.884806000	13.708901000
6	2.534447000	8.447833000	11.801053000
1	3.007749000	7.665895000	12.413549000
1	2.995380000	9.401103000	12.087799000
1	2.786052000	8.243054000	10.754472000
6	0.509665000	6.983465000	11.876865000
1	0.965606000	6.344366000	12.647555000
1	0.795094000	6.573793000	10.900093000
1	-0.579336000	6.914868000	11.991761000
5	-3.141713000	8.246998000	12.622985000
1	-3.010836000	8.950275000	11.562607000
1	-2.695807000	8.759435000	13.632475000
1	-2.588039000	7.201297000	12.361402000
1	-4.349961000	8.106979000	12.712740000
1	-4.584913000	7.588375000	10.939854000
8	-4.822969000	7.174379000	10.096838000
6	-4.251284000	5.893363000	10.081582000
1	-4.551388000	5.289775000	10.950511000
1	-3.151191000	5.921831000	10.057904000
1	-4.596791000	5.380921000	9.178272000

90

M06_*anti*-1·MeOH_DHB_IIab_toluene

E= -2142.97925809 Ha

46	-1.755425000	10.280317000	11.925444000
44	0.229784000	13.128015000	13.310862000
15	-3.665817000	11.616721000	12.495286000
15	0.295442000	9.711793000	10.863312000
6	-0.974427000	12.103696000	11.745772000
6	0.329528000	12.405146000	11.240890000
6	0.489456000	13.827599000	11.265615000
1	1.353014000	14.382577000	10.919645000
6	-0.704364000	14.399164000	11.815956000
1	-0.891593000	15.456953000	11.955928000
6	-1.599507000	13.329854000	12.136478000
6	0.552569000	11.938441000	15.138544000
1	0.194364000	10.924351000	15.266620000
6	1.817924000	12.327065000	14.608357000
1	2.605478000	11.662540000	14.276995000
6	1.885005000	13.749505000	14.617693000
1	2.722472000	14.349027000	14.286958000
6	0.661765000	14.243596000	15.155033000
1	0.405689000	15.284438000	15.301441000
6	-0.158732000	13.125635000	15.477051000
1	-1.147121000	13.172476000	15.915964000
6	-2.968983000	13.330893000	12.738008000
1	-3.632900000	14.080948000	12.292365000
1	-2.931199000	13.545622000	13.809505000
6	1.246056000	11.319465000	10.773794000
1	2.136711000	11.248210000	11.403747000
1	1.602781000	11.481430000	9.749578000
6	-4.854990000	11.846060000	11.041350000
6	-4.093849000	12.603283000	9.938036000
1	-4.718929000	12.618065000	9.033196000
1	-3.146290000	12.112922000	9.682171000
1	-3.878897000	13.644869000	10.206418000
6	-6.114115000	12.642832000	11.405819000
1	-6.677775000	12.848199000	10.483226000
1	-5.881875000	13.610470000	11.870876000
1	-6.777056000	12.081405000	12.074705000
6	-5.257938000	10.476278000	10.477322000
1	-5.955482000	10.630463000	9.640399000
1	-5.753585000	9.837159000	11.216608000
1	-4.385775000	9.927968000	10.099640000
6	-4.557775000	11.237637000	14.110716000
6	-3.438963000	10.874107000	15.104499000
1	-3.888420000	10.662181000	16.086310000
1	-2.720077000	11.695580000	15.236576000
1	-2.876468000	9.985669000	14.784814000
6	-5.360672000	12.416425000	14.680523000
1	-5.774079000	12.113657000	15.654305000
1	-6.202412000	12.702953000	14.041842000
1	-4.740072000	13.304921000	14.853975000
6	-5.479499000	10.022872000	13.939068000
1	-5.839526000	9.710742000	14.931144000
1	-4.955965000	9.168841000	13.488869000
1	-6.361285000	10.256421000	13.329043000
6	-0.006504000	9.258519000	9.055152000
6	-0.668753000	10.481822000	8.395959000
1	-0.925519000	10.222518000	7.358539000
1	-0.014534000	11.362304000	8.365005000
1	-1.596896000	10.759737000	8.912379000
6	1.275845000	8.906059000	8.291288000
1	1.030639000	8.793766000	7.224470000
1	1.702829000	7.953963000	8.628067000
1	2.046059000	9.685548000	8.371428000
6	-0.998491000	8.088325000	8.966287000
1	-1.222186000	7.899150000	7.905733000
1	-1.942790000	8.313541000	9.478848000
1	-0.602705000	7.161164000	9.393674000
6	1.451445000	8.503138000	11.734601000
6	1.372446000	8.871899000	13.226252000
1	2.073688000	8.237940000	13.788644000
1	0.366956000	8.704887000	13.634542000
1	1.643896000	9.920770000	13.404549000
6	2.914893000	8.600306000	11.277071000
1	3.504804000	7.873274000	11.854942000
1	3.351687000	9.589741000	11.463503000
1	3.046386000	8.359879000	10.216851000
6	0.958944000	7.059602000	11.564865000
1	1.523164000	6.415788000	12.255500000
1	1.128980000	6.681162000	10.549222000
1	-0.106597000	6.952744000	11.808713000
5	-2.999352000	7.713012000	12.056438000
1	-2.319820000	6.766810000	11.717982000
1	-2.128936000	8.589031000	12.397542000
1	-3.612868000	7.493082000	13.087366000
1	-3.731165000	8.095364000	11.177047000
1	-2.028099000	7.712374000	14.158752000
8	-1.669221000	7.725893000	15.058673000
6	-2.665763000	7.223019000	15.909012000
1	-2.945174000	6.189170000	15.659428000
1	-2.274477000	7.230890000	16.930806000
1	-3.583113000	7.832375000	15.893855000

9

M06_TFE_toluene

E= -452.732042009 Ha

1	-2.071495000	-0.671526000	-0.617858000
8	-1.974434000	-0.074434000	0.131126000
6	-0.882731000	0.762111000	-0.083648000
6	0.423323000	0.012785000	0.008781000
1	-0.902291000	1.265029000	-1.060596000
1	-0.879622000	1.530302000	0.695186000
9	0.479013000	-0.973219000	-0.901271000
9	1.454898000	0.830819000	-0.222106000
9	0.607614000	-0.547600000	1.203384000

93

M06_*syn*-1·TFE_DHB_Ia_toluene

E= -2480.02877014 Ha

46	-2.038677000	10.386838000	11.939205000
44	0.058909000	13.302087000	13.133436000
15	-3.853903000	11.930232000	12.241602000
15	0.044422000	9.544646000	11.119369000
6	-1.063272000	12.103683000	11.646484000
6	0.302538000	12.237118000	11.239040000
6	0.571722000	13.627857000	11.042547000
1	1.506822000	14.059009000	10.706198000
6	-0.621882000	14.356135000	11.351772000
1	-0.740372000	15.431035000	11.288524000
6	-1.628210000	13.414669000	11.735710000
6	0.027742000	12.440603000	15.159141000
1	-0.500153000	11.528740000	15.409423000
6	1.378665000	12.531594000	14.714866000
1	2.062969000	11.702824000	14.584418000
6	1.681838000	13.905063000	14.492101000
1	2.631806000	14.300991000	14.159014000
6	0.517813000	14.666596000	14.797969000
1	0.428468000	15.743000000	14.739118000
6	-0.503452000	13.762826000	15.208813000
1	-1.501607000	14.039892000	15.523427000
6	-3.054677000	13.616445000	12.129732000
1	-3.603112000	14.241668000	11.414784000
1	-3.133179000	14.116442000	13.097912000
6	1.165188000	11.033297000	11.042035000
1	1.921078000	10.950519000	11.827292000
1	1.706272000	11.049019000	10.088675000
6	-5.014254000	11.857307000	10.752762000
6	-4.166409000	12.188403000	9.511501000
1	-4.796350000	12.074840000	8.617401000
1	-3.316085000	11.500770000	9.411807000
1	-3.780160000	13.215613000	9.517396000
6	-6.187419000	12.841779000	10.833693000
1	-6.740605000	12.807606000	9.883289000
1	-5.856602000	13.878613000	10.983717000
1	-6.893005000	12.579180000	11.630626000
6	-5.546234000	10.424489000	10.586141000
1	-6.138260000	10.369281000	9.660723000
1	-6.191217000	10.108687000	11.413261000
1	-4.725751000	9.700617000	10.503135000
6	-4.797372000	11.983494000	13.878850000
6	-3.741699000	11.722797000	14.967342000
1	-4.217597000	11.810779000	15.955283000
1	-2.917564000	12.448296000	14.921587000
1	-3.316512000	10.714862000	14.878001000
6	-5.472746000	13.335848000	14.159124000
1	-6.032171000	13.248856000	15.102495000
1	-6.184845000	13.627943000	13.380011000
1	-4.749932000	14.150375000	14.290514000
6	-5.856436000	10.875244000	13.946936000
1	-6.246203000	10.830133000	14.974649000
1	-5.437442000	9.890194000	13.708572000
1	-6.706068000	11.072570000	13.281692000
6	-0.122297000	8.999954000	9.318289000
6	-0.489772000	10.248007000	8.495760000
1	-0.726040000	9.931972000	7.469461000
1	0.330960000	10.973716000	8.437174000
1	-1.372094000	10.759394000	8.900889000
6	1.156926000	8.385668000	8.736345000
1	1.007546000	8.217303000	7.659359000
1	1.392990000	7.415193000	9.188550000
1	2.026937000	9.046881000	8.848115000
6	-1.282014000	7.998100000	9.197155000
1	-1.401401000	7.717609000	8.140359000
1	-2.225818000	8.445592000	9.538313000
1	-1.106828000	7.080008000	9.771123000
6	1.001637000	8.301067000	12.165360000
6	0.822691000	8.776897000	13.618933000
1	1.415016000	8.129608000	14.282276000
1	-0.227579000	8.720739000	13.932588000
1	1.166350000	9.811884000	13.761690000
6	2.503218000	8.242183000	11.843909000
1	2.972883000	7.525154000	12.533738000
1	3.006505000	9.206247000	11.989128000
1	2.706180000	7.897122000	10.824884000
6	0.399618000	6.896172000	12.029053000
1	0.869559000	6.239149000	12.775856000
1	0.588780000	6.458649000	11.040743000
1	-0.681370000	6.893843000	12.220515000
5	-3.117472000	8.275109000	12.917111000
1	-3.002622000	8.837288000	11.776305000
1	-2.520833000	8.826250000	13.822494000
1	-2.693872000	7.152898000	12.732196000
1	-4.313272000	8.281497000	13.149919000
1	-4.893881000	7.252050000	11.915696000
8	-5.352856000	6.723374000	11.239749000
6	-4.409092000	6.082144000	10.450709000
1	-4.412058000	4.992299000	10.604857000
1	-3.386937000	6.444083000	10.625761000
6	-4.715563000	6.310934000	8.994841000
9	-4.683094000	7.603900000	8.655816000
9	-3.811385000	5.676319000	8.229076000
9	-5.920897000	5.847343000	8.648750000

93

M06_*syn*-1·TFE_DHB_IIa_toluene

E= -2480.02972179 Ha

46	-1.939758000	10.401023000	11.811056000
44	0.069781000	13.307149000	13.244119000
15	-3.804681000	11.817410000	12.301734000
15	0.186098000	9.719378000	10.957366000
6	-1.045901000	12.182461000	11.688322000
6	0.296240000	12.418866000	11.252622000
6	0.492803000	13.833772000	11.174472000
1	1.393927000	14.339480000	10.849291000
6	-0.722381000	14.472267000	11.583741000
1	-0.893989000	15.541303000	11.619279000
6	-1.667643000	13.450913000	11.915138000
6	0.175111000	12.271464000	15.180907000
1	-0.275409000	11.304469000	15.366076000
6	1.498964000	12.505229000	14.707111000
1	2.240237000	11.747944000	14.485216000
6	1.689871000	13.912642000	14.600136000
1	2.594813000	14.409211000	14.276578000
6	0.483904000	14.551947000	15.007553000
1	0.311527000	15.619142000	15.047257000
6	-0.450572000	13.538781000	15.366225000
1	-1.455183000	13.707225000	15.732841000
6	-3.088099000	13.541308000	12.368828000
1	-3.686839000	14.218701000	11.748343000
1	-3.157783000	13.917136000	13.392545000
6	1.208480000	11.282552000	10.923003000
1	2.020216000	11.195951000	11.649245000
1	1.683270000	11.396268000	9.941372000
6	-4.997663000	11.869680000	10.839930000
6	-4.202419000	12.410404000	9.637913000
1	-4.836712000	12.347996000	8.741619000
1	-3.297903000	11.815470000	9.452999000
1	-3.904305000	13.459378000	9.760137000
6	-6.218933000	12.766241000	11.076284000
1	-6.785968000	12.845072000	10.136536000
1	-5.940103000	13.785369000	11.376870000
1	-6.894939000	12.349633000	11.832605000
6	-5.459472000	10.445267000	10.493518000
1	-6.130151000	10.494801000	9.622842000
1	-6.006051000	9.961790000	11.310536000
1	-4.610417000	9.800345000	10.233050000
6	-4.693222000	11.623424000	13.957863000
6	-3.582662000	11.316619000	14.978713000
1	-4.029089000	11.226485000	15.980396000
1	-2.823367000	12.110344000	15.015789000
1	-3.072798000	10.374224000	14.740466000
6	-5.449964000	12.881918000	14.411153000
1	-5.941164000	12.659736000	15.370396000
1	-6.230371000	13.187216000	13.705623000
1	-4.784377000	13.736979000	14.583256000
6	-5.667980000	10.438498000	13.920098000
1	-6.019769000	10.243572000	14.944299000
1	-5.188312000	9.522584000	13.551826000
1	-6.550939000	10.650404000	13.303813000
6	0.068426000	9.204764000	9.145056000
6	-0.445171000	10.427217000	8.363154000
1	-0.631704000	10.123318000	7.322773000
1	0.277017000	11.252896000	8.340954000
1	-1.389085000	10.806332000	8.777392000
6	1.409609000	8.758718000	8.550060000
1	1.278378000	8.590802000	7.470468000
1	1.761204000	7.816439000	8.986683000
1	2.196252000	9.516026000	8.670443000
6	-0.967289000	8.079942000	8.989038000
1	-1.044394000	7.819294000	7.923049000
1	-1.960029000	8.397317000	9.333359000
1	-0.697388000	7.171147000	9.537531000
6	1.205551000	8.511789000	11.991561000
6	0.924295000	8.907463000	13.452303000
1	1.508159000	8.259831000	14.123103000
1	-0.137748000	8.786674000	13.699961000
1	1.201913000	9.951183000	13.656719000
6	2.718500000	8.590669000	11.735650000
1	3.211916000	7.836891000	12.367143000
1	3.142433000	9.564695000	12.009586000
1	2.987498000	8.375456000	10.695533000
6	0.736068000	7.066823000	11.773353000
1	1.196234000	6.429667000	12.543051000
1	1.043402000	6.677121000	10.794861000
1	-0.352050000	6.965816000	11.868921000
5	-2.930975000	8.136863000	12.500257000
1	-2.846106000	8.850136000	11.451840000
1	-2.408124000	8.643739000	13.482241000
1	-2.379158000	7.096969000	12.194951000
1	-4.118676000	7.975952000	12.679457000
1	-1.922197000	6.836050000	14.042492000
8	-1.839171000	6.350279000	14.880906000
6	-2.658587000	6.958923000	15.819733000
1	-3.158749000	6.200662000	16.436065000
1	-3.432789000	7.594832000	15.367756000
6	-1.863913000	7.825864000	16.764717000
9	-2.678906000	8.403485000	17.663137000
9	-0.953256000	7.125640000	17.449911000
9	-1.207110000	8.807262000	16.136675000

93

M06_*anti*-1·TFE_DHB_IIab_toluene

E= -2480.02245527 Ha

46	-1.753249000	10.267885000	11.931232000
44	0.217315000	13.100873000	13.347535000
15	-3.672464000	11.598857000	12.496571000
15	0.298288000	9.713264000	10.862751000
6	-0.976015000	12.093118000	11.767570000
6	0.329490000	12.400487000	11.269513000
6	0.487838000	13.822460000	11.310278000
1	1.352599000	14.381636000	10.974313000
6	-0.708950000	14.387485000	11.860531000
1	-0.897510000	15.443619000	12.010683000
6	-1.605120000	13.314812000	12.165850000
6	0.535538000	11.896124000	15.168002000
1	0.183659000	10.878914000	15.288956000
6	1.801578000	12.296383000	14.648897000
1	2.595595000	11.639160000	14.318834000
6	1.860171000	13.719070000	14.670321000
1	2.696350000	14.326148000	14.350310000
6	0.630703000	14.201373000	15.204160000

1	0.367545000	15.239409000	15.357740000
6	-0.185118000	13.075891000	15.511398000
1	-1.176039000	13.112890000	15.945381000
6	-2.978305000	13.310453000	12.758206000
1	-3.639658000	14.063327000	12.313485000
1	-2.948088000	13.517046000	13.831523000
6	1.247715000	11.321379000	10.790540000
1	2.138307000	11.243230000	11.419924000
1	1.604385000	11.495091000	9.768134000
6	-4.844410000	11.836823000	11.030091000
6	-4.066992000	12.595050000	9.939075000
1	-4.682267000	12.618785000	9.027803000
1	-3.119942000	12.099645000	9.691086000
1	-3.847891000	13.633678000	10.215524000
6	-6.104934000	12.637233000	11.381644000
1	-6.657084000	12.846148000	10.452912000
1	-5.874577000	13.603367000	11.850685000
1	-6.777877000	12.077381000	12.041880000
6	-5.246071000	10.470586000	10.456343000
1	-5.926797000	10.631225000	9.606933000
1	-5.760632000	9.834335000	11.185102000
1	-4.371107000	9.916777000	10.093202000
6	-4.585909000	11.212150000	14.097789000
6	-3.483794000	10.838409000	15.106334000
1	-3.951598000	10.622959000	16.078568000
1	-2.763437000	11.654874000	15.258393000
1	-2.916272000	9.952532000	14.787586000
6	-5.391854000	12.389933000	14.665650000
1	-5.821043000	12.081404000	15.630756000
1	-6.222687000	12.685810000	14.017152000
1	-4.769704000	13.273781000	14.855792000
6	-5.510237000	10.001990000	13.907519000
1	-5.879930000	9.682535000	14.893921000
1	-4.986545000	9.150824000	13.452262000
1	-6.386549000	10.243700000	13.293048000
6	-0.018268000	9.276771000	9.053396000
6	-0.670838000	10.510627000	8.404595000
1	-0.940118000	10.258331000	7.368656000
1	-0.004531000	11.381822000	8.370821000
1	-1.590418000	10.800490000	8.929682000
6	1.254875000	8.915372000	8.278594000
1	1.001320000	8.813437000	7.212708000
1	1.673799000	7.956428000	8.605673000
1	2.033748000	9.686077000	8.359115000
6	-1.022882000	8.116902000	8.966446000
1	-1.255743000	7.933747000	7.906876000
1	-1.961517000	8.350085000	9.485986000
1	-0.633743000	7.183959000	9.387667000
6	1.457401000	8.494230000	11.714193000
6	1.397413000	8.856101000	13.208219000
1	2.097970000	8.212973000	13.760712000
1	0.394690000	8.696697000	13.625378000
1	1.680464000	9.901454000	13.389190000
6	2.916056000	8.587134000	11.240664000
1	3.510631000	7.861165000	11.814991000
1	3.356664000	9.576399000	11.418717000
1	3.035702000	8.342343000	10.180189000
6	0.956083000	7.054007000	11.542018000
1	1.527296000	6.403115000	12.220095000
1	1.110150000	6.681571000	10.521656000
1	-0.106410000	6.949382000	11.799776000
5	-3.001336000	7.695232000	12.083381000
1	-2.354759000	6.730723000	11.732984000
1	-2.096960000	8.554288000	12.361647000
1	-3.578179000	7.499105000	13.142361000
1	-3.768920000	8.075438000	11.235359000
1	-2.047568000	7.695215000	14.116151000
8	-1.631247000	7.693641000	14.994991000
6	-2.581435000	7.249661000	15.905439000
1	-2.784369000	6.170465000	15.829211000
1	-3.542949000	7.780463000	15.821130000
6	-2.060967000	7.505692000	17.291986000
9	-1.852627000	8.805064000	17.528738000
9	-2.947544000	7.073272000	18.201951000
9	-0.908394000	6.873872000	17.529091000

12

M06_HFIP_toluene

E= -452.732042009 Ha

8	8.602441000	0.492090000	-11.046343000
6	8.653602000	-0.824151000	-10.619907000
1	9.677325000	-1.216513000	-10.522960000
6	8.005557000	-0.974055000	-9.240671000
6	7.978184000	-1.658183000	-11.705304000
9	8.730765000	-1.645421000	-12.803965000
9	6.779678000	-1.193048000	-12.028215000
9	7.841610000	-2.925468000	-11.317933000
9	6.700646000	-0.737248000	-9.253619000
9	8.206677000	-2.185619000	-8.730452000
9	8.571685000	-0.087780000	-8.413242000
1	9.275155000	1.011187000	-10.593498000

96

M06_*syn*-1·HFIP_DHB_Ia*_toluene

E= -2817.06032685 Ha

46	-2.098335000	10.406970000	11.914116000
44	0.063476000	13.227593000	13.153962000
15	-3.873729000	11.997267000	12.224491000
15	-0.043552000	9.516822000	11.067807000
6	-1.079586000	12.098716000	11.630609000
6	0.294339000	12.197561000	11.240932000
6	0.607688000	13.583411000	11.076524000
1	1.559309000	13.992787000	10.759907000
6	-0.566205000	14.341733000	11.389542000
1	-0.650908000	15.420828000	11.347775000
6	-1.605756000	13.424227000	11.741684000
6	-0.020462000	12.328932000	15.161856000
1	-0.590701000	11.437371000	15.391904000
6	1.335645000	12.365771000	14.726036000
1	1.981862000	11.509244000	14.582376000
6	1.703557000	13.727583000	14.532037000
1	2.672683000	14.085234000	14.210953000
6	0.574767000	14.536392000	14.847715000
1	0.535983000	15.616767000	14.810314000
6	-0.489579000	13.673420000	15.235853000
1	-1.473774000	13.991907000	15.554357000
6	-3.030414000	13.662228000	12.122795000
1	-3.555756000	14.301449000	11.402817000
1	-3.105642000	14.163766000	13.090483000
6	1.122721000	10.971376000	11.032213000
1	1.865100000	10.850035000	11.825268000
1	1.676025000	10.988306000	10.085907000
6	-5.026464000	11.949263000	10.727796000
6	-4.169344000	12.278486000	9.492663000
1	-4.794940000	12.173905000	8.594379000
1	-3.323148000	11.585749000	9.395183000
1	-3.775953000	13.302848000	9.505467000
6	-6.190489000	12.944621000	10.804703000
1	-6.735031000	12.922559000	9.848944000
1	-5.850294000	13.976858000	10.964706000
1	-6.906295000	12.684076000	11.592970000
6	-5.571357000	10.522091000	10.551820000
1	-6.160944000	10.477732000	9.624198000
1	-6.220697000	10.206699000	11.375942000
1	-4.755840000	9.792330000	10.470411000
6	-4.831284000	12.073378000	13.852699000
6	-3.791265000	11.810989000	14.955559000
1	-4.277908000	11.914707000	15.936635000
1	-2.957442000	12.525209000	14.913214000
1	-3.378824000	10.796921000	14.881803000
6	-5.495224000	13.434889000	14.115137000
1	-6.046840000	13.367597000	15.064692000
1	-6.212477000	13.717729000	13.337782000
1	-4.766593000	14.247219000	14.225803000
6	-5.901069000	10.975342000	13.918187000
1	-6.302337000	10.941785000	14.941879000
1	-5.488172000	9.984682000	13.692211000
1	-6.741803000	11.174566000	13.242337000
6	-0.214707000	9.028937000	9.250495000
6	-0.542716000	10.308319000	8.460280000
1	-0.782097000	10.026732000	7.424597000
1	0.298925000	11.011217000	8.424990000
1	-1.411333000	10.834690000	8.875315000
6	1.051710000	8.396531000	8.658945000
1	0.908190000	8.270514000	7.575474000
1	1.253988000	7.404072000	9.078419000
1	1.940538000	9.025841000	8.801575000
6	-1.397066000	8.060090000	9.092527000
1	-1.513944000	7.810015000	8.027988000
1	-2.334539000	8.521382000	9.435285000
1	-1.244664000	7.121303000	9.639891000
6	0.865453000	8.209378000	12.078538000
6	0.685092000	8.641557000	13.545497000
1	1.254553000	7.958344000	14.192428000
1	-0.368749000	8.602630000	13.849386000
1	1.053809000	9.662200000	13.724031000
6	2.368002000	8.118934000	11.769352000
1	2.810306000	7.364445000	12.436829000
1	2.896063000	9.062662000	11.955007000
1	2.572202000	7.805686000	10.740347000
6	0.226612000	6.826355000	11.888852000
1	0.667041000	6.133115000	12.620593000
1	0.415999000	6.413069000	10.890384000
1	-0.856110000	6.845921000	12.070093000
5	-3.219284000	8.345753000	12.939023000
1	-3.089080000	8.868216000	11.780029000
1	-2.688304000	8.959190000	13.843123000
1	-2.738098000	7.239067000	12.828827000
1	-4.425233000	8.312731000	13.119437000
1	-4.801368000	6.964744000	12.162143000
8	-5.161776000	6.361412000	11.481699000
6	-4.154102000	6.039726000	10.600436000
1	-3.290342000	6.718820000	10.675329000
6	-4.702051000	6.189984000	9.183829000
9	-4.909713000	7.482654000	8.921998000
9	-3.845691000	5.727709000	8.267787000
9	-5.858041000	5.558489000	9.012404000
6	-3.605322000	4.637911000	10.882804000
9	-3.325753000	4.513673000	12.175621000
9	-4.464513000	3.671326000	10.559994000
9	-2.471951000	4.417720000	10.205452000

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M06_*syn*-1·HFIP_DHB_IIa_toluene

E= -2817.06095991 Ha

46	-2.112210000	10.507142000	11.853911000
44	0.087194000	13.239114000	13.241643000
15	-3.859511000	12.123930000	12.165525000
15	-0.053864000	9.597294000	11.041595000
6	-1.050919000	12.186049000	11.659753000
6	0.330660000	12.268516000	11.295297000
6	0.676115000	13.652077000	11.186385000
1	1.641561000	14.051336000	10.900122000
6	-0.486599000	14.424809000	11.506345000
1	-0.547711000	15.506298000	11.501448000
6	-1.550924000	13.518182000	11.808746000
6	-0.052071000	12.284029000	15.218423000
1	-0.641085000	11.396466000	15.413673000
6	1.313818000	12.311747000	14.812619000
1	1.951314000	11.450699000	14.658654000
6	1.706431000	13.672640000	14.666596000
1	2.687510000	14.023786000	14.376152000
6	0.583684000	14.489857000	14.982022000
1	0.562128000	15.571364000	14.974669000
6	-0.501731000	13.632878000	15.322675000
1	-1.488553000	13.956121000	15.627920000
6	-2.977547000	13.771140000	12.173022000
1	-3.472674000	14.462151000	11.480149000
1	-3.061498000	14.217967000	13.167048000
6	1.136664000	11.033723000	11.053895000
1	1.873775000	10.877180000	11.845527000
1	1.694418000	11.068860000	10.110572000
6	-4.955962000	12.176749000	10.627784000
6	-4.053955000	12.561341000	9.442484000
1	-4.646231000	12.502008000	8.517760000
1	-3.205156000	11.871925000	9.342814000
1	-3.660473000	13.582893000	9.518252000
6	-6.109407000	13.182764000	10.724438000
1	-6.609186000	13.241574000	9.746041000
1	-5.765279000	14.194675000	10.978665000
1	-6.863721000	12.873514000	11.457427000
6	-5.517113000	10.771641000	10.356789000
1	-6.117998000	10.797878000	9.435464000
1	-6.158420000	10.406141000	11.165949000
1	-4.710579000	10.040112000	10.212321000
6	-4.867443000	12.146376000	13.762655000
6	-3.853253000	11.864078000	14.885404000
1	-4.372252000	11.913131000	15.853887000
1	-3.038397000	12.601130000	14.899992000
1	-3.411514000	10.864766000	14.782831000
6	-5.555823000	13.491374000	14.045569000
1	-6.073161000	13.412531000	15.013416000
1	-6.307344000	13.750163000	13.292933000
1	-4.846689000	14.324317000	14.127189000
6	-5.923160000	11.033067000	13.764883000
1	-6.354484000	10.963205000	14.774528000
1	-5.491358000	10.054365000	13.520947000
1	-6.746775000	11.242111000	13.070817000
6	-0.205640000	9.138953000	9.215220000
6	-0.499783000	10.434077000	8.437709000
1	-0.735829000	10.169716000	7.396654000
1	0.356546000	11.119726000	8.418397000
1	-1.360972000	10.974166000	8.851432000
6	1.060549000	8.494179000	8.636385000
1	0.935208000	8.387202000	7.548629000
1	1.238936000	7.492328000	9.044291000
1	1.956735000	9.106619000	8.805049000
6	-1.401547000	8.190781000	9.027427000
1	-1.484119000	7.924794000	7.963395000
1	-2.340775000	8.678403000	9.326490000
1	-1.295266000	7.261032000	9.599062000
6	0.819105000	8.261625000	12.048417000
6	0.610238000	8.671338000	13.517811000
1	1.147116000	7.963789000	14.166468000
1	-0.452361000	8.650062000	13.792862000
1	0.995863000	9.679904000	13.724283000
6	2.326337000	8.157625000	11.768620000
1	2.743766000	7.381059000	12.426810000
1	2.864769000	9.088201000	11.987238000
1	2.547023000	7.865328000	10.736698000
6	0.168699000	6.889971000	11.825322000
1	0.593209000	6.179372000	12.549819000
1	0.365119000	6.492086000	10.822119000
1	-0.914592000	6.921164000	11.993486000
5	-3.327106000	8.404269000	12.745268000
1	-3.119245000	9.000862000	11.635502000
1	-2.882598000	8.967788000	13.724664000
1	-2.816177000	7.310976000	12.605293000
1	-4.543950000	8.335189000	12.801117000
1	-4.627717000	6.565835000	12.269369000
8	-4.936225000	5.916066000	11.610464000
6	-4.502375000	6.350765000	10.377234000
1	-3.828367000	7.218915000	10.449800000
6	-5.688146000	6.807606000	9.529193000
9	-6.421277000	7.678252000	10.217984000
9	-5.280850000	7.422605000	8.413074000
9	-6.485679000	5.802271000	9.170543000
6	-3.686388000	5.237066000	9.727146000
9	-2.554146000	5.062160000	10.411902000
9	-4.326600000	4.073080000	9.709618000
9	-3.352216000	5.538024000	8.468376000

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M06_*anti*-1·HFIP_DHB_IIa_toluene

E= -2817.05750508 Ha

46	-1.753266000	10.253642000	11.948191000
44	0.157450000	13.248454000	13.246252000
15	-3.670567000	11.532823000	12.633292000
15	0.341857000	9.727073000	10.896070000
6	-1.019717000	12.094752000	11.734884000
6	0.269321000	12.429230000	11.214840000
6	0.371129000	13.855995000	11.169903000
1	1.210138000	14.427922000	10.792513000
6	-0.842533000	14.402078000	11.699619000
1	-1.075471000	15.456166000	11.789778000
6	-1.691043000	13.311544000	12.072055000
6	0.514141000	12.197221000	15.150775000
1	0.162320000	11.196363000	15.370174000
6	1.769163000	12.536705000	14.565902000
1	2.543955000	11.841726000	14.267402000
6	1.843658000	13.955199000	14.468295000
1	2.675561000	14.522982000	14.073616000
6	0.634560000	14.496013000	14.992279000
1	0.387103000	15.546561000	15.065767000
6	-0.185159000	13.411064000	15.414323000
1	-1.161383000	13.499457000	15.874375000
6	-3.059537000	13.297976000	12.669899000
1	-3.759403000	13.941903000	12.125527000
1	-3.049263000	13.656680000	13.702073000
6	1.232528000	11.367952000	10.796598000
1	2.110030000	11.345637000	11.447548000
1	1.607287000	11.524471000	9.778993000
6	-5.050078000	11.596472000	11.341391000
6	-4.404408000	12.135524000	10.051111000
1	-5.160845000	12.126367000	9.253155000
1	-3.567074000	11.502835000	9.727338000
1	-4.039058000	13.165682000	10.148415000
6	-6.214353000	12.508741000	11.750487000
1	-6.895458000	12.611931000	10.892530000
1	-5.892024000	13.519166000	12.035846000
1	-6.795784000	12.081110000	12.576189000
6	-5.595035000	10.193405000	11.038254000
1	-6.337284000	10.277488000	10.230440000
1	-6.093608000	9.735160000	11.898628000
1	-4.804228000	9.512257000	10.704708000
6	-4.320284000	11.211716000	14.378248000
6	-3.065017000	10.933738000	15.223754000
1	-3.362475000	10.751927000	16.267170000
1	-2.367900000	11.782600000	15.209656000
1	-2.517766000	10.054439000	14.857944000
6	-5.075048000	12.395837000	15.001314000
1	-5.422806000	12.094849000	16.000798000
1	-5.956012000	12.691001000	14.421709000
6	-4.437455000	13.278780000	15.135809000
1	-5.225225000	9.970583000	14.406800000
1	-5.364108000	9.660027000	15.453539000
1	-4.796174000	9.122748000	13.854792000
1	-6.220015000	10.179472000	13.993372000
6	0.179427000	9.232912000	9.076799000
6	-0.587023000	10.380574000	8.393006000
1	-0.748253000	10.114104000	7.338343000
1	-0.045881000	11.334946000	8.414372000
1	-1.571807000	10.532140000	8.855198000
6	1.536349000	9.037839000	8.386640000
1	1.364877000	8.906016000	7.307811000
1	2.048451000	8.137464000	8.746564000
1	2.210865000	9.895794000	8.507717000
6	-0.654311000	7.954225000	8.909573000
1	-0.798459000	7.774096000	7.833821000
1	-1.642529000	8.047865000	9.373057000
1	-0.165915000	7.069109000	9.329817000
6	1.506415000	8.595145000	11.859236000
6	1.294064000	8.968377000	13.336370000
1	1.973307000	8.370319000	13.961685000
1	0.264806000	8.759502000	13.655029000
1	1.500308000	10.030772000	13.524282000
6	2.991660000	8.774015000	11.511333000
1	3.573573000	8.054508000	12.106531000
1	3.365241000	9.774563000	11.763176000
1	3.209073000	8.578830000	10.455536000
6	1.116069000	7.123393000	11.665959000
1	1.634818000	6.520354000	12.425563000
1	1.418597000	6.745204000	10.681763000
1	0.037938000	6.958653000	11.793143000
5	-2.823045000	7.920821000	11.931244000
1	-2.168450000	6.902708000	11.763186000
1	-2.137177000	8.615220000	12.744478000
1	-3.877224000	7.711771000	12.492728000
1	-3.005839000	8.453798000	10.854665000
1	-2.080368000	6.461552000	13.422056000
8	-1.909314000	6.194292000	14.347111000
6	-2.714846000	6.936139000	15.183936000
1	-3.107677000	7.846493000	14.704472000
6	-1.869932000	7.406229000	16.363068000
9	-0.919725000	8.236523000	15.926546000
9	-2.602249000	8.073872000	17.259027000
9	-1.266140000	6.405342000	16.995737000
6	-3.940818000	6.121455000	15.598182000
9	-4.595405000	5.728695000	14.508337000

9	-3.621970000	5.031413000	16.293533000
9	-4.788796000	6.843098000	16.337448000

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M06_*syn,syn*-[{Pd(^tBu^PC^Ru^P)}$_2$(μ,η^{1,2}:η^{1,2}-BH_4)]$^+$ (2)

toluene E= -4026.96229632 Ha

44	12.907870000	-3.183229000	4.266142000
46	11.013843000	-0.093072000	5.365868000
15	9.144556000	-1.235797000	4.300603000
15	12.824089000	0.187190000	6.900262000
6	10.883271000	-3.151277000	5.161160000
6	11.594262000	-1.986037000	5.615153000
6	12.764118000	-2.434453000	6.330656000
6	12.751435000	-3.870311000	6.349894000
1	13.471853000	-4.508158000	6.840534000
6	11.592364000	-4.313475000	5.623228000
1	11.293266000	-5.340935000	5.476211000
6	9.600720000	-3.044315000	4.408827000
1	8.794579000	-3.595090000	4.905557000
1	9.688443000	-3.468599000	3.406772000
6	8.770407000	-0.973824000	2.462042000
6	10.147642000	-0.829952000	1.791537000
1	10.009874000	-0.755922000	0.702542000
1	10.787465000	-1.699185000	1.993414000
1	10.672545000	0.069245000	2.139991000
6	8.030936000	-2.149841000	1.802786000
1	7.805097000	-1.872117000	0.762651000
1	7.081667000	-2.389025000	2.292296000
1	8.638460000	-3.061965000	1.763897000
6	7.959699000	0.310031000	2.226748000
1	7.981883000	0.544609000	1.151170000
1	8.379582000	1.170454000	2.762449000
1	6.907256000	0.188903000	2.512285000
6	7.588667000	-1.109725000	5.362810000
6	6.402457000	-1.916991000	4.820793000
1	5.590338000	-1.887535000	5.562201000
1	6.646614000	-2.973271000	4.646870000
1	6.010290000	-1.492722000	3.888569000
6	7.175439000	0.362076000	5.511211000
1	6.361550000	0.426072000	6.249550000
1	6.807597000	0.789498000	4.572385000
1	8.008151000	0.983465000	5.866736000
6	7.968490000	-1.630560000	6.760080000
1	7.088302000	-1.553756000	7.414704000
1	8.771258000	-1.025515000	7.202079000
1	8.289628000	-2.679734000	6.760284000
6	13.688864000	-1.455064000	6.973519000
1	14.644266000	-1.387918000	6.446927000
1	13.921014000	-1.714430000	8.012340000
6	12.154351000	0.430238000	8.647778000
6	11.447689000	-0.873687000	9.060026000
1	10.909341000	-0.694678000	10.001931000
1	12.153430000	-1.695032000	9.235439000
1	10.719130000	-1.207598000	8.310852000
6	11.112887000	1.559433000	8.625053000
1	10.718296000	1.708098000	9.641171000
1	10.269159000	1.311214000	7.966157000
1	11.540182000	2.511307000	8.286641000
6	13.243122000	0.743416000	9.680732000
1	12.790904000	0.728467000	10.683161000
1	13.682885000	1.736982000	9.534328000
1	14.048316000	-0.003427000	9.672429000
6	14.189644000	1.404662000	6.458204000
6	13.711701000	2.845190000	6.674002000
1	14.460146000	3.536697000	6.257911000
1	13.594243000	3.089945000	7.737534000
1	12.758699000	3.029149000	6.161247000
6	15.500366000	1.179357000	7.225853000
1	16.251261000	1.884317000	6.839579000
1	15.904748000	0.169108000	7.087614000
1	15.398518000	1.365876000	8.299733000
6	14.444622000	1.186845000	4.955000000
1	15.266115000	1.843813000	4.632372000
1	13.551989000	1.423873000	4.360267000
1	14.733485000	0.150899000	4.728679000
6	12.906059000	-3.328085000	2.052720000
1	12.022516000	-3.409452000	1.438553000
6	13.565718000	-2.113772000	2.436488000
1	13.258485000	-1.110599000	2.181657000
6	14.722775000	-2.466067000	3.203719000
1	15.444821000	-1.777358000	3.615515000
6	14.777791000	-3.892803000	3.296487000
1	15.542958000	-4.467467000	3.794052000
6	13.655249000	-4.425915000	2.585423000
1	13.428533000	-5.471886000	2.452087000
5	10.597979000	2.233670000	4.339981000
1	9.532042000	2.403030000	3.799194000
1	11.363988000	1.614019000	3.641060000
1	10.376513000	1.695495000	5.465289000
1	11.172423000	3.310800000	4.696015000
44	7.809481000	6.383227000	1.600659000
46	10.362843000	4.740269000	3.751838000
15	11.781183000	4.861713000	1.793603000
15	9.056680000	5.655878000	5.558613000
6	9.963298000	6.844382000	1.551181000
6	9.631984000	6.374628000	2.873129000
6	8.655442000	7.276414000	3.432004000
6	8.414253000	8.317516000	2.470665000
1	7.760276000	9.166782000	2.601857000
6	9.221517000	8.050874000	1.311147000
1	9.274936000	8.664939000	0.424259000
6	10.975681000	6.142159000	0.709737000
1	11.731395000	6.825506000	0.305934000
1	10.510116000	5.650573000	-0.147775000
6	11.998682000	3.378329000	0.646223000
6	10.611423000	2.714219000	0.576401000
1	10.645968000	1.892694000	-0.154440000
1	9.833822000	3.419636000	0.249440000
1	10.313661000	2.303645000	1.549531000
6	12.432915000	3.753463000	-0.780038000
1	12.529308000	2.824103000	-1.360790000
1	13.401595000	4.261851000	-0.816259000
1	11.693770000	4.377804000	-1.295202000
6	13.005646000	2.375272000	1.226031000
1	12.978750000	1.459375000	0.616478000
1	12.758523000	2.100260000	2.258611000
1	14.033314000	2.757776000	1.197166000
6	13.436624000	5.643867000	2.259864000
6	14.444220000	5.710868000	1.106785000
1	15.321560000	6.283494000	1.442584000
1	14.032238000	6.228652000	0.230530000
1	14.799015000	4.721125000	0.797847000
6	14.031389000	4.857724000	3.438560000
1	14.976174000	5.330038000	3.746148000
1	14.245280000	3.812650000	3.182297000
1	13.347142000	4.868423000	4.298911000
6	13.154139000	7.080384000	2.732731000
1	14.074360000	7.489381000	3.174019000
1	12.365446000	7.115574000	3.493452000
1	12.860547000	7.741292000	1.908316000
6	8.116724000	7.077658000	4.810453000
1	7.051730000	6.836685000	4.792835000
1	8.222394000	7.972429000	5.433339000
6	10.180431000	6.460955000	6.847666000
6	10.924067000	7.611866000	6.150019000
1	11.646821000	8.039206000	6.859820000
1	10.258311000	8.421364000	5.827712000
1	11.482543000	7.256325000	5.275778000
6	11.233275000	5.439979000	7.303805000
1	11.936070000	5.932457000	7.992313000
1	11.805684000	5.063152000	6.445789000
1	10.790301000	4.586494000	7.831470000
6	9.436012000	7.019490000	8.065833000
1	10.150694000	7.580558000	8.685854000
1	9.012836000	6.225216000	8.691890000
1	8.632761000	7.713444000	7.784740000
6	7.714949000	4.593582000	6.349777000
6	8.356834000	3.547216000	7.270289000
1	7.588922000	2.824231000	7.584932000
1	8.771449000	4.001622000	8.179202000
1	9.154553000	2.990987000	6.758114000
6	6.657234000	5.388294000	7.130555000
1	5.896700000	4.681029000	7.493499000
1	6.138808000	6.128063000	6.507579000
1	7.068705000	5.901825000	8.004302000
6	7.020896000	3.880602000	5.175853000
1	6.206592000	3.253365000	5.567061000
1	7.721838000	3.239366000	4.627026000
1	6.585885000	4.596213000	4.464942000
6	7.225055000	4.818071000	0.137968000
1	7.911500000	4.292371000	-0.507616000
6	6.810737000	4.404948000	1.446390000
1	7.141099000	3.518934000	1.969146000
6	5.861554000	5.365846000	1.927201000
1	5.334254000	5.326278000	2.867957000
6	5.693141000	6.368296000	0.919662000
1	5.026330000	7.214375000	0.972028000
6	6.535456000	6.029288000	-0.186825000
1	6.617226000	6.576904000	-1.112390000

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M06_Pd(^tBu^PC^Ru^P)(H) (3) toluene

E= -2000.62918148 Ha

46	-1.899286000	10.452938000	11.750863000
44	0.144950000	13.383354000	13.179920000
15	-3.722332000	11.860377000	12.215781000
15	0.176348000	9.766081000	10.900447000
6	-0.977958000	12.259491000	11.595791000
6	0.373686000	12.477976000	11.192953000
6	0.594467000	13.892952000	11.120278000
1	1.505258000	14.393363000	10.812496000
6	-0.621687000	14.546973000	11.516243000
1	-0.775043000	15.619270000	11.552961000
6	-1.583277000	13.529952000	11.828933000
6	0.218798000	12.358756000	15.125779000
1	-0.250047000	11.402813000	15.321388000
6	1.549672000	12.561997000	14.656304000
1	2.275839000	11.788088000	14.441545000
6	1.770064000	13.964682000	14.541552000
1	2.686560000	14.440271000	14.218628000
6	0.575331000	14.631619000	14.937835000
1	0.425267000	15.702514000	14.969722000
6	-0.382404000	13.640531000	15.298144000
1	-1.384884000	13.832896000	15.659110000
6	-3.013146000	13.604049000	12.275644000
1	-3.616816000	14.270461000	11.647507000
1	-3.096331000	13.989249000	13.295979000
6	1.259907000	11.303398000	10.899119000
1	2.035180000	11.187152000	11.661897000
1	1.784380000	11.392987000	9.940204000
6	-4.936788000	11.930644000	10.768425000
6	-4.128371000	12.423679000	9.554025000
1	-4.777586000	12.401805000	8.666291000
1	-3.266059000	11.771551000	9.360061000
1	-3.761348000	13.451140000	9.671179000
6	-6.129936000	12.866540000	10.994179000
1	-6.692334000	12.959147000	10.052599000
1	-5.824073000	13.877969000	11.294818000
1	-6.821619000	12.472433000	11.748798000
6	-5.447226000	10.518871000	10.440483000
1	-6.046977000	10.565013000	9.519103000
1	-6.083536000	10.106006000	11.230691000
1	-4.615195000	9.821628000	10.277493000
6	-4.593027000	11.649001000	13.876147000
6	-3.459783000	11.384750000	14.884483000
1	-3.892265000	11.269828000	15.889744000
1	-2.736040000	12.210926000	14.916748000
1	-2.911811000	10.465821000	14.632979000
6	-5.398660000	12.869660000	14.342608000
1	-5.836693000	12.645268000	15.327046000
1	-6.223186000	13.116325000	13.664834000
1	-4.773722000	13.763745000	14.463346000
6	-5.507514000	10.416811000	13.842985000
1	-5.813451000	10.175623000	14.871866000
1	-4.993230000	9.538617000	13.430064000
1	-6.420961000	10.598797000	13.263235000
6	0.075117000	9.290533000	9.073023000
6	-0.335411000	10.557438000	8.300017000
1	-0.528358000	10.281391000	7.252793000
1	0.445685000	11.327854000	8.299599000
1	-1.253544000	11.000932000	8.706980000
6	1.391482000	8.758626000	8.494332000
1	1.279114000	8.637951000	7.406118000
1	1.652316000	7.776271000	8.906795000
1	2.232558000	9.444669000	8.664312000
6	-1.035393000	8.246279000	8.877805000
1	-1.124165000	8.017818000	7.805082000
1	-2.002442000	8.625828000	9.233310000
6	-0.831748000	7.307767000	9.405358000
6	1.149763000	8.509937000	11.916525000
6	0.935734000	8.944098000	13.378788000
1	1.495746000	8.268185000	14.042188000
1	-0.127703000	8.900726000	13.652641000
1	1.287833000	9.969477000	13.560533000
6	2.656501000	8.468489000	11.624594000
1	3.127747000	7.756034000	12.318513000
1	3.143145000	9.440185000	11.778609000
1	2.879887000	8.131339000	10.606974000
6	0.555197000	7.107007000	11.735240000
1	1.002179000	6.432740000	12.481005000
1	0.774247000	6.692108000	10.743145000
1	-0.532287000	7.105581000	11.888301000
1	-2.643237000	8.965813000	11.890878000

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M06_*syn*-Pd(^tBu^PC^Ru^P)(η^{1,2}-BH_4) (*syn*-1) thf

E= -2027.28775011 Ha

46	0.113707000	-1.030582000	-0.138289000
44	-0.077027000	2.730870000	-0.675656000
15	-2.257910000	-0.933720000	-0.511795000
15	2.450124000	-0.706011000	-0.576195000
6	0.018901000	0.600295000	-1.287037000
6	1.137097000	1.312819000	-1.825748000
6	0.635596000	2.330838000	-2.696153000
1	1.229185000	3.023020000	-3.281605000
6	-0.795515000	2.259882000	-2.681002000
1	-1.466779000	2.889182000	-3.253409000
6	-1.175745000	1.198892000	-1.800074000
6	-0.062447000	3.015876000	1.506252000
1	-0.018780000	2.200179000	2.217871000
6	1.054563000	3.699647000	0.941394000
1	2.097946000	3.501331000	1.152660000
6	0.559078000	4.703488000	0.060015000
1	1.158293000	5.399837000	-0.511866000
6	-0.864803000	4.641897000	0.078442000
1	-1.536528000	5.283114000	-0.477079000
6	-1.248363000	3.600389000	0.971449000
1	-2.264871000	3.314629000	1.211148000
6	-2.522707000	0.662180000	-1.443406000
6	-3.148886000	0.479914000	-2.324846000
1	-3.076348000	1.357556000	-0.807302000
6	2.537463000	0.918864000	-1.488529000
1	3.016371000	1.661246000	-0.845156000
1	3.174375000	0.816340000	-2.374791000
6	-2.776735000	-2.278296000	-1.731008000
6	-2.015984000	-2.017681000	-3.043033000
1	-2.219233000	-2.849854000	-3.732837000
1	-0.930741000	-1.972018000	-2.880636000
1	-2.332417000	-1.091501000	-3.539156000
6	-4.281790000	-2.290706000	-2.024534000
1	-4.474858000	-3.006420000	-2.837799000
1	-4.651737000	-1.309882000	-2.352964000
1	-4.866694000	-2.614526000	-1.155688000
6	-2.341112000	-3.652691000	-1.198785000
1	-2.624020000	-4.419718000	-1.934946000
1	-2.817480000	-3.909539000	-0.246051000
1	-1.253329000	-3.701434000	-1.057954000
6	-3.437287000	-0.801571000	0.956511000
6	-2.740611000	0.145020000	1.950206000
1	-3.403321000	0.303764000	2.813708000
1	-2.526666000	1.125872000	1.502642000
1	-4.114300000	-1.252895000	-2.983338000
1	-4.982411000	-1.984566000	-1.615757000
6	-2.938692000	-3.716195000	-0.834312000
1	-2.038631000	-3.943886000	-0.250892000
1	-3.084963000	-4.531484000	-1.558472000
1	-3.806129000	-3.714324000	-0.162446000
6	-3.314954000	-0.798287000	1.047523000
1	-2.944363000	0.553395000	1.678192000
1	-3.468097000	0.645313000	2.641125000
1	-3.251224000	1.397765000	1.049481000
6	2.259735000	-1.755972000	-3.127818000
1	2.513281000	-2.560746000	-3.833173000
1	2.496756000	-0.801467000	-3.614576000
1	1.177050000	-1.793644000	-2.948940000
6	4.555157000	-1.857127000	-2.151506000
1	4.792294000	-2.547024000	-2.975369000
1	5.184136000	-2.136214000	-1.298206000
1	4.832843000	-0.845845000	-2.478417000
6	2.749776000	-3.392599000	-1.321414000
1	3.098673000	-4.119991000	-2.069335000
1	1.670453000	-3.539484000	-1.181813000
1	3.247598000	-3.620754000	-0.372263000
6	3.648392000	-0.484489000	0.865384000
6	2.886166000	0.362461000	1.899981000
1	3.549787000	0.562089000	2.754311000
1	1.995484000	-0.161921000	2.270533000
1	2.567640000	1.329870000	1.486400000
6	4.945842000	0.247296000	0.486853000
1	5.561134000	0.338669000	1.394580000
1	4.766188000	1.263507000	0.114980000
1	5.536131000	-0.295208000	-0.258801000
6	4.003599000	-1.835265000	1.499832000
1	4.561105000	-1.646624000	2.429401000
1	4.644492000	-2.442704000	0.849000000
1	3.108962000	-2.415196000	1.759145000
5	0.206377000	-2.752436000	1.809521000
1	0.220148000	-2.726427000	0.535164000
1	0.104955000	-1.653974000	2.330490000
1	1.253293000	-3.287061000	2.115078000
1	-0.749936000	-3.452280000	2.078990000

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M06_*anti*-Pd(^tBu^PC^Ru^P)(η^{1,2}-BH_4) (*syn*-1) thf

E= -2027.28381752 Ha

46	0.159115000	-1.010440000	-0.099681000
44	-0.195006000	2.766982000	-0.619653000
15	-2.221363000	-0.997542000	-0.474665000
15	2.489363000	-0.543946000	-0.444701000
6	0.013949000	0.622156000	-1.241157000
6	1.107714000	1.403611000	-1.730832000
6	0.580610000	2.399460000	-2.612460000
1	1.154256000	3.128361000	-3.172941000
6	-0.844771000	2.257985000	-2.634715000
1	-1.531047000	2.855004000	-3.223712000
6	-1.195231000	1.172197000	-1.770262000
6	-0.172748000	3.132783000	1.555222000
1	-0.087398000	2.352685000	2.301458000
6	0.911285000	3.832350000	0.948479000
1	1.964006000	3.679921000	1.153140000
6	0.367963000	4.783504000	0.037207000
1	0.934132000	5.475647000	-0.572387000
6	-1.052309000	4.672413000	0.079615000
1	-1.754015000	5.267095000	-0.490384000
6	-1.385600000	3.654446000	1.017165000
1	-2.386584000	3.350215000	1.290747000
6	-2.515843000	0.524744000	-1.519943000
1	-2.968218000	0.214419000	-2.466979000
1	-3.238949000	1.187965000	-1.035089000
6	2.512873000	1.098741000	-1.328347000
1	2.909394000	1.861435000	-0.653470000
1	3.197427000	1.055084000	-2.182474000
6	-2.814655000	-2.396733000	-1.608492000
6	-1.719438000	-2.545866000	-2.680886000
1	-2.033702000	-3.314322000	-3.402732000
1	-0.766512000	-2.862312000	-2.236924000
1	-1.550930000	-1.613024000	-3.238212000
6	-4.152137000	-2.121727000	-2.315393000
1	-4.388012000	-2.996393000	-2.939996000
1	-4.114300000	-1.252895000	-2.983338000
1	-4.982411000	-1.984566000	-1.615757000
6	-2.938692000	-3.716195000	-0.834312000
1	-2.038631000	-3.943886000	-0.250892000
1	-3.084963000	-4.531484000	-1.558472000
1	-3.806129000	-3.714324000	-0.162446000
6	-3.314954000	-0.798287000	1.047523000
6	-2.944363000	0.553395000	1.678192000
1	-3.468097000	0.645313000	2.641125000
1	-3.251224000	1.397765000	1.049481000

1	-1.864524000	0.631813000	1.868416000
6	-4.814922000	-0.809275000	0.731088000
1	-5.081297000	-0.097340000	-0.062187000
1	-5.367174000	-0.519217000	1.637626000
1	-5.162600000	-1.807481000	0.439836000
6	-2.991191000	-1.895293000	2.071879000
1	-3.601655000	-1.722416000	2.970597000
1	-1.934875000	-1.867897000	2.367137000
1	-3.215946000	-2.901726000	1.703187000
6	3.307594000	-1.698869000	-1.697891000
6	2.508521000	-1.555274000	-3.007165000
1	2.897322000	-2.285980000	-3.731258000
1	2.605695000	-0.559820000	-3.458497000
1	1.440770000	-1.765715000	-2.856669000
6	4.778835000	-1.351161000	-1.960025000
1	5.133585000	-1.955355000	-2.808551000
1	5.412119000	-1.592960000	-1.097965000
1	4.928791000	-0.295276000	-2.222268000
6	3.209352000	-3.162433000	-1.247045000
1	3.657521000	-3.795641000	-2.027312000
1	2.167028000	-3.474350000	-1.111702000
1	3.746268000	-3.354830000	-0.311771000
6	3.534990000	-0.268074000	1.100531000
6	2.620122000	0.498032000	2.072951000
1	3.184911000	0.723423000	2.989678000
1	1.737338000	-0.094882000	2.349303000
1	2.273180000	1.449599000	1.645916000
6	4.804272000	0.563017000	0.861365000
1	5.317802000	0.689419000	1.826302000
1	4.585392000	1.567071000	0.476648000
1	5.505520000	0.075059000	0.176575000
6	3.922129000	-1.608458000	1.737715000
1	4.345676000	-1.413197000	2.734037000
1	4.685963000	-2.134312000	1.151669000
1	3.056223000	-2.271758000	1.864309000
5	0.344661000	-3.382456000	1.015364000
1	0.304445000	-2.150522000	1.341032000
1	0.227472000	-3.585281000	-0.178564000
1	-0.581674000	-3.879132000	1.626429000
1	1.423457000	-3.777503000	1.413713000

80

M06_Pd(^{tBu}PC^{Ru}P)(H) (3) thf

E= -2000.63422752 Ha

46	-1.903372000	10.449912000	11.772492000
44	0.165427000	13.381402000	13.172824000
15	-3.730482000	11.869061000	12.230818000
15	0.174732000	9.756551000	10.905063000
6	-0.983740000	12.252123000	11.612924000
6	0.360374000	12.470129000	11.182647000
6	0.577226000	13.885118000	11.100579000
1	1.480543000	14.384323000	10.768823000
6	-0.632636000	14.539678000	11.516141000
1	-0.789045000	15.611979000	11.547489000
6	-1.586893000	13.523974000	11.852461000
6	0.289373000	12.346601000	15.111111000
1	-0.155968000	11.379635000	15.308879000
6	1.609053000	12.579554000	14.622392000
1	2.346541000	11.821262000	14.389756000
6	1.798455000	13.988058000	14.514149000
1	2.701493000	14.485227000	14.184691000
6	0.595783000	14.627610000	14.934330000
1	0.424899000	15.695328000	14.978695000
6	-0.336064000	13.614316000	15.302126000
1	-1.338150000	13.781959000	15.676698000
6	-3.007591000	13.601116000	12.325432000
1	-3.617314000	14.291627000	11.730509000
1	-3.067614000	13.951056000	13.360157000
6	1.246192000	11.299247000	10.877095000
1	2.037138000	11.189564000	11.624424000
1	1.749702000	11.387066000	9.907252000
6	-4.914105000	11.959164000	10.760511000
6	-4.109397000	12.527208000	9.577720000
1	-4.741345000	12.495538000	8.677935000
1	-3.209504000	11.929513000	9.379510000
1	-3.805813000	13.570190000	9.732702000
6	-6.138355000	12.848662000	11.004986000
1	-6.690107000	12.956836000	10.058782000
1	-5.862738000	13.856717000	11.343499000
1	-6.825317000	12.407471000	11.737282000
6	-5.373899000	10.545275000	10.373217000
1	-6.012883000	10.614723000	9.480236000
1	-5.954909000	10.057668000	11.163837000
1	-4.517892000	9.900426000	10.134114000
6	-4.631900000	11.644986000	13.871530000
6	-3.521415000	11.367089000	14.901145000
1	-3.978876000	11.233977000	15.892862000
1	-2.804936000	12.198154000	14.966718000
1	-2.962900000	10.454064000	14.650641000
6	-5.437674000	12.868313000	14.331740000
1	-5.875542000	12.645129000	15.316449000
1	-6.261568000	13.110040000	13.652065000
1	-4.812491000	13.762436000	14.449392000
6	-5.557198000	10.422476000	13.808102000
1	-5.909847000	10.194608000	14.824937000
1	-5.035802000	9.534406000	13.426094000
1	-6.440742000	10.609959000	13.185183000
6	0.054515000	9.261757000	9.084915000
6	-0.381064000	10.515222000	8.304262000
1	-0.567377000	10.227021000	7.259194000
1	0.385914000	11.299747000	8.298773000
1	-1.309993000	10.941038000	8.706915000
6	1.372999000	8.742052000	8.500086000
1	1.249100000	8.606298000	7.414950000
1	1.651358000	7.769347000	8.923567000
1	2.204406000	9.443474000	8.653339000
6	-1.041821000	8.199912000	8.908052000
1	-1.131346000	7.960274000	7.837933000
1	-2.013869000	8.570624000	9.259724000
1	-0.820434000	7.269713000	9.443021000
6	1.161392000	8.515517000	11.926405000
6	0.954729000	8.954882000	13.387774000
1	1.523643000	8.283690000	14.048329000
1	-0.106124000	8.906484000	13.671854000
1	1.306052000	9.981959000	13.561506000
6	2.666835000	8.488920000	11.625464000
1	3.145139000	7.775441000	12.313397000
1	3.145163000	9.463755000	11.784649000
1	2.886657000	8.160269000	10.604410000
6	0.583629000	7.104564000	11.754450000
1	1.046177000	6.441058000	12.500267000
1	0.800950000	6.690338000	10.761952000
1	-0.502667000	7.086445000	11.915895000
1	-2.653799000	8.952559000	11.922481000

13

M06_THF_thf

E= -232.355003306 Ha

8	-0.343137000	-0.807885000	5.418371000
6	-1.108755000	-1.890155000	4.920717000
1	-1.958539000	-1.484604000	4.365722000
1	-1.500361000	-2.485222000	5.763361000
6	-0.145771000	-2.721985000	4.075004000
1	-0.362302000	-3.790678000	4.154459000
1	-0.220465000	-2.448162000	3.018803000
6	1.237380000	-2.349503000	4.641498000
1	1.798135000	-3.215990000	5.001857000
1	1.847018000	-1.853342000	3.880636000
6	0.901582000	-1.381808000	5.771947000
1	0.803830000	-1.920679000	6.730201000
1	1.627647000	-0.575904000	5.905882000

17

M06_THF·BH_3_thf

E= -258.986305433 Ha

5	-0.328451000	0.518367000	4.540774000
1	0.323715000	1.302738000	5.184159000
1	0.193736000	0.205613000	3.493063000
1	-1.487797000	0.828498000	4.423149000
8	-0.362206000	-0.810693000	5.448778000
6	-1.129574000	-1.921809000	4.908758000
1	-1.976449000	-1.498807000	4.369238000
1	-1.492333000	-2.491646000	5.770290000
6	-0.145485000	-2.712464000	4.064469000
1	-0.362689000	-3.781225000	4.123510000
1	-0.211163000	-2.415405000	3.015202000
6	1.236127000	-2.355166000	4.645611000
1	1.769900000	-3.228758000	5.026163000
1	1.864229000	-1.884071000	3.885915000
6	0.934721000	-1.383008000	5.773099000
1	0.815406000	-1.887049000	6.737531000
1	1.635777000	-0.555816000	5.879895000

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M06_*syn*-Pd(^{tBu}PC^{Ru}P)(η^{1,2}-BH_4) (*syn*-1)+THF_thf

E= -2027.28775011 Ha

46	0.060909000	-1.136863000	-0.198629000
44	-0.140277000	2.666149000	-0.571185000
15	-2.305317000	-1.019006000	-0.570032000
15	2.401197000	-0.758387000	-0.548307000
6	-0.027923000	0.555398000	-1.256815000
6	1.093036000	1.292765000	-1.754382000
6	0.597126000	2.340615000	-2.592882000
1	1.194368000	3.056163000	-3.145667000
6	-0.833790000	2.262806000	-2.597842000
1	-1.501420000	2.908981000	-3.155522000
6	-1.218726000	1.168235000	-1.761175000
6	-0.144251000	2.879116000	1.620688000
1	-0.099606000	2.039402000	2.303970000
6	0.970693000	3.590216000	1.086648000
1	2.014557000	3.395284000	1.298967000
6	0.473847000	4.618370000	0.234774000
1	1.071554000	5.338152000	-0.309075000
6	-0.949389000	4.545061000	0.240507000
1	-1.622411000	5.199000000	-0.298444000
6	-1.330554000	3.471837000	1.095873000
1	-2.346526000	3.171579000	1.319579000
6	-2.567003000	0.612306000	-1.440143000
1	-3.182686000	0.464146000	-2.335048000
1	-3.129551000	1.280024000	-0.782714000
6	2.490903000	0.894257000	-1.411823000
1	2.959467000	1.619784000	-0.742210000
1	3.138079000	0.822386000	-2.293356000
6	-2.850782000	-2.316486000	-1.826607000
6	-2.096671000	-2.020155000	-3.135105000
1	-2.309968000	-2.828836000	-3.849417000
1	-1.009815000	-1.986721000	-2.978343000
1	-2.409970000	-1.076781000	-3.599685000
6	-4.359102000	-2.300692000	-2.102497000
1	-4.570622000	-2.983356000	-2.939286000
1	-4.722682000	-1.304220000	-2.388210000
1	-4.935810000	-2.651267000	-1.238306000
6	-2.428639000	-3.714232000	-1.346782000
1	-2.737915000	-4.451417000	-2.102678000
1	-2.892365000	-3.994731000	-0.394336000
1	-1.339548000	-3.785316000	-1.228124000
6	-3.452662000	-0.926838000	0.925720000
6	-2.719081000	-0.020484000	1.930023000
1	-3.332413000	0.078750000	2.838723000
1	-2.550739000	0.986614000	1.523551000
1	-1.744600000	-0.437989000	2.216984000
6	-4.831675000	-0.319672000	0.625405000
1	-5.395290000	-0.274308000	1.569576000
1	-5.415345000	-0.922967000	-0.077819000
1	-4.770837000	0.704553000	0.237389000
6	-3.647044000	-2.313712000	1.551935000
1	-4.149543000	-2.190999000	2.523484000
1	-2.692755000	-2.825208000	1.729327000
1	-4.282930000	-2.956242000	0.929570000
6	3.101280000	-1.977475000	-1.808474000
6	2.332154000	-1.753448000	-3.122887000
1	2.640034000	-2.527018000	-3.841412000
1	2.542050000	-0.777161000	-3.577631000
1	1.247004000	-1.841468000	-2.977131000
6	4.601166000	-1.793301000	-2.069123000
1	4.894192000	-2.445117000	-2.905881000
1	5.207027000	-2.079828000	-1.201148000
1	4.854238000	-0.761873000	-2.349388000
6	2.830689000	-3.417998000	-1.347184000
1	3.227071000	-4.108280000	-2.106723000
1	1.754620000	-3.609831000	-1.242213000
1	3.312154000	-3.656956000	-0.392431000
6	3.518884000	-0.547261000	0.959029000
6	2.684007000	0.254144000	1.974937000
1	3.298438000	0.433859000	2.870558000
1	1.779522000	-0.293276000	2.275447000
1	2.374127000	1.229784000	1.574501000
6	4.816461000	0.224005000	0.671047000
1	5.385768000	0.295346000	1.610088000
1	4.632364000	1.249253000	0.327089000
1	5.453429000	-0.278959000	-0.064116000
6	3.872690000	-1.907848000	1.572861000
1	4.363136000	-1.736221000	2.543254000
1	4.573694000	-2.471472000	0.944493000
1	2.981574000	-2.522842000	1.751175000
5	0.166664000	-3.009182000	1.603105000
1	0.151377000	-2.886044000	0.335550000
1	0.118398000	-1.952102000	2.207026000
1	1.205567000	-3.596456000	1.837081000
1	-0.803978000	-3.698681000	1.851879000
8	-0.507175000	-0.185667000	4.878384000
6	-1.035704000	-1.509334000	4.974791000
1	-1.401686000	-1.806058000	3.983555000
1	-1.886006000	-1.514550000	5.670105000
6	0.101874000	-2.412475000	5.445592000
1	0.035661000	-2.586580000	6.526148000
1	0.089144000	-3.383419000	4.942977000
6	1.342298000	-1.586449000	5.122815000
1	2.204904000	-1.836135000	5.746940000
1	1.620888000	-1.712965000	4.069583000
6	0.826838000	-0.183819000	5.362349000
1	0.841816000	0.057356000	6.439649000
1	1.381888000	0.598733000	4.833713000

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M06_*syn*-Pd(^{tBu}PC^{Ru}P)(η^{1,2}-BH_4)+THF_TS_{SN2}_thf

E= -2259.61563108 Ha

46	-0.173087000	-1.138961000	0.531469000
44	-0.062396000	2.560334000	-0.474694000
15	-2.449654000	-0.965549000	-0.038142000
15	2.179690000	-0.959826000	0.329740000
6	-0.071460000	0.351237000	-0.841089000
6	1.125544000	0.932421000	-1.356348000
6	0.761069000	1.881431000	-2.367316000
1	1.436757000	2.468566000	-2.978867000
6	-0.673164000	1.901900000	-2.453251000
1	-1.254115000	2.505988000	-3.140858000
6	-1.182921000	0.965709000	-1.494416000
6	-0.162435000	3.095478000	1.655702000
1	-0.210926000	2.369575000	2.457919000
6	1.026214000	3.649321000	1.092427000
1	2.042408000	3.424085000	1.392629000
6	0.645756000	4.572157000	0.075412000
1	1.319066000	5.165218000	-0.529740000
6	-0.777692000	4.589526000	0.006945000
1	-1.375020000	5.198402000	-0.659208000
6	-1.276316000	3.678637000	0.982342000
1	-2.320967000	3.478635000	1.185681000
6	-2.578897000	0.540731000	-1.152270000
1	-3.178421000	0.299056000	-2.038045000
1	-3.120624000	1.327320000	-0.619140000
6	2.460229000	0.485677000	-0.843178000
1	2.974001000	1.289068000	-0.308868000
1	3.135279000	0.175516000	-1.649690000
6	-2.990138000	-2.397305000	-1.145235000
6	-2.168288000	-2.300977000	-2.443488000
1	-2.373059000	-3.194622000	-3.051388000
1	-1.089548000	-2.270905000	-2.240114000
1	-2.430210000	-1.422856000	-3.047153000
6	-4.481953000	-2.374293000	-1.497692000
1	-4.680904000	-3.156205000	-2.246356000
1	-4.793969000	-1.414390000	-1.931608000
1	-5.111769000	-2.586435000	-0.625317000
6	-2.637347000	-3.731400000	-0.467779000
1	-2.931580000	-4.555253000	-1.135424000
1	-3.154271000	-3.871914000	0.488539000
1	-1.557551000	-3.807865000	-0.281480000
6	-3.675084000	-0.621149000	1.353084000
6	-2.966073000	0.405802000	2.255575000
1	-3.632440000	0.668311000	3.090811000
1	-2.719823000	1.330126000	1.713847000
1	-2.034404000	-0.004228000	2.670571000
6	-5.017513000	-0.033888000	0.893550000
1	-5.620081000	0.192577000	1.786307000
1	-5.592995000	-0.732649000	0.277411000
1	-4.898821000	0.903464000	0.335410000
6	-3.930465000	-1.894371000	2.170006000
1	-4.485456000	-1.623251000	3.080762000
1	-2.993001000	-2.376379000	2.479112000
1	-4.537656000	-2.622664000	1.617578000
6	2.910474000	-2.433186000	-0.602433000
6	2.191200000	-2.486380000	-1.962845000
1	2.549027000	-3.369067000	-2.513132000
1	2.386901000	-1.604847000	-2.586321000
1	1.104576000	-2.585854000	-1.833042000
6	4.423004000	-2.330933000	-0.832323000
1	4.741369000	-3.168722000	-1.471288000
1	4.985709000	-2.402125000	0.106525000
1	4.709076000	-1.401008000	-1.342506000
6	2.587733000	-3.742192000	0.136893000
1	2.905825000	-4.587356000	-0.492187000
1	1.510016000	-3.840562000	0.323896000
1	3.108634000	-3.827089000	1.096304000
6	3.189961000	-0.520660000	1.866561000
6	2.290230000	0.426154000	2.680517000
1	2.833086000	0.753337000	3.580800000
1	1.362326000	-0.073600000	2.994513000
1	2.014452000	1.319538000	2.103478000
6	4.519092000	0.189533000	1.571030000
1	5.051696000	0.340026000	2.522383000
1	4.372489000	1.180814000	1.124372000
1	5.174364000	-0.392865000	0.913140000
6	3.467472000	-1.772016000	2.710090000
1	3.862830000	-1.453153000	3.687164000
1	4.220626000	-2.422155000	2.247702000
1	2.552892000	-2.353333000	2.887375000
5	-0.276771000	-3.016749000	3.685142000
1	-0.288930000	-2.384992000	1.658222000
1	-0.450312000	-1.872367000	3.977339000
1	0.820216000	-3.409709000	3.433780000
1	-1.212216000	-3.715997000	3.436066000
8	-0.144242000	-3.609722000	5.687776000
6	0.820990000	-4.653322000	5.841269000
1	0.732501000	-5.318949000	4.979786000
1	0.575172000	-5.221211000	6.749590000
6	2.177274000	-3.956472000	5.969154000
1	2.780668000	-4.423626000	6.752124000
1	2.742420000	-4.015614000	5.034460000
6	1.813567000	-2.498963000	6.304178000
1	2.349276000	-2.112606000	7.174837000
1	2.028776000	-1.841629000	5.454554000
6	0.314801000	-2.560258000	6.540856000
1	0.081188000	-2.828114000	7.582290000
1	-0.228187000	-1.649594000	6.280764000

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M06_Pd(^{tBu}PC^{Ru}P)(H) (3)+THF·BH_3_thf

E= -2259.63061459 Ha

46	0.138480000	-1.212205000	-0.237577000
44	-0.194234000	2.592508000	-0.694669000
15	-2.186681000	-1.178608000	-0.664710000
15	2.433622000	-0.796040000	-0.571486000
6	0.026415000	0.467736000	-1.373731000
6	1.133669000	1.251248000	-1.820357000
6	0.632083000	2.282707000	-2.680238000
1	1.217116000	3.023199000	-3.213847000
6	-0.797623000	2.150388000	-2.736135000
1	-1.465049000	2.774430000	-3.319613000
6	-1.167418000	1.038554000	-1.909551000
6	-0.323984000	2.806505000	1.493714000
1	-0.304084000	1.970574000	2.183434000
6	0.809681000	3.530822000	1.021520000
1	1.841610000	3.346348000	1.293853000
6	0.349235000	4.553201000	0.142156000
1	0.967633000	5.280361000	-0.368030000
6	-1.071222000	4.462225000	0.067831000
1	-1.720972000	5.108641000	-0.507743000
6	-1.485979000	3.383870000	0.901656000
1	-2.509677000	3.073174000	1.069907000
6	-2.498813000	0.422174000	-1.600413000

1	-3.085239000	0.213676000	-2.503286000
1	-3.113881000	1.081425000	-0.981125000
6	2.524601000	0.887492000	-1.395429000
1	2.922413000	1.605746000	-0.672737000
1	3.236461000	0.861872000	-2.229150000
6	-2.678906000	-2.520390000	-1.901697000
6	-1.880441000	-2.246743000	-3.189105000
1	-2.067614000	-3.067873000	-3.896721000
1	-0.800443000	-2.210064000	-2.991158000
1	-2.174664000	-1.311226000	-3.681340000
6	-4.175761000	-2.539329000	-2.232773000
1	-4.344229000	-3.230307000	-3.072813000
1	-4.553824000	-1.553175000	-2.534875000
1	-4.774365000	-2.899534000	-1.387483000
6	-2.253975000	-3.900331000	-1.375721000
1	-2.480914000	-4.654814000	-2.143917000
1	-2.785352000	-4.184752000	-0.460624000
1	-1.176430000	-3.933717000	-1.168168000
6	-3.364620000	-1.096856000	0.807766000
6	-2.706914000	-0.104181000	1.782711000
1	-3.345125000	0.000283000	2.673529000
1	-2.585395000	0.892967000	1.337665000
1	-1.713460000	-0.450336000	2.101796000
6	-4.778989000	-0.599673000	0.476786000
1	-5.348889000	-0.525568000	1.415624000
1	-5.322347000	-1.281738000	-0.185384000
1	-4.777120000	0.398185000	0.020035000
6	-3.455038000	-2.466910000	1.494004000
1	-3.936675000	-2.340068000	2.475932000
1	-2.462641000	-2.908937000	1.658327000
1	-4.064262000	-3.174646000	0.917611000
6	3.178740000	-1.965326000	-1.856512000
6	2.463039000	-1.689383000	-3.191115000
1	2.793462000	-2.439629000	-3.924593000
1	2.699121000	-0.699526000	-3.601169000
1	1.372771000	-1.770834000	-3.092147000
6	4.687742000	-1.781067000	-2.056634000
1	5.009366000	-2.403177000	-2.905643000
1	5.260991000	-2.101152000	-1.178114000
1	4.954397000	-0.741150000	-2.289034000
6	2.884035000	-3.420837000	-1.460791000
1	3.294689000	-4.086918000	-2.234561000
1	1.802890000	-3.601145000	-1.390111000
1	3.337020000	-3.699777000	-0.502688000
6	3.522375000	-0.628406000	0.959516000
6	2.654622000	0.137462000	1.974567000
1	3.219537000	0.267866000	2.911091000
1	1.729837000	-0.411721000	2.199894000
1	2.367573000	1.134981000	1.610636000
6	4.829638000	0.143896000	0.733587000
1	5.356258000	0.225985000	1.696584000
1	4.655350000	1.165106000	0.371646000
1	5.501072000	-0.361172000	0.031032000
6	3.841285000	-2.013405000	1.538148000
1	4.298080000	-1.884879000	2.531436000
1	4.556768000	-2.564714000	0.915162000
1	2.935327000	-2.623348000	1.657472000
5	-0.264453000	0.645089000	4.706520000
1	0.246701000	-2.599410000	0.708977000
1	0.569701000	1.349158000	5.222376000
1	0.023434000	0.303157000	3.584043000
1	-1.390368000	1.072398000	4.800016000
8	-0.264720000	-0.697617000	5.597598000
6	-1.209052000	-1.721867000	5.176510000
1	-2.103283000	-1.212002000	4.817205000
1	-1.452904000	-2.303169000	6.072655000
6	-0.458798000	-2.535495000	4.145030000
1	-0.822865000	-3.565180000	4.115477000
6	-0.586200000	-2.106612000	3.146285000
6	1.011868000	-2.433993000	4.586103000
1	1.394077000	-3.383662000	4.968193000
1	1.645231000	-2.131680000	3.748038000
6	1.015918000	-1.384538000	5.691397000
1	1.050516000	-1.831277000	6.689765000
1	1.792478000	-0.623882000	5.609041000

11

M06_Py_toluene

E= -248.161169630 Ha

6	-20.203453000	3.780293000	-3.165888000
6	-20.203453000	4.972910000	-2.458776000
6	-20.203453000	4.917921000	-1.071803000
7	-20.203453000	3.780293000	-0.381147000
6	-20.203453000	2.642665000	-1.071803000
6	-20.203453000	2.587676000	-2.458776000
1	-20.203453000	3.780293000	-4.251909000
1	-20.203453000	5.931099000	-2.967915000
1	-20.203453000	5.837644000	-0.488848000
1	-20.203453000	1.722942000	-0.488848000
1	-20.203453000	1.629487000	-2.967915000

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M06_ Py·BH_3_toluene

E= -274.810099136 Ha

6	-20.208231000	3.776869000	-3.164602000
6	-20.328231000	4.968778000	-2.470228000
6	-20.318448000	4.942154000	-1.088099000
7	-20.197193000	3.800068000	-0.402971000
6	-20.080113000	2.644343000	-1.072508000
6	-20.081852000	2.593585000	-2.449900000
1	-20.212098000	3.767433000	-4.249712000
1	-20.428956000	5.916996000	-2.985033000
1	-20.408315000	5.841067000	-0.488588000
1	-19.983727000	1.755688000	-0.457228000
1	-19.984097000	1.637572000	-2.950637000
5	-20.202478000	3.777636000	1.213189000
1	-21.192203000	3.157832000	1.535739000
1	-19.188705000	3.204112000	1.543838000
1	-20.232755000	4.930420000	1.572157000

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M06_*syn*-Pd(^{tBu}PC^{Ru}P)($\eta^{1,2}$-BH_4) (*syn*-1)+Py_toluene

E= -2275.44955500 Ha

46	-1.965728000	10.109973000	11.042867000
44	-0.692742000	12.007607000	14.071312000
15	-4.031359000	11.205030000	11.573002000
15	0.356602000	9.869952000	10.535233000
6	-1.249927000	11.747692000	11.937570000
6	0.129755000	12.111997000	12.045096000
6	0.201536000	13.402145000	12.659012000
1	1.102790000	13.970027000	12.856164000
6	-1.135115000	13.825665000	12.951763000
1	-1.414387000	14.768689000	13.405975000
6	-2.029776000	12.797620000	12.515422000
6	-1.028219000	10.202711000	15.277785000
1	-1.454367000	9.291206000	14.875747000
6	0.357159000	10.537682000	15.318973000
1	1.174795000	9.920359000	14.968919000
6	0.486130000	11.822098000	15.920325000
1	1.413002000	12.349855000	16.101143000
6	-0.819175000	12.284754000	16.252045000
1	-1.057779000	13.224519000	16.731697000
6	-1.753521000	11.285526000	15.856453000
1	-2.825905000	11.335182000	15.994475000
6	-3.521621000	12.726846000	12.535240000
1	-3.986980000	13.616836000	12.094249000
1	-3.905914000	12.653455000	13.555849000
6	1.201864000	11.215059000	11.516782000
1	1.772720000	10.755853000	12.327762000
1	1.927875000	11.743853000	10.887439000
6	-4.833938000	11.893113000	10.007950000
6	-3.805993000	12.838494000	9.361621000
1	-4.216417000	13.204567000	8.409147000
1	-2.866103000	12.314200000	9.143284000
1	-3.576071000	13.714022000	9.982302000
6	-6.132552000	12.664458000	10.273595000
1	-6.451811000	13.153211000	9.340813000
1	-6.009879000	13.450823000	11.030986000
1	-6.945646000	11.999527000	10.588297000
6	-5.106604000	10.752548000	9.014484000
1	-5.507794000	11.184735000	8.085484000
1	-5.836829000	10.027135000	9.388452000
1	-4.188603000	10.204713000	8.766737000
6	-5.280318000	10.353315000	12.706798000
6	-4.426240000	9.657903000	13.781593000
1	-5.092516000	9.167618000	14.507398000
1	-3.792504000	10.370591000	14.326586000
1	-3.777421000	8.892067000	13.337422000
6	-6.258375000	11.315588000	13.398831000
1	-6.923606000	10.719293000	14.041239000
1	-6.889938000	11.862372000	12.690693000
1	-5.753632000	12.043837000	14.045733000
6	-6.082099000	9.287543000	11.947638000
1	-6.626698000	8.671599000	12.678830000
1	-5.434241000	8.616724000	11.369477000
1	-6.824476000	9.735428000	11.274639000
6	0.694719000	10.330866000	8.735422000
6	0.308082000	11.811213000	8.564727000
1	0.345920000	12.060195000	7.494100000
1	0.993400000	12.490779000	9.086496000
1	-0.710182000	12.011481000	8.921838000
6	2.159553000	10.155473000	8.315810000
1	2.286740000	10.566507000	7.303048000
1	2.457989000	9.101260000	8.279493000
1	2.852252000	10.694012000	8.976807000
6	-0.213434000	9.496374000	7.818089000
1	-0.010730000	9.773585000	6.772913000
1	-1.274366000	9.691297000	8.022618000
1	-0.048250000	8.417783000	7.918399000
6	1.254406000	8.292258000	11.054646000
6	0.653678000	7.921153000	12.423083000
1	1.177916000	7.037000000	12.815535000
1	-0.414540000	7.682378000	12.336099000
1	0.762227000	8.733514000	13.156009000
6	2.773724000	8.463091000	11.210100000
1	3.197280000	7.496537000	11.521837000
1	3.040854000	9.194877000	11.982645000
1	3.267123000	8.751510000	10.275985000
6	0.972757000	7.149662000	10.069930000
1	1.358405000	6.213665000	10.500828000
1	1.476772000	7.298025000	9.106779000
1	-0.102183000	7.015220000	9.895171000
1	-2.590873000	8.866750000	9.868702000
5	-2.847981000	7.769723000	10.481558000
1	-4.025351000	7.581931000	10.257458000
1	-2.628426000	7.810201000	11.681774000
1	-2.140861000	6.951368000	9.931849000
7	-5.523618000	6.146124000	14.322881000
6	-4.413884000	6.114170000	13.587289000
1	-4.539929000	6.095210000	12.505611000
6	-3.134646000	6.125623000	14.130282000
1	-2.272231000	6.104795000	13.471547000
6	-4.150485000	6.218885000	16.286623000
1	-4.097514000	6.263556000	17.369728000
6	-5.381094000	6.193202000	15.647043000
1	-6.300064000	6.215686000	16.231535000
6	-3.001896000	6.182662000	15.507961000
1	-2.019199000	6.200135000	15.970808000

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M06_*syn*-Pd(^{tBu}PC^{Ru}P)($\eta^{1,2}$-BH_4)+Py_TS_{SN2}_toluene

E= -2275.41761969 Ha

46	-2.125886000	10.136929000	11.520922000
44	0.019080000	12.824762000	13.273714000
15	-3.896586000	11.558268000	12.122265000
15	-0.050238000	9.435764000	10.660791000
6	-1.125584000	11.899305000	11.584654000
6	0.235271000	12.103260000	11.207554000
6	0.509300000	13.508999000	11.272358000
1	1.440468000	14.000978000	11.016504000
6	-0.684497000	14.168624000	11.722126000
1	-0.798603000	15.237602000	11.859389000
6	-1.686589000	13.164764000	11.931158000
6	0.044917000	11.605647000	15.103466000
1	-0.439458000	10.641134000	15.189320000
6	1.387337000	11.837991000	14.682054000
1	2.109301000	11.080904000	14.402664000
6	1.626085000	13.242017000	14.715155000
1	2.554266000	13.736077000	14.460518000
6	0.432194000	13.880628000	15.157637000
1	0.294439000	14.944638000	15.296757000
6	-0.544210000	12.871152000	15.396034000
1	-1.551523000	13.039169000	15.756337000
6	-3.115624000	13.252027000	12.377043000
1	-3.684025000	14.010855000	11.825781000
1	-3.188690000	13.524628000	13.433644000
6	1.078949000	10.934950000	10.793675000
1	1.862512000	10.726854000	11.527617000
1	1.590603000	11.101388000	9.838009000
6	-5.098573000	11.833345000	10.691072000
6	-4.274585000	12.447414000	9.544218000
1	-4.917090000	12.530459000	8.655299000
1	-3.416427000	11.813428000	9.283360000
1	-3.900546000	13.452080000	9.777767000
6	-6.264442000	12.769574000	11.029489000
1	-6.828136000	12.984026000	10.108711000
1	-5.926067000	13.731331000	11.439184000
1	-6.963693000	12.313510000	11.741173000
6	-5.643736000	10.482423000	10.199919000
1	-6.248312000	10.654060000	9.296421000
1	-6.282887000	9.989458000	10.940380000
1	-4.829962000	9.789590000	9.947135000
6	-4.778236000	11.194506000	13.749527000
6	-3.659479000	10.752569000	14.711024000
1	-4.094442000	10.553684000	15.702018000
1	-2.886027000	11.524366000	14.826194000
1	-3.171454000	9.834056000	14.355122000
6	-5.518867000	12.391970000	14.361373000
1	-5.968159000	12.074086000	15.314483000
1	-6.329486000	12.759379000	13.722507000
1	-4.848872000	13.232240000	14.584099000
6	-5.753816000	10.022996000	13.577394000
1	-6.085026000	9.691456000	14.573075000
1	-5.278500000	9.166321000	13.080555000
1	-6.649307000	10.311030000	13.012378000
6	-0.140338000	9.103626000	8.803779000
6	-0.568541000	10.426490000	8.142185000
1	-0.737942000	10.242972000	7.070895000
1	0.191958000	11.213078000	8.227523000
1	-1.505127000	10.806019000	8.572386000
6	1.184113000	8.640053000	8.186767000
1	1.077488000	8.615905000	7.091489000
1	1.454629000	7.627508000	8.510402000
1	2.017942000	9.316296000	8.420950000
6	-1.237534000	8.064748000	8.520814000
1	-1.345602000	7.951552000	7.431465000
1	-2.204040000	8.382099000	8.934690000
1	-1.004794000	7.079038000	8.938599000
6	0.869941000	8.079234000	11.595315000
6	0.630526000	8.401550000	13.082015000
1	1.165360000	7.665906000	13.701527000
1	-0.439130000	8.353640000	13.330845000
1	0.994680000	9.403287000	13.349842000
6	2.381367000	8.027189000	11.332317000
1	2.816334000	7.228245000	11.951975000
1	2.890320000	8.960299000	11.605614000
1	2.619998000	7.799085000	10.287816000
6	0.252292000	6.707719000	11.291146000
1	0.651026000	5.974380000	12.008936000
1	0.509220000	6.354573000	10.284346000
1	-0.841082000	6.719893000	11.394970000
1	-2.976146000	8.688228000	11.429001000
5	-3.624345000	7.009541000	11.908291000
1	-4.744573000	7.403331000	11.761244000
1	-3.090958000	7.086815000	12.977311000
1	-3.033324000	6.541444000	10.980825000
7	-4.373588000	4.959739000	12.446012000
6	-5.640807000	4.580985000	12.323548000
1	-6.335597000	5.342628000	11.972975000
6	-6.072331000	3.295643000	12.618599000
1	-7.117888000	3.029907000	12.503738000
6	-3.813259000	2.764244000	13.188566000
1	-3.050407000	2.072878000	13.530660000
6	-3.479937000	4.071302000	12.868611000
1	-2.453865000	4.429620000	12.950751000
6	-5.137690000	2.371337000	13.060056000
1	-5.437277000	1.355845000	13.301303000

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M06_Pd(^{tBu}PC^{Ru}P)(H) (3)+Py·BH_3_toluene

E= -2275.45035050 Ha

46	-2.286250000	10.382684000	11.703882000
44	-0.035972000	12.909332000	13.520878000
15	-3.977970000	11.940463000	12.160041000
15	-0.225558000	9.536539000	10.933294000
6	-1.178355000	12.084640000	11.778288000
6	0.205903000	12.196362000	11.454382000
6	0.575528000	13.578701000	11.548224000
1	1.547590000	14.006486000	11.332132000
6	-0.585219000	14.316726000	11.961459000
1	-0.628365000	15.389503000	12.109106000
6	-1.660801000	13.383088000	12.123435000
1	-0.164911000	11.667363000	15.331506000
1	-0.717558000	10.737909000	15.385766000
6	1.206019000	11.811432000	14.963854000
1	1.885208000	11.010499000	14.699315000
6	1.539503000	13.194730000	15.030662000
1	2.508669000	13.626151000	14.818672000
6	0.375936000	13.908994000	15.436623000
1	0.306734000	14.977914000	15.588215000
6	-0.675855000	12.966443000	15.621980000
1	-1.682617000	13.198931000	15.945814000
6	-3.095732000	13.559690000	12.523971000
1	-3.589831000	14.385182000	11.997471000
1	-3.188334000	13.777660000	13.592028000
6	0.982976000	10.976652000	11.059804000
1	1.755911000	10.737673000	11.795242000
1	1.502557000	11.104128000	10.102453000
6	-5.009030000	12.327356000	10.623857000
6	-4.065217000	12.984937000	9.600201000
1	-4.602926000	13.088401000	8.646257000
1	-3.170367000	12.375524000	9.419673000
1	-3.740219000	13.987162000	9.906213000
6	-6.188447000	13.271179000	10.885643000
1	-6.643233000	13.545990000	9.921845000
1	-5.878858000	14.202114000	11.380175000
1	-6.969200000	12.795674000	11.491614000
6	-5.521894000	11.013957000	10.011596000
1	-6.087517000	11.244610000	9.096389000
1	-6.186546000	10.463285000	10.686911000
1	-4.689531000	10.348929000	9.746088000
6	-5.050764000	11.640253000	13.682549000
6	-4.073106000	11.121812000	14.753695000
1	-4.622637000	10.943134000	15.690134000
1	-3.270673000	11.843620000	14.962542000
1	-3.600699000	10.180477000	14.438428000
6	-5.763948000	12.887684000	14.223688000
1	-6.312827000	12.611235000	15.136665000
1	-6.491241000	13.297851000	13.515265000
1	-5.063091000	13.686747000	14.496455000
6	-6.085226000	10.543931000	13.395058000
1	-6.559008000	10.243837000	14.341840000
1	-5.618411000	9.653687000	12.951977000
1	-6.881634000	10.892536000	12.725255000
6	-0.278849000	9.160652000	9.082194000
6	-0.661949000	10.478987000	8.384447000
1	-0.773975000	10.284454000	7.307695000
1	0.094042000	11.265757000	8.503081000
1	-1.620390000	10.862771000	8.759951000
6	1.051197000	8.654005000	8.512061000
1	0.968362000	8.594757000	7.416306000
1	1.294114000	7.647299000	8.873139000
1	1.892418000	9.322524000	8.742420000
6	-1.389992000	8.140417000	8.785027000
1	-1.486889000	8.027451000	7.694766000
1	-2.357249000	8.477802000	9.181304000
1	-1.184543000	7.146054000	9.196920000
6	0.594511000	8.147700000	11.917581000
6	0.291244000	8.471273000	13.391447000
1	0.774322000	7.719203000	14.033783000
1	-0.790849000	8.456713000	13.586865000
1	0.670038000	9.461528000	13.678980000
6	2.115612000	8.043021000	11.736413000
1	2.479738000	7.186142000	12.323458000
1	2.642738000	8.932253000	12.104751000

1	2.408349000	7.875769000	10.694085000
6	-0.050655000	6.797716000	11.576174000
1	0.268591000	6.054846000	12.323511000
1	0.254079000	6.425088000	10.590458000
1	-1.146687000	6.859467000	11.604293000
1	-3.210303000	8.994926000	11.648675000
5	-2.902663000	4.663904000	9.572855000
1	-3.494166000	5.556182000	9.013692000
1	-1.707043000	4.693060000	9.358748000
1	-3.366826000	3.568052000	9.347223000
7	-3.069305000	4.909577000	11.158927000
6	-3.594597000	6.039214000	11.644771000
1	-3.917188000	6.773502000	10.913727000
6	-3.689358000	6.275528000	13.005445000
1	-4.097616000	7.220707000	13.345437000
6	-2.684435000	4.141267000	13.377576000
1	-2.308941000	3.361557000	14.030044000
6	-2.619932000	3.975062000	12.012094000
1	-2.201389000	3.085524000	11.552539000
6	-3.230333000	5.313891000	13.886850000
1	-3.289996000	5.473407000	14.958663000

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M06_*syn*-Pd(^{tBu}PC^{Ru}P)(η^1-OC(O)H) (4) toluene

E= -2189.21569342 Ha

44	3.776708000	0.822137000	10.106307000
46	0.472661000	-0.976490000	9.720315000
15	1.552949000	-2.689043000	10.963920000
15	0.082153000	0.605216000	7.996047000
6	2.343507000	-0.612178000	9.188023000
6	3.499898000	-1.308083000	9.663145000
6	4.636973000	-0.808279000	8.951437000
1	5.660177000	-1.149153000	9.054440000
6	4.185028000	0.217217000	8.057779000
1	4.810377000	0.778913000	7.374269000
6	2.769271000	0.351554000	8.218813000
6	2.953781000	1.930181000	11.820539000
1	1.948861000	1.786903000	12.197695000
6	4.118280000	1.223114000	12.240338000
1	4.159518000	0.459091000	13.006070000
6	5.228676000	1.713839000	11.495255000
1	6.254674000	1.384318000	11.590236000
6	4.752743000	2.726050000	10.613313000
1	5.353527000	3.298984000	9.919682000
6	3.349068000	2.858366000	10.813908000
1	2.699573000	3.556147000	10.300910000
6	3.378044000	-2.384851000	10.696339000
1	3.832989000	-2.085068000	11.644577000
1	3.874412000	-3.315306000	10.395421000
6	1.776681000	1.242804000	7.538074000
1	1.896869000	1.258601000	6.448337000
1	1.869713000	2.278896000	7.875882000
6	1.238092000	-4.375078000	10.175426000
6	1.921684000	-5.539382000	10.901318000
1	3.000041000	-5.377415000	11.036344000
1	1.798079000	-6.453568000	10.301274000
1	1.471885000	-5.729916000	11.883062000
6	1.774440000	-4.294131000	8.734734000
1	1.296783000	-3.478222000	8.176356000
1	1.540241000	-5.237741000	8.220743000
1	2.861562000	-4.152697000	8.688586000
6	-0.276050000	-4.628484000	10.093742000
1	-0.733555000	-4.769594000	11.078990000
1	-0.449015000	-5.546029000	9.511511000
1	-0.800031000	-3.799807000	9.599913000
6	1.330468000	-2.706494000	12.834168000
6	2.414677000	-3.486981000	13.590772000
1	2.427181000	-4.552396000	13.336896000
1	2.210377000	-3.407118000	14.669162000
1	3.419976000	-3.079793000	13.422376000
6	1.388332000	-1.226044000	13.254494000
1	2.329782000	-0.748938000	12.948027000
1	1.318133000	-1.165111000	14.350827000
1	0.554369000	-0.655311000	12.822237000
6	-0.052034000	-3.263629000	13.202887000
1	-0.855309000	-2.791618000	12.621943000
1	-0.244579000	-3.051748000	14.264859000
1	-0.107377000	-4.351001000	13.067616000
6	-0.536305000	-0.255825000	6.434091000
6	0.592414000	-1.182212000	5.947164000
1	1.462717000	-0.628959000	5.572789000
1	0.208229000	-1.794971000	5.118708000
1	0.933313000	-1.861709000	6.738733000
6	-0.910081000	0.705006000	5.299821000
1	-1.803550000	1.294441000	5.537666000
1	-1.135547000	0.117340000	4.397115000
1	-0.092036000	1.394066000	5.048565000
6	-1.743973000	-1.134733000	6.797435000
1	-1.491435000	-1.856656000	7.585171000
1	-2.060465000	-1.691967000	5.902960000
1	-2.601788000	-0.550687000	7.149321000
6	-0.917128000	2.139146000	8.428879000
6	-0.408095000	2.562332000	9.819806000
1	-0.613717000	1.790262000	10.574495000
1	-0.925517000	3.485117000	10.121608000
1	0.672447000	2.765174000	9.819639000
6	-0.737646000	3.307783000	7.449618000
1	0.310689000	3.618838000	7.353705000
1	-1.298101000	4.172709000	7.835161000
1	-1.123763000	3.085686000	6.449322000
6	-2.406944000	1.786260000	8.543057000
1	-2.860901000	1.582796000	7.564802000
1	-2.938951000	2.642115000	8.983793000
1	-2.572549000	0.920535000	9.197612000
6	-2.097353000	-0.842058000	11.219527000
1	-3.152592000	-1.154779000	11.415261000
8	-1.580063000	-1.444716000	10.228406000
8	-1.590306000	0.005145000	11.949060000

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M06_*syn*-Pd(^{tBu}PC^{Ru}P)(η^1-OC(O)OH) (5) toluene

E= -2264.46234160 Ha

46	2.040527000	17.033219000	3.029469000
44	4.162146000	14.115643000	1.933595000
15	4.123767000	18.139651000	3.299082000
15	0.344678000	15.395604000	3.295518000
8	0.785573000	18.763601000	2.679727000
8	0.925817000	18.558737000	0.441561000
8	-0.267063000	20.190333000	1.397314000
1	-0.385259000	20.344888000	0.453150000
6	3.177814000	15.463500000	3.407579000
6	4.596699000	15.483469000	3.593131000
6	5.011774000	14.157472000	3.937754000
1	6.020563000	13.841936000	4.175308000
6	3.852632000	13.314422000	3.933344000
1	3.841433000	12.256682000	4.167136000
6	2.720544000	14.119063000	3.587038000
6	3.773337000	14.657025000	-0.162285000
1	3.161304000	15.500521000	-0.456099000
6	5.179762000	14.679176000	0.069769000
1	5.829994000	15.538151000	-0.035009000
6	5.590696000	13.366815000	0.439751000
1	6.601203000	13.058359000	0.672114000
6	4.438825000	12.529042000	0.436823000
1	4.420194000	11.472237000	0.667286000
6	3.317962000	13.325466000	0.065341000
1	2.300673000	12.971609000	-0.041550000
6	5.371459000	16.759047000	3.466749000
1	6.018798000	16.751231000	2.584896000
1	6.022455000	16.944554000	4.329530000
6	1.268027000	13.778654000	3.451277000
1	0.885266000	13.203200000	4.302895000
1	1.079007000	13.175257000	2.558688000
6	4.189819000	19.036555000	4.957283000
6	5.494437000	19.804628000	5.197671000
1	5.502264000	20.173750000	6.234385000
1	5.583987000	20.677270000	4.539739000
1	6.384577000	19.173864000	5.065421000
6	4.029999000	17.966770000	6.052816000
1	3.954175000	18.473865000	7.025749000
1	4.881619000	17.276731000	6.104179000
1	3.116283000	17.375518000	5.908849000
6	2.991345000	19.993597000	5.059103000
1	2.979584000	20.441111000	6.064001000
1	2.040733000	19.467869000	4.902619000
1	3.039220000	20.809444000	4.330254000
6	4.742729000	19.197541000	1.870676000
6	6.250364000	19.483986000	1.903861000
1	6.519046000	20.040635000	0.993401000
1	6.853129000	18.566607000	1.911201000
1	6.545942000	20.096438000	2.762146000
6	4.410885000	18.384157000	0.605761000
1	4.790961000	18.924478000	-0.274086000
1	3.326354000	18.252133000	0.486132000
1	4.881373000	17.391199000	0.622177000
6	3.967815000	20.522131000	1.814300000
1	4.183516000	21.016239000	0.855616000
1	4.266258000	21.210484000	2.614804000
1	2.881914000	20.366834000	1.869690000
6	-0.521829000	15.614328000	4.957129000
6	0.542838000	15.413020000	6.050397000
1	0.091096000	15.647772000	7.025202000
1	1.400634000	16.082744000	5.906827000
1	0.915625000	14.382382000	6.098216000
6	-1.671690000	14.628765000	5.194136000
1	-2.027891000	14.741638000	6.229273000
1	-1.360897000	13.582821000	5.065028000
1	-2.524133000	14.825134000	4.532910000
6	-1.038586000	17.058005000	5.066982000
1	-1.471629000	17.203545000	6.067978000
1	-1.815421000	17.287982000	4.329871000
1	-0.229428000	17.786747000	4.930207000
6	-0.860159000	15.139919000	1.873045000
6	0.007193000	15.207694000	0.601918000
1	-0.632242000	15.019076000	-0.273448000
1	0.804369000	14.451134000	0.606814000
1	0.469167000	16.197995000	0.483082000
6	-1.598277000	13.794114000	1.907703000
1	-2.220770000	13.715907000	1.003694000
1	-2.261790000	13.696439000	2.773438000
1	-0.910762000	12.938304000	1.902219000
6	-1.880272000	16.286783000	1.826440000
1	-2.426211000	16.232791000	0.873028000
1	-1.396746000	17.271683000	1.876376000
1	-2.619219000	16.217581000	2.634551000
6	0.543650000	19.085457000	1.485606000