A low-valent dinuclear ruthenium diazadiene complex catalyzes the oxidation of dihydrogen and reversible hydrogenation of quinones

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Contents

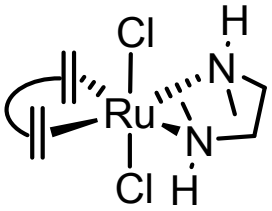
1 General Methods

All experiments were performed under argon atmosphere using standard Schlenk and glove-box techniques. THF, DME, Et_2O, *n*-hexane were dried by Innovative Technology solvent purification system and stored with 4Å molecular sieves under argon. THF-d_8 was purchased from Euriso-Top, degassed and distilled from sodium/benzophenone. NMR spectra were recorded on Bruker 400 or 500 MHz spectrometer with respect to ^1H. Reactions for isotope effect were monitored by ^1H NMR spectroscopy with a Bruker 400 spectrometer. Quaternary carbon atoms are indicated as C^{quat}, aromatic units as CH^{ar} and CH^{ar}. The olefinic protons and carbon atoms of the $C{=}C_{dbcot}$ unit in the central seven-membered ring are indicated as CH^{olefin} and CH^{olefin}. The protons and carbones in dad moieties are indicated as CH^{dad} and CH^{dad}. $RuCl_3 \cdot 3H_2O$ and N,N'-Dimethylethylenediamine were purchased from Aldrich-Fine Chemicals. KO*t*Bu was purchased from ABCR-Chemicals. Vitamin K_3 was purchased from Apollo Scientific Ltd. Vitamin K_2 was purchased from Sigma-Fine Chemicals. These chemcials were used as received. 1,4-benzoquinone was purified by sublimation before use and dbcot was synthesized according to published method.[S1] Single crystals suitable for X-ray diffraction were protected with polyisobutylene oil in glovebox then transferred to the goniometer of an Oxford XCalibur, a Bruker SMART APEX or a Bruker APEX diffractometer. The structures were solved using direct methods (SHELXS) on OLEX2 and refined by full-matrix leastsquares procedures. DFT geometry optimization of the 2,5-di-*tert*butyl-*p*-benzoquinone was performed using TURBOMOLE[S2] coupled to the PQS Baker optimizer[S3], [S4] via the BOpt package[S5] at the BP86,[S6],[S7] def2-TZVP[S8],[S9] level of theory (m4 grid), on full models (including *t*Bu groups) in the gas phase, using Grimme's version 3 (disp3, "zero damping") dispersion corrections.[S10] The minimum energy (no imaginary frequenciy) was characterized by numerically calculating the Hessian matrix. EPR parameters were calculated with the ORCA[S11] Program system at the B3LYP/TZ2P level, using the coordinates from the structures optimized in Turbomole as input. The EPR spectrum was recorded on a Bruker EMX X-band spectrometer equipped with a He cryostat. The spectrum was analyzed and simulated using the W95EPR program of Prof. F. Neese.

2 Synthesis of complexes

$[RuCl_2(dbcot)]_x$, Complex 1,

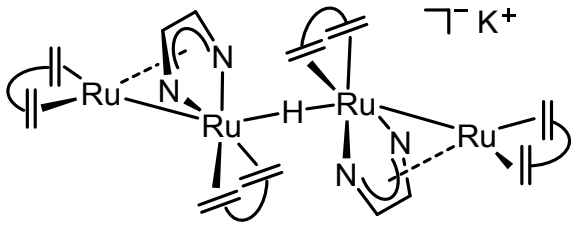
In a 500 mL three-necked flask, $RuCl_3 \cdot 3H_2O$ (4.5 g, 17.2 mmol) and dbcot (7 g, 34.4 mmol) were dissolved in a mixture of 150 mL ethanol and 30 mL THF (both degassed). The solution was refluxed for 24 h. A brownish powder was precipitated with quantitative yield. It was filtered, washed with dry THF (3×20 mL), and then dried under vacuum. Anal. Calcd for $C_{16}H_{12}Cl_2Ru$ (found): C, 51.08 (50.56); H, 3.21 (3.46); Cl, 18.84 (18.61).



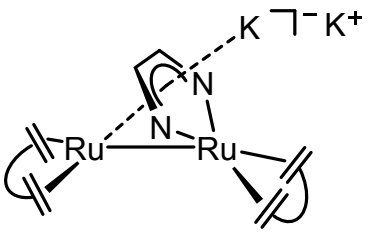
$[RuCl_2(Me_2en)(dbcot)]$, Complex 2.

N,*N*′-dimethylethylenediamine (0.62 mL, 5.6 mmol) was added to a suspension of complex **1** (2.0 g, 5.3 mmol) in 20 mL THF. The mixture was heated at 65 °C for 1 h before removing the solvent under vacuum. The obtained solid was washed with Et_2O (3×5 mL). After drying under vacuum, 2.3 g of **2** was obtained as an orange powder with 93% yield. ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C): δ 6.91-7.01 (m, 8H, C*H*^{ar}), 5.26 (d, J_{HH} = 9.0 Hz, 2H, C*H*^{olef}), 5.11 (d, J_{HH} = 9.0 Hz, 2H, C*H*^{olef}), 4.03 (b, 2H, N*H*), 3.26-3.19 (m, 2H, CH_2), 2.73-2.69 (m, 2H, CH_2), 2.43 (s, 3H, CH_3), 2.41 (s, 3H, CH_3). ^{13}C NMR (125.78 MHz, $CDCl_3$, 25 °C): δ 144.6 (*C*^{quat}), 143.7 (*C*^{quat}), 127.1 (*C*H^{ar}), 126.8 (*C*H^{ar}), 125.9 (*C*H^{ar}), 125.9 (*C*H^{ar}), 93.1 (*C*H^{olef}), 89.2 (*C*H^{olef}), 52.4 (*C*H_2), 35.9 (*C*H_3). Anal. Calcd for $C_{20}H_{24}Cl_2N_2Ru \cdot 0.5\ CH_2Cl_2$ (found): C, 48.58 (48.49); H, 4.97 (5.03); N, 5.53 (5.79).

[K][Ru$_4$(μ-H)(Me$_2$dad)$_2$(dbcot)$_4$], Complex [K][3$_2$(μ-H)].



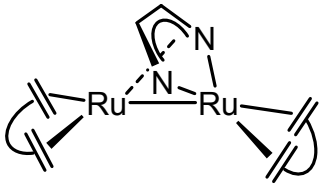
KO*t*Bu (27 mg, 0.22 mmol) dissolved in 2 mL THF was added to a THF (5 mL) solution of complex **2** (50 mg, 0.11 mmol) with stirring at room temperature. The mixture was filtered after 0.5 h. The volatiles of the filtrate was removed under vacuum, the residue was washed with Et_2O/DME (1:1) before extracting by THF. **[K][3$_2$(μ-H)]** as green crystals (17 mg, 40% yield) were obtained by layering with DME and hexane on the top of the THF solution. The 18-crown-6 coordinated product was obtained by adding 18-crown-6 in the THF solution of **[K][3$_2$(μ-H)].** ^{1}H NMR (500 MHz, THF-d_8, 25 °C): δ 6.72-6.70 (m, 4H, C*H*^{ar}), 6.50-6.48 (m, 4H, C*H*^{ar}), 6.42-6.32 (m, 16H, C*H*^{ar}), 6.30 (s, 4H, C*H*^{dad}), 6.30-6.27 (m, 4H), 5.96-5.93 (m, 4H), 3.91 (s, 2H, C*H*^{olef}), 3.89 (s, 2H, C*H*^{olef}), 3.60 (s, 24H, CH_2), 3.08 (s, 8H, C*H*^{olef}), 3.05 (s, 2H, C*H*^{olef}), 3.02 (s, 2H, C*H*^{olef}), 1.55 (s, 12H, CH_3), -9.46 (s, 1H, Ru-*H*-Ru). ^{13}C NMR (125.78 MHz, THF-d_8, 25 °C): δ 152.0 (*C*^{quat}), 151.6 (*C*^{quat}), 127.85 (*C*H^{ar}), 126.7 (*C*H^{ar}), 124.7 (*C*H^{ar}), 123.5 (*C*H^{ar}), 123.3 (*C*H^{ar}), 112.9 (*C*H^{dad}), 76.8 (*C*H^{olef}), 75.6 (*C*H^{olef}), 71.4 (*C*H$_2$), 66.7 (*C*H^{olef}), 59.4 (*C*H^{olef}), 37.8 (*C*H$_3$). Anal. Calcd for $C_{72}H_{65}KN_4Ru$·dme (found): C, 60.06 (59.74); H, 4.97 (5.04); N, 3.69 (3.86).



[K]$_2$[Ru$_2$(Me$_2$dad)(dbcot)$_2$], Complex [K]$_2$[3].

KC_8 (15 mg, 111.9 μmol) was portionly added to a THF (8 mL) solution of complex **[K][3$_2$(μ-H)]** (50 mg, 32.90 μmol) at -30 °C. The reaction was slowly warmed up to room temperature. And the color changed from green to brown. After stirring for 2 h at room temperature, the mixture was filtered and the solvent was removed under vacuum. The obtained solid was dissolved in THF. Crystals (53 mg, 84%

yield) were obtained by layering DME and hexane (containing 18-crown-6) on the top of the THF solution. ^{1}H NMR (500 MHz, THF-d_8, 25 °C): δ 6.71-6.66 (m, 4H, CH^{ar}), 6.60-6.56 (m, 4H, CH^{ar}), 6.45-6.36 (m, 8H, CH^{ar}), 5.20 (s, 2H, CH^{dad}), 3.20-2.80 (b, 2H, CH^{olef}), 3.18 (s, 1H, CH^{olef}), 3.13 (s, 1H, CH^{olef}), 3.10 (s, 1H, CH^{olef}), 2.84 (s, 1H, CH^{olef}), 2.45 (s, 1H, CH^{olef}), 2.42 (s, 1H, CH^{olef}), 2.29 (s, 6H, CH_3). ^{13}C NMR (125.78 MHz, THF-d_8, 25 °C): δ 156.7 (C^{quat}), 155.8 (C^{quat}), 126.4 (CH^{ar}), 126.3 (CH^{ar}), 122.9 (CH^{ar}), 107.1 (CH^{dad}), 96.9 (CH^{olef}), 71.2 (CH$_2$), 61.2 (CH^{olef}), 58.4 (CH^{olef}), 53.1 (CH^{olef}), 39.2 (CH$_3$). Anal. Calcd for $C_{36}H_{32}K_2N_2Ru_2$·2(18-crown-6) (found): C, 55.37 (55.21); H, 6.19 (6.36); N, 2.15 (2.38).



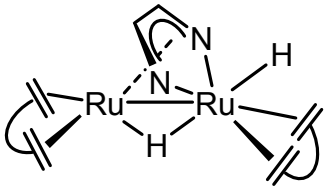
[Ru$_2$(Me$_2$dad)(dbcot)$_2$], Complex 3.

Method 1. [Fc][PF$_6$] (48 mg, 105 μmol) was slowly added to a THF (8 mL) solution of **[K]$_2$[3]** (50 mg, 52.5 μmol) at room temperature. After 2 h stirring, the mixture was filtered and the solvent was removed under vacuum. After washing with hexane, **3** (28 mg, 40.3 μmol) was obtained from toluene extraction in 77% yield.

Method 2. [Fc][PF$_6$] (3.5 mg, 10.6 μmol) was slowly added to a THF (5mL) solution of **[K][3$_2$(μ-H)]** (18 mg, 10.6 μmol) at -30 °C with strring. The reaction was warmed up to room temperature slowly. After 1.5 h, the mixture was filtered and the solvent was removed under vacuum. The residue was washed with Et$_2$O (3×2 mL) and dried under vaccum. Yield 12 mg, 80%.

^{1}H NMR (400 MHz, THF-d_8, 0 °C): δ 6.94 (s, 2H, CH^{dad}), 6.88-6.85 (m, 2H, CH^{ar}), 6.69-6.67 (m, 2H, CH^{ar}), 6.63-6.58 (m, 4H, CH^{ar}), 6.42-6.40 (m, 2H, CH^{ar}), 6.37-6.31 (m, 4H, CH^{ar}), 6.16-6.14 (m, 2H, CH^{ar}), 4.56 (d, J_{HH} = 8.8 Hz, 2H, CH^{olef}), 3.70 (d, J_{HH} = 8.8 Hz, 2H, CH^{olef}), 3.61 (d, J_{HH} = 8.3 Hz, 2H, CH^{olef}), 3.30 (d, J_{HH} = 8.3 Hz, 2H, CH^{olef}), 2.23 (s, 6H, CH_3). ^{13}C NMR (125.78 MHz, THF-d_8, 0 °C): δ 151.8 (C^{quat}), 151.0 (C^{quat}), 149.5 (C^{quat}), 149.5 (C^{quat}), 127.6 (CH^{ar}), 127.2 (CH^{ar}), 126.9 (CH^{dad}), 126.6 (CH^{ar}), 125.4 (CH^{ar}), 124.8 (CH^{ar}), 124.6 (CH^{ar}), 124.4 (CH^{ar}), 124.2 (CH^{ar}), 117.6 (CH^{ar}), 82.9 (CH^{olef}),

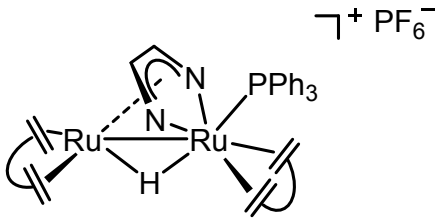
79.0 (*C*H^{olef}), 70.7 (*C*H^{olef}), 63.8 (*C*H^{olef}), 37.0 (*C*H$_3$). MALDI HRMS (m/z): {Ru$_2$(Me$_2$dad)(dbcot)$_2$H}$^+$ calcd. For $C_{36}H_{33}N_2Ru_2$ 697.0731; found: 697.0725.



[Ru$_2$H(μ-H)(Me$_2$dad)(dbcot)$_2$], Complex 3(μ-H)H.

3 (50 mg, 72 μmol) dissolved in 10 mL THF in a J-Young Schlenk was degassed three times by freeze-pump-thaw and placed under 1 bar H_2. The mixture was stirred at 40 °C overnight, subsequently the solvent was removed under vacuum. **3(μ-H)H** (48 mg) was obtained as a yellowish powder in 96 % yield. ^{1}H NMR (500 MHz, THF-d_8, 25 °C): δ 6.90 (s, 2H, C*H*^{dad}), 6.79-6.76 (m, 4H, C*H*^{ar}), 6.74-6.72 (m, 2H, C*H*^{ar}), 6.71-6.70 (m, 4H, C*H*^{ar}), 6.68-6.63 (m, 4H, C*H*^{ar}), 6.61-6.60 (m, 2H, C*H*^{ar}), 3.94 (d, J_{HH} = 8.8 Hz, 2H, C*H*^{olef}), 3.72 (d, J_{HH} = 8.7 Hz, 2H, C*H*^{olef}), 3.64 (d, J_{HH} = 8.8 Hz, 2H, C*H*^{olef}), 3.53 (d, J_{HH} = 8.7 Hz, 2H, C*H*^{olef}), 1.87 (s, 6H, C*H*$_3$), -0.74 (d, J_{HH} = 8.7 Hz, 1H, Ru-(μ-*H*)), -2.74 (d, J_{HH} = 8.7 Hz, 1H, Ru-(t-*H*)). ^{13}C NMR (125.78 MHz, THF-d_8, 25 °C): δ 152.3 (*C*^{quat}), 148.7 (*C*^{quat}), 148.6 (*C*^{quat}), 148.5 (*C*^{quat}), 148.4 (*C*^{quat}), 127.8 (*C*H^{ar}), 127.0 (*C*H^{ar}), 126.8 (*C*H^{ar}), 126.6 (*C*H^{ar}), 125.9 (*C*H^{ar}), 125.1 (*C*H^{ar}), 113.1 (*C*H^{dad}), 70.0(*C*H^{olef}), 67.4 (*C*H^{olef}), 67.0 (*C*H^{olef}), 61.1 (*C*H^{olef}), 38.7 (*C*H$_3$). MALDI HRMS (m/z): {Ru$_2$H(Me$_2$dad)(dbcot)$_2$}$^+$ calcd. For $C_{36}H_{33}N_2Ru_2$ 697.0731; found: 697.0721.

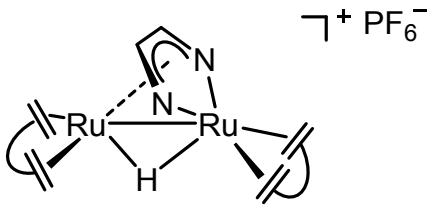
[Ru$_2$(μ-H)(Me$_2$dad)(dbcot)$_2$(PPh$_3$)][PF$_6$], Complex [3(μ-H)(PPh$_3$)][PF$_6$]



3(μ-H)H (5 mg, 7.2 μmol) and PPh_3 (1.88 mg, 7.2 μmol) were dissolved in 0.4 mL THF-d_8 in a J-Young NMR tube. Subsequently, Cp_2FePF_6 (2.4 mg, 7.2 μmol) was added to the solution. The reaction was checked by ^{1}H NMR after 0.5 h. **[3(μ-H)(PPh$_3$)][PF$_6$]** was quantitatively formed using the residual solvent signal as internal standard. ^{1}H NMR (500 MHz, THF-d_8, 25 °C): δ 7.50-6.30 (m, 33H, , C*H*^{ar} and C*H*^{dad}),

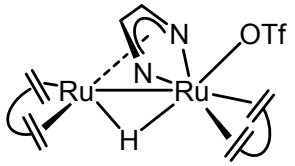
4.82 (d, J_{HH} = 9.2 Hz, 2H, C*H*^{olef}), 4.51 (d, J_{HH} = 9.2 Hz, 2H, C*H*^{olef}), 3.94 (d, J_{HH} = 8.6 Hz, 2H, C*H*^{olef}), 3.70 (d, J_{HH} = 4.8 Hz, 2H, C*H*^{olef}), 1.95 (s, 6H, CH_3), -1.70 (d, J_{HP} = 33.1 Hz, 1H, Ru-*H*). ^{13}C NMR (125.78 MHz, THF-d_8, 25 °C): δ 147.4 (*C*^{quat}), 146.8 (*C*^{quat}), 146.1 (*C*^{quat}), 142.5 (*C*^{quat}), 138.6 (*C*^{quat}), 135.6 (*C*H), 135.5 (*C*H), 132.8 (*C*^{quat}), 132.4 (*C*^{quat}), 132.1 (*C*H^{ar}), 131.3 (*C*H^{ar}), 131.3 (*C*H^{ar}), 131.1 (*C*H^{ar}), 131.0 (*C*H^{ar}), 130.5 (*C*H^{ar}), 129.7 (*C*H^{ar}), 129.1 (*C*H^{ar}), 129.1 (*C*H^{ar}), 128.9 (*C*H^{ar}), 128.1 (*C*H^{ar}), 128.0 (*C*H^{ar}), 127.7 (*C*H^{ar}), 126.9 (*C*H^{ar}), 126.7 (*C*H^{ar}), 126.5 (*C*H^{ar}), 126.4 (*C*H^{ar}), 126.1 (*C*H^{ar}), 126.1 (*C*H^{ar}), 125.8 (*C*H^{ar}), 125.6 (*C*H^{ar}), 118.2 (*C*H^{dad}), 85.3 (*C*H^{olef}), 78.1 (*C*H^{olef}), 75.2 (*C*H^{olef}), 68.5 (*C*H^{olef}), 41.6 (*C*H_3). ^{31}P NMR (202.5 MHz, 25 °C): δ 32.8 (s, *P*Ph_3), -144.22 (hept, J_{PF} = 709.8 Hz, *P*F_6^-). ^{19}F NMR (470.6 MHz, 25 °C): δ -73.29 (d, J_{FP} = 709.8 Hz, P*F*$_6^-$). MALDI HRMS (m/z): {[$Ru_2H(Me_2dad)(dbcot)_2$][PPh_3]}$^+$ calcd. For $C_{54}H_{48}N_2PRu_2$ 959.1642; found: 959.1637.

[Ru_2(μ-H)(Me_2dad)(dbcot)$_2$][PF_6], Complex [3(μ-H)][PF_6].



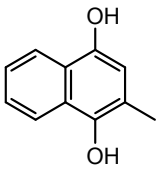
3(μ-H)H (5 mg, 7.2 μmol) was dissolved in 0.4 mL THF-d_8 in a J-Young NMR tube, subsequently [Fc][PF_6] (2.4 mg, 7.2 μmol) was added at 0 °C. The reaction was checked by ^{1}H NMR after 10 minutes. **[3(μ-H)]**$^+$ was formed quantitatively using the residual solvent signal as internal standard. ^{1}H NMR (500 MHz, THF-d_8, 25 °C): δ 7.77 (s, 2H, C*H*^{dad}), 7.25-6.64 (m, 16H, C*H*^{ar}), 4.94 (d, J_{HH} = 9.1 Hz, 2H, C*H*^{olef}), 4.70 (d, J_{HH} = 9.1 Hz, 2H, C*H*^{olef}), 4.14 (d, J_{HH} = 8.5 Hz, 2H, C*H*^{olef}), 4.02 (d, J_{HH} = 8.5 Hz, 2H, C*H*^{olef}), 2.22 (s, 6H, CH_3), -10.34 (s, 1H, Ru-*H*). ^{13}C NMR (125.78 MHz, THF-d_8, 25 °C): δ 147.6 (*C*^{quat}), 147.2 (*C*^{quat}), 146.1 (*C*^{quat}), 143.4 (*C*^{quat}), 138.5 (*C*^{quat}), 129.7 (*C*H^{ar}), 128.9 (*C*H^{ar}), 128.5 (*C*H^{ar}), 128.0 (*C*H^{ar}), 126.8 (*C*H^{ar}), 126.6 (*C*H^{ar}), 126.56 (*C*H^{ar}), 126.2 (*C*H^{ar}), 126.1 (*C*H^{ar}), 125.8 (*C*H^{ar}), 123.1 (*C*H^{dad}), 87.2 (*C*H^{olef}), 81.8 (*C*H^{olef}), 77.8 (*C*H^{olef}), 71.2 (*C*H^{olef}), 40.2 (*C*H_3). ^{31}P NMR (202.5 MHz, 25 °C): δ -144.22

(hept, J_{PF} = 709.8 Hz, , PF_6^-). ^{19}F NMR (470.6 MHz, 25 °C): δ -73.29 (d, J_{FP} = 709.8 Hz, , PF_6^-). MALDI HRMS (m/z): $\{Ru_2H(Me_2dad)(dbcot)_2\}^+$ calcd. For $C_{36}H_{33}N_2Ru_2$ 697.0731; found: 697.0725.

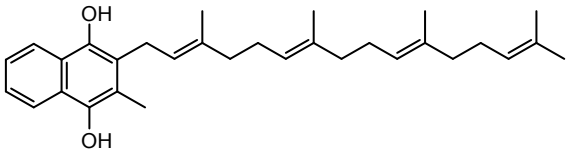


[Ru_2(μ-H)(OTf)(Me_2dad)(dbcot)$_2$], Complex [3(μ-H)(OTf)].

3(μ-H)H (50 mg, 71.8 μmol) was dissolved in 8 mL THF in a vial and [Fc][OTf] (24 mg, 71.8 μmol) was added at 0 °C. After stirring for 1 h, the solvent was removed under vacuum. **[3(μ-H)(OTf)]** (55 mg, 90% yield) was obtained after washing with hexane (3×5 mL) and drying under vacuum. ^{1}H NMR spectrum shows that 89% of complex exist in the form of **[3(μ-H)(OTf)]**, while the rest 11% (Ru-H, –10.3 ppm, free OTf, –79.82 ppm) exist in the form of **[3(μ-H)][OTf]**, since it has the same proton spectrum as that of **[3(μ-H)][PF_6]**. **[3(μ-H)(OTf)]**: ^{1}H NMR (500 MHz, THF-d_8, 25 °C): δ 7.61 (s, 2H, CH^{dad}), 6.98-6.95 (m, 2H, CH^{ar}), 6.87-6.85 (m, 2H, CH^{ar}), 6.80-6.77 (m, 8H, CH^{ar}), 6.71-6.68 (m, 2H, CH^{ar}), 6.62-6.58 (m, 2H, CH^{ar}), 4.81 (d, J_{HH} = 9.0 Hz, 2H, CH^{olef}), 4.75 (d, J_{HH} = 9.0 Hz, 2H, CH^{olef}), 4.02 (d, J_{HH} = 8.5 Hz, 2H, CH^{olef}), 3.92 (d, J_{HH} = 8.5 Hz, 2H, CH^{olef}), 2.17 (s, 6H, CH_3), -10.18 (s, 1H, Ru-*H*). ^{13}C NMR (125.78 MHz, THF-d_8, 25 °C): δ 147.7 (C^{quat}), 147.4 (C^{quat}), 145.6 (C^{quat}), 143.6 (C^{quat}), 138.5 (C^{quat}), 128.4 (CH^{ar}), 128.0 (CH^{ar}), 126.9 (CH^{ar}), 126.8 (CH^{ar}), 126.4 (CH^{ar}), 126.2 (CH^{ar}), 125.7 (CH^{ar}), 122.2 (CH^{dad}), 84.6 (CH^{olef}), 81.0 (CH^{olef}), 75.7 (CH^{olef}), 69.1 (CH^{olef}), 40.1 (CH_3). ^{19}F NMR (470.6 MHz, 25 °C): δ -79.05 (2). MALDI HRMS (m/z): $\{Ru_2H(Me_2dad)(dbcot)_2\}^+$ calcd. For $C_{36}H_{33}N_2Ru_2$ 697.0731; found: 697.0742.

Compound VK_3H_2. 

^{1}H NMR (500 MHz, THF-d_8, 25 °C): δ 8.20-8.07 (m, 2H), 7.41-7.24 (m, 2H), 6.56 (s, 1H), 2.32 (s, 3H).



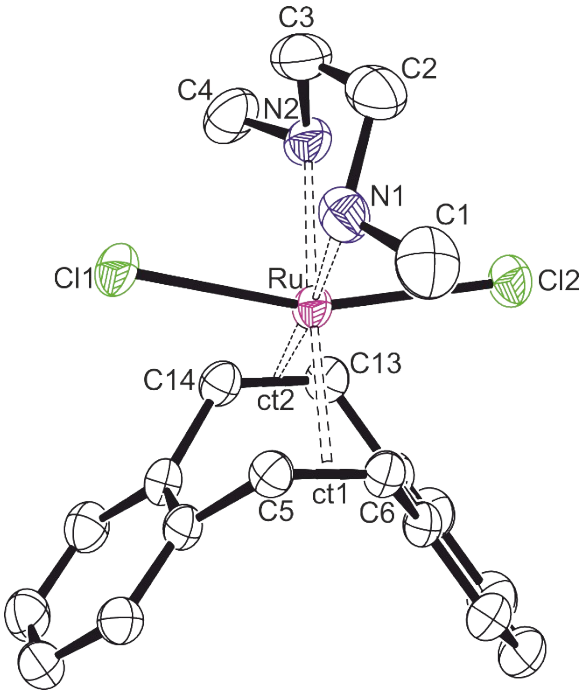
Compound VK_2H_2. ^{1}H NMR (500 MHz, THF-d_8, 25 °C): δ 8.22-8.14 (m, 2H), 7.40-7.38 (dd, J_{HH} = 6.5 Hz, 3.3 Hz, 2H), 7.36 (b, 2H), 5.24-5.17(m, 4H), 3.69 (d, J_{HH} = 6.7 Hz, 2H), 2.43 (s, 3H), 2.20-2.03 (m, 12H), 1.93 (s, 3H), 1.74 (s, 3H), 1.67 (s, 6H), 1.66 (s, 3H).

3 Crystallographic Data

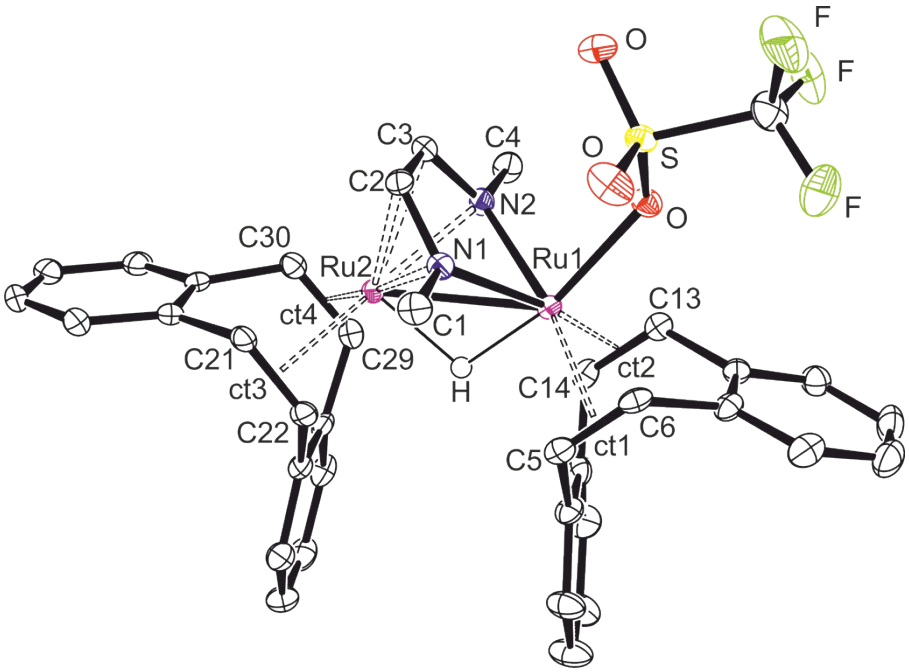
Supplementary Table 1. Selected crystal data of **2**, **[K][3$_2$(μ-H)]**, **[K]$_2$[3]**, **3(μ-H)H**, **[3(μ-H)][OTf]**.

	2	**[K][3$_2$(μ-H)]**	**[K]$_2$[3]**	**3(μ-H)H**	**[3(μ-H)(OTf)]**
N1-C2	1.479(2)	1.381(3)	1.399(4)	1.379(3), 1.378(2)	1.371(3), 1.366(4)
C2-C3	1.508(3)	1.382(4)	1.406(4)	1.400(3), 1.397(3)	1.400(4), 1.403(4)
C3-N2	1.477(3)	1.379(2)	1.390(3)	1.371(3), 1.372(2)	1.368(4), 1.373(4)
C5-C6	1.389(3)	1.437(3)	1.450(4)	1.426(3), 1.424(3)	1.395(4), 1.419(4)
C13-C14	1.399(3)	1.430(3)	1.451(3)	1.420(3), 1.425(3)	1.411(4), 1.403(4)
Ru1-N1	2.162(2)	2.106(2)	2.055(2)	2.088(2), 2.093(2)	2.136(2), 2.126(2)
Ru1-N2	2.165(1)	2.108(2)	2.078(2)	2.095(1), 2.097(1)	2.116(2), 2.145(2)
Ru1-ct1	2.098(2)	2.011(2)	1.986(2)	2.019, 2.017	2.074, 2.064
Ru1-ct2	2.095(2)	2.017(2)	1.984(2)	2.034, 2.027	2.073, 2.077
C21-C22		1.449(3)	1.454(4)	1.427(3), 1.427(3)	1.437(4), 1.429(4)
C29-C30		1.446(2)	1.459(4)	1.430(3), 1.429(2)	1.419(4), 1.441(4)
Ru1-Ru2		2.6947(5)	2.8239(8)	2.7388(3), 2.7213(3)	2.6725(6), 2.6723(5)
Ru2-N1		2.176(2)	2.476(2)	2.182(2), 2.188(2)	2.150(2), 2.143(2)
Ru2-N2		2.171(2)	2.293(2)	2.171(2), 2.177(2)	2.152(2), 2.161(2)
Ru2-C2		2.229(2)	2.188(3)	2.224(2), 2.229(2)	2.245(3), 2.248(3)
Ru2-C3		2.224(2)	2.165(2)	2.229(2), 2.235(2)	2.256(3), 2.249(3)
Ru2-ct3		1.991(3)	1.973(3)	2.022, 2.019	2.012, 2.020

Ru2-ct4		1.992(2)	1.968(3)	2.017, 2.015	2.030, 2.018



Supplementary Figure 1. X-ray crystal structure of **2**. Ellipsoids are drawn at a 50 % probability level. Hydrogen atoms have been removed for clarity. *Ct* is the centroid of the C=C_{dbcot} bond.



Supplementary Figure 2. X-ray crystal structure of **[3(μ-H)(OTf)]**. Ellipsoids are drawn at a 50 % probability level. Non-relevant hydrogen atoms have been removed for clarity. Ct is the centroid of the C=C_{dbcot} bond.

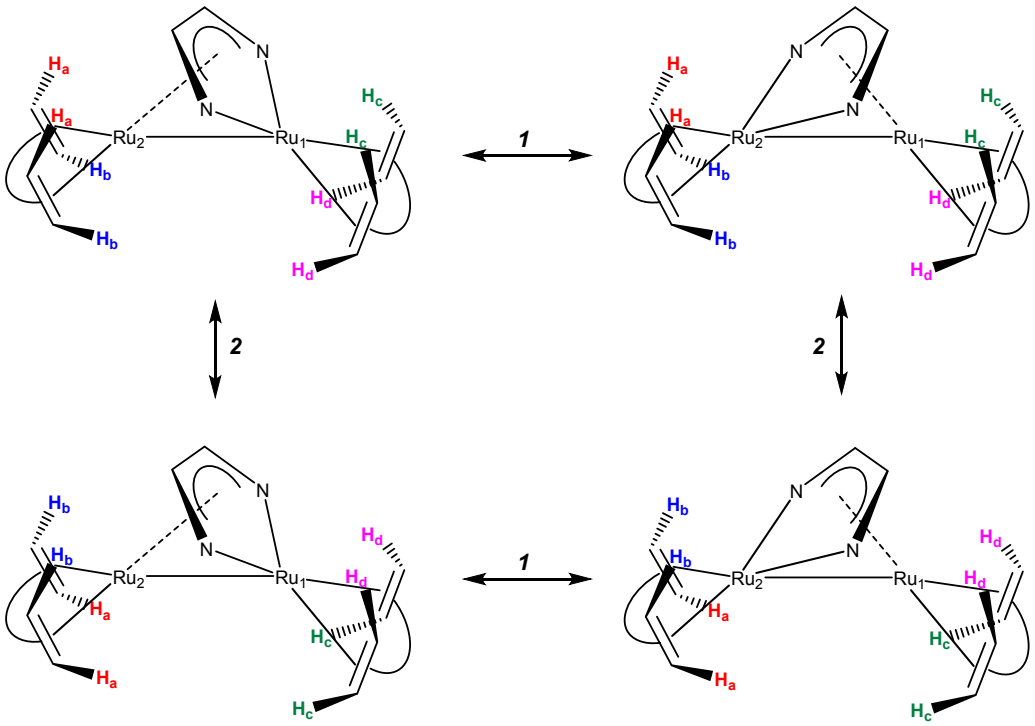
4 Selected ^{1}H and ^{13}C chemical shifts

Supplementary Table 2. Selected ^{1}H and ^{13}C chemical shifts of **2**, **[K][3$_2$(μ-H)]**, **[K]$_2$[3]**, **3**, **3(μ-H)H**, **[3(μ-H)][PF$_6$]**, measured in THF-d_8 if not otherwise noted. Chemical shifts given on the δ scale are expressed in ppm.

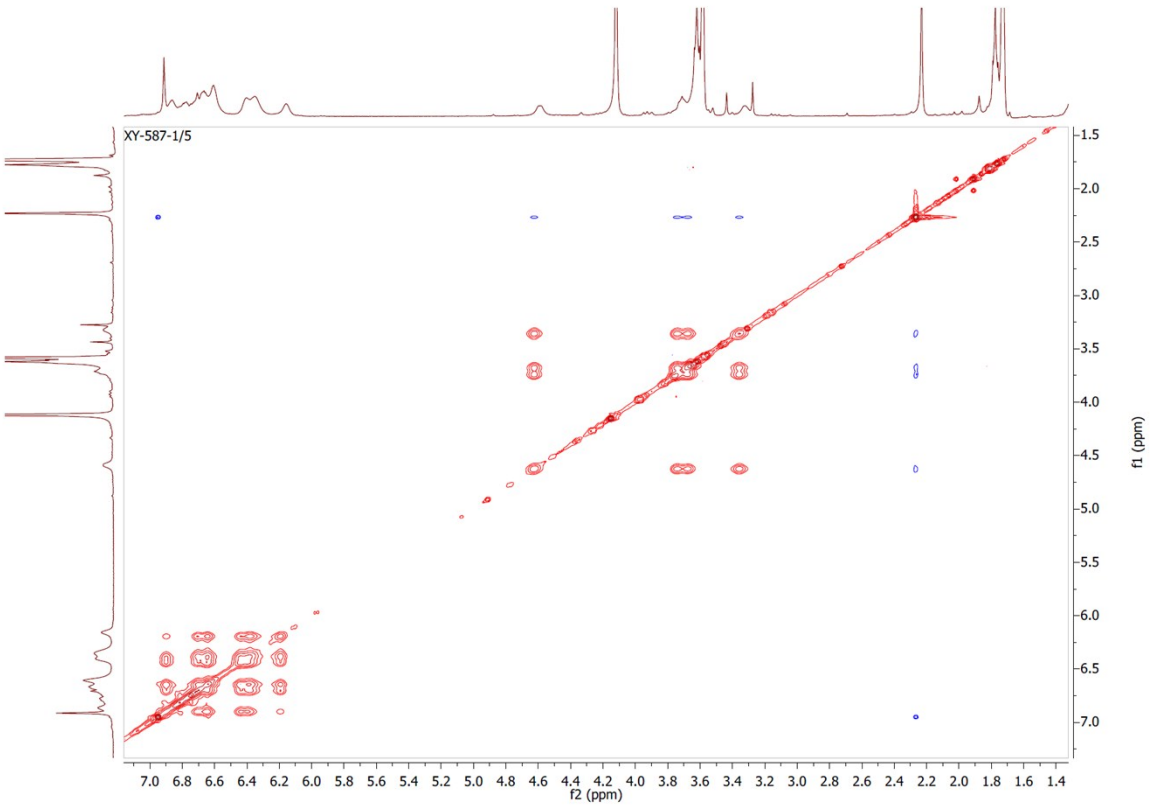
	δ Ru-H	**δ $^{1}H_{HC=N\ or\ (N-CH=)}$**	**δ $^{13}C_{HC=N\ or\ (N-CH=)}$**	**δ $^{1}H_{olef}$**	**δ $^{13}C_{olef}$**
2 (in $CDCl_3$)		3.23, 2.72 (CH_2)	52.4 (CH_2)	5.26, 5.11	93.1, 89.2
[K][3$_2$(μ-H)]	-9.46	6.30	112.9	3.91, 3.89, 3.08, 3.05, 3.02	76.8, 75.6, 66.7, 59.4
[K]$_2$[3]		5.20	107.1	3.10, 2.80-3.20, 2.45, 2.42	96.9, 61.2, 58.4, 53.1
3		6.94	126.9	4.56, 3.70, 3.61, 3.30	82.9, 79.0, 70.7, 63.8
3(μ-H)H	-0.74，-2.74	6.90	113.1	3.94, 3.72, 3.64, 3.53	70.0, 67.4, 67.0, 61.1
[3(μ-H)][PF$_6$]	-10.34	7.77	123.1	4.94, 4.70, 4.14, 4.02	87.2, 81.8, 77.8, 71.2

5 NOESY experiment of 3

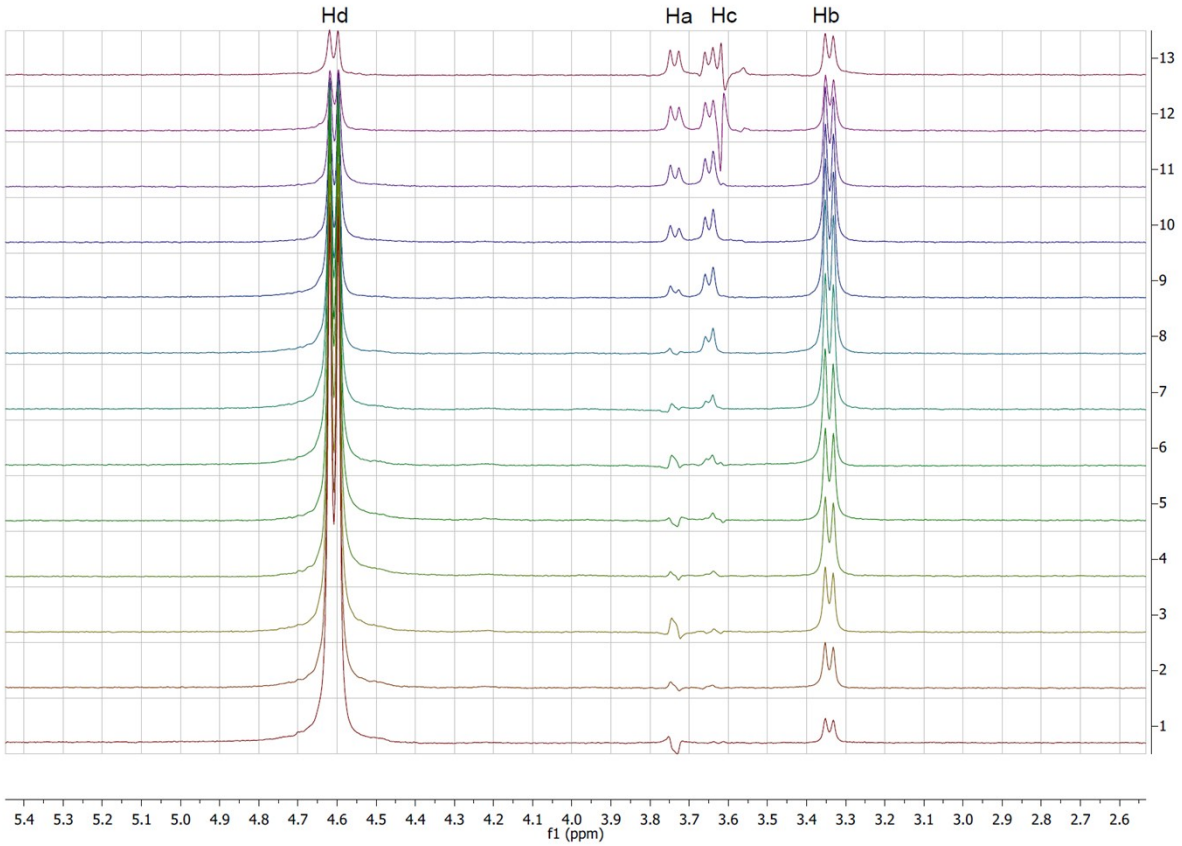
a)



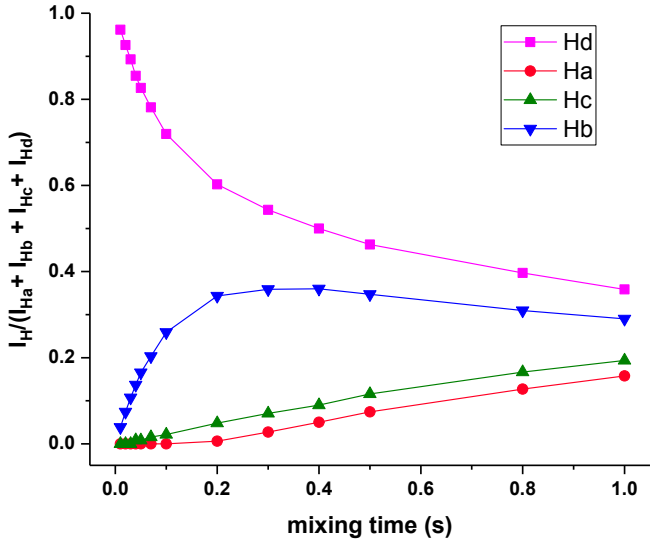
b)



c)



d)



Supplementary Figure 3. a). The dynamic processes of **3** in THF-d_8. b). The NOESY spectrum of complex **3** at room temperature. c). ^{1}H NMR spectra of complex **3** with different D8 from the selective gradient NOESY experiment at T = 283 K. d). The relative intensities of H_a, H_b, H_c and H_d plotted against the D8 (mixing time). The lines in the figure are only lines connecting the data.

6 Hydrogenation and dehydrogenation reactions

6.1 PPh_3 and [Fc][PF_6]

3(μ-H)H catalyzed H_2 spliting to protons and electrons.

5 mg of **3(μ-H)H**, 18.8 mg of PPh_3, 24 mg of [Fc][PF_6] were charged in to a J-Young NMR tube, to which 0.4 ml THF was added. The reaction was heated at 40 °C under 1 bar H_2. The reaction was followed by ^{31}P NMR. The stability of the catalyst was tested by adding 18.8 mg of PPh_3, 24 mg of [Fc][PF_6] and H_2 to the reaction mixture every 1.5 h. Catalytic acitivity was still observed after the 6th addition.

6.2 Vitamin K

Supplementary Table 3. Interconversion of VK_2 and VK_3 with VK_2H_2 and VK_3H_2.

Entry	Substance	H_2 / bar	**3(μ-H)H** / mol%	solvent	T / °C	Time / h	TOF / h^{-1}	TON
1	VK_3	1	0.33	THF	40	80	-	252
2	VK_3	15	0.5	THF	70	24	-	130
3	VK_3	15	0.13	THF	40	15	2.2	33
					70	4	10	40
						108	-	217
4	VK_2	1.5	1.2	THF	r.t.	20 ~ 65	0.5	81
5	VK_3H_2	-	0.2	THF	40	48	-	70
6	VK_3H_2	-	7.7	THF	40	3.5	3.7	13
7	VK_2H_2	-	0.2	THF	40	40	0.6	24

Hydrogenation of VK_3 by 3(μ-H)H. 4 mg of **3(μ-H)H** and 50 mg of VK_3 were dissolved in 0.4 mL THF-d_8 in a J-Young NMR tube. The solution was degassed by freeze-pump-thaw for three times, subsequently it was heated to 40 °C under 1 bar H_2 . 50 mg of VK_3 was repeatedly added every 80 h. 300 mg VK_3 in total was added and 84% of which was hydrogenated to dihydrovitamin K_3. The TON is 252.

General procedure for the hydrogenation of VK_3 by 3(μ-H)H under high pressure. 3(μ-H)H and VK_3 were dissolved in 5 mL THF. The solution was injected into a 100 mL autoclave under Ar. Subsequently, the autoclave was purged by H_2 three times and pressurized with 15 bar H_2. After a certain time, a small portion of the reaction was taken out of the autoclave to remove solvent under vacuum. Conversion was calculated according to the ratio of VK_3 to dihydrovitamin K_3 in ^1H NMR spectrum.

Hydrogenation of VK_2 by 3(μ-H)H. 5 mg of **3(μ-H)H** and 30 mg of VK_2 were dissolved in 0.4 mL THF-d_8 in a J-Young NMR tube. The solution was degassed by freeze-pump-thaw for three times and pressurized with 1.5 bar H_2. The tube was kept in dark at room temperature until complete consumption of VK_2 (20-65 h), confirmed by in-situ ^1H NMR. 30 mg VK_2 was charged each time until it took 65 h to fully consume. 270 mg of VK_2 in total was added, and the ratio of VK_2 hydroquinone to tautomerization product is 22:1. The TON is 81.

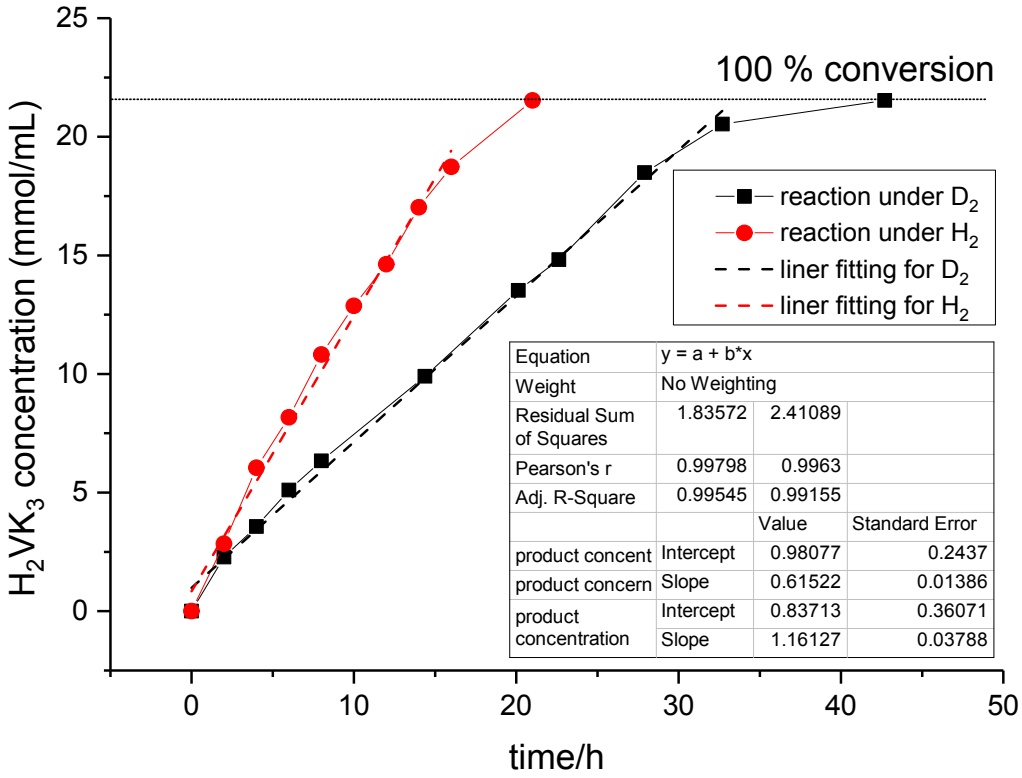
General procedure for the dehydrogenation of dihydrovitamin K_3 by 3(μ-H)H. Dihydrovitamin K_3 and **3(μ-H)H** were dissolved in 2 mL THF in a 50 mL two-necked round bottom flask, equipped with a reflux condenser. The solution was heated at 40 °C under Ar. After 3.5 h or 48 h, the conversion was determined according to the ratio of VK_3 to dihydrovitamin K_3 in ^1H NMR spectrum.

Dehydrogenation of VK_2 hydroquinone by 3(μ-H)H. 1 mg **3(μ-H)H** was added to the hydrogenation reaction mixture under Ar with stirring at 40 °C. After 40 h, 77.5 mg VK_2 hydroquinone was dehydrogenated to VK_2 and tautomerized VK_2. The TON is 24.

7 Mechanistic Studies

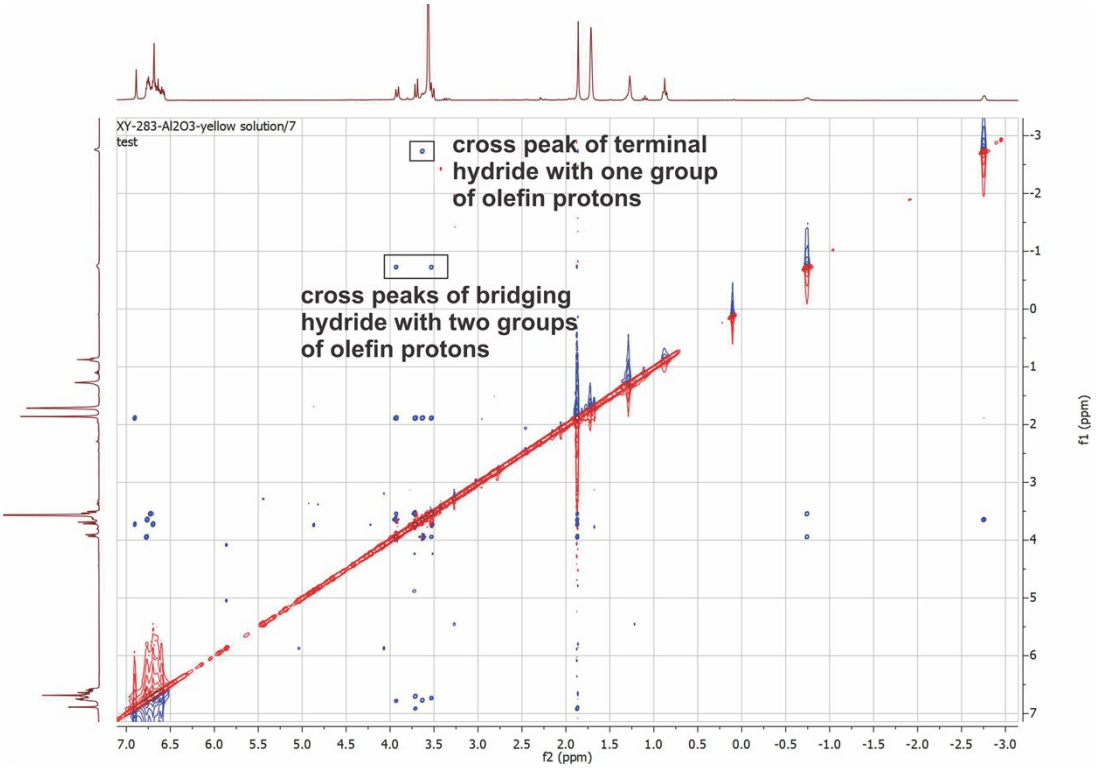
7.1 Isotope effect measurement

In a 2.7 mL J-Young NMR tube, 4.0 mg (5.7 µmol) of **3(µ-H)H** and 15.0 mg (86.1 µmol) of VK_3 were dissolved in 0.4 mL THF-d_8. The solution was degassed by freeze-pump-thaw for three times and placed under 1 bar H_2 or D_2 at room temperature. The reaction was heated at 40 °C. ^{1}H NMR spectra (number of scan: 64) were recorded at room temperature. Resonances of the methyl group in VK_3 and VK_3H_2 were integrated. The concentrations of VK_3H_2 were calculated from conversions. These reactions follow pseudo-zero-order kinetics. A linear fit was used to determine reaction constants (k_{obs}). The isotope effect was determined by using the ratio of the slopes of the zero order appearance of VK_3H_2. k_H/k_D = 1.9(2).



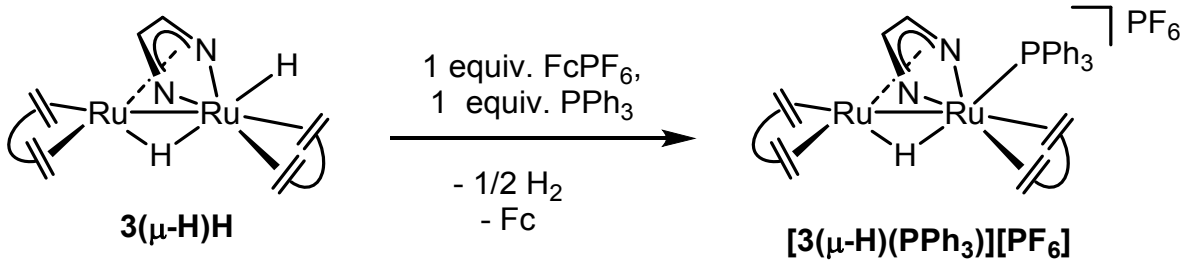
Supplementary Figure 4. Representative zero-order plot ([VK_3H_2] vs time) of **3(µ-H)H** catalyzed hydrogenation of VK_3 at 40 °C in THF-d_8. The lines in the figure are only lines connecting the data.

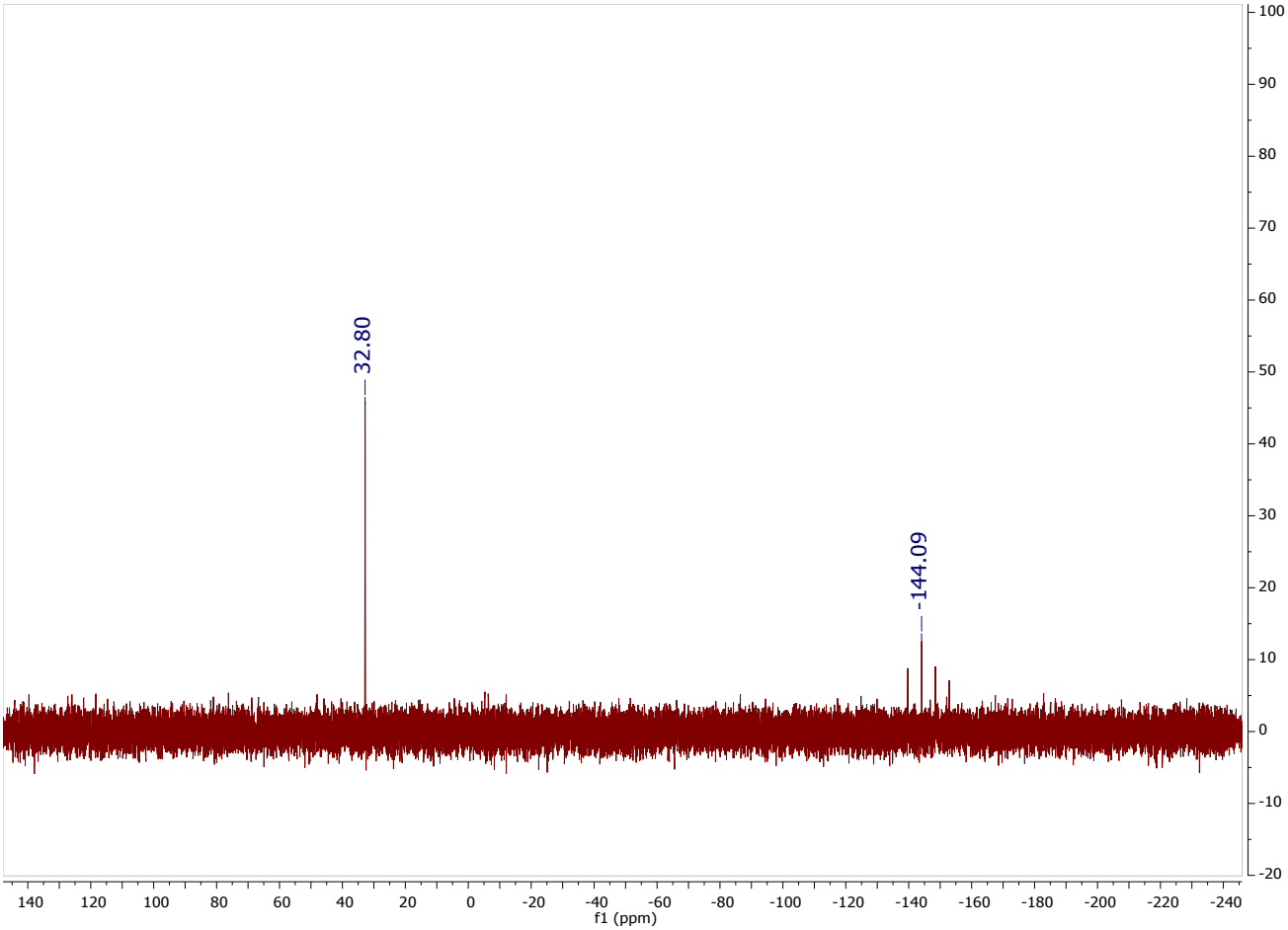
7.2 NMR



Supplementary Figure 5. NOESY spectrum of **3(μ-H)H** in THF-d_8.

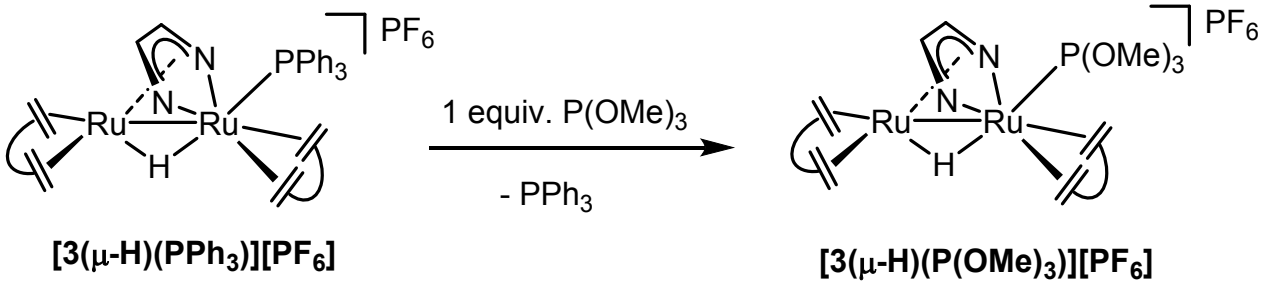
Equimolar reaction between 3(μ-H)H, PPh_3 and [Fc][PF_6] in the absence of H_2 . 5 mg of **3(μ-H)H ,** 2 mg of PPh_3, and 2.4 mg of [Fc][PF_6] were dissolved in 0.4 mL of THF-d_8 in a J-Young NMR tube. The reaction mixture was heated at 40 °C under Ar. After 0.5 h, a ^{31}P NMR spectrum was recorded showing **[3(μ-H)(PPh_3)][PF_6]** as only product (See Supplementary Fig. 6).



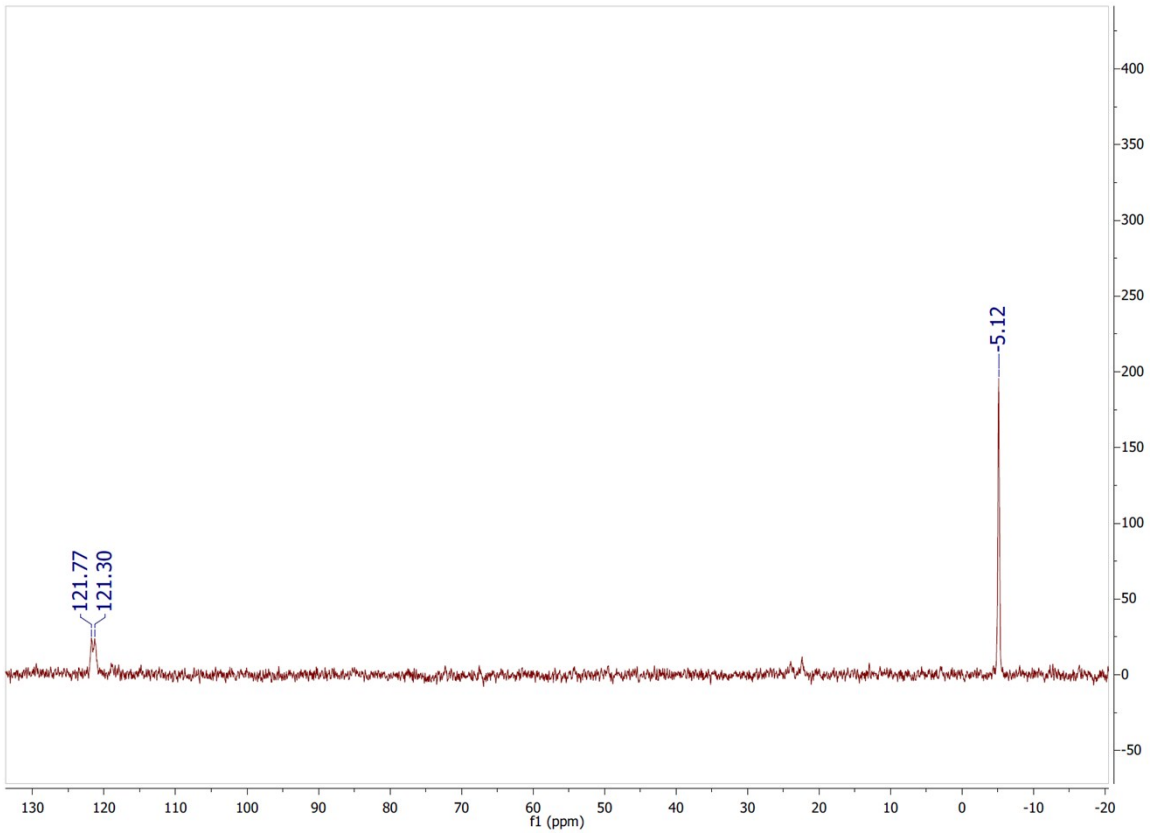


Supplementary Figure 6. The ^{31}P NMR spectrum of the reaction of **3(μ-H)H** with PPh_3 and [Fc][PF_6] (1:1:1) in THF-d_8.

Reaction between [3(μ-H)(PPh$_3$)][PF$_6$] and P(OMe)$_3$. 5 mg of **[3(μ-H)(PPh$_3$)][PF$_6$],** and 1μL of P(OMe)$_3$ were dissolved in 0.4 mL of THF-d_8 in a J-Young NMR tube. The reaction mixture was heated at 40 °C under Ar. After 10 h, a ^{31}P NMR spectrum was recorded showing free PPh$_3$ at -5 ppm and a bound P(OMe)$_3$ at 121 ppm (See Supplementary Fig. 7).

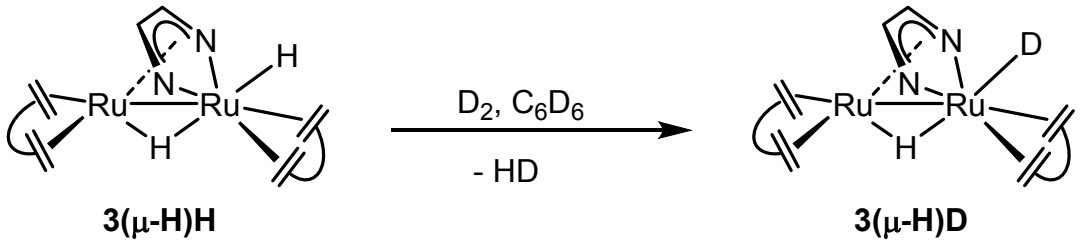


[3(μ-H)(PPh$_3$)][PF$_6$] **[3(μ-H)(P(OMe)$_3$)][PF$_6$]**

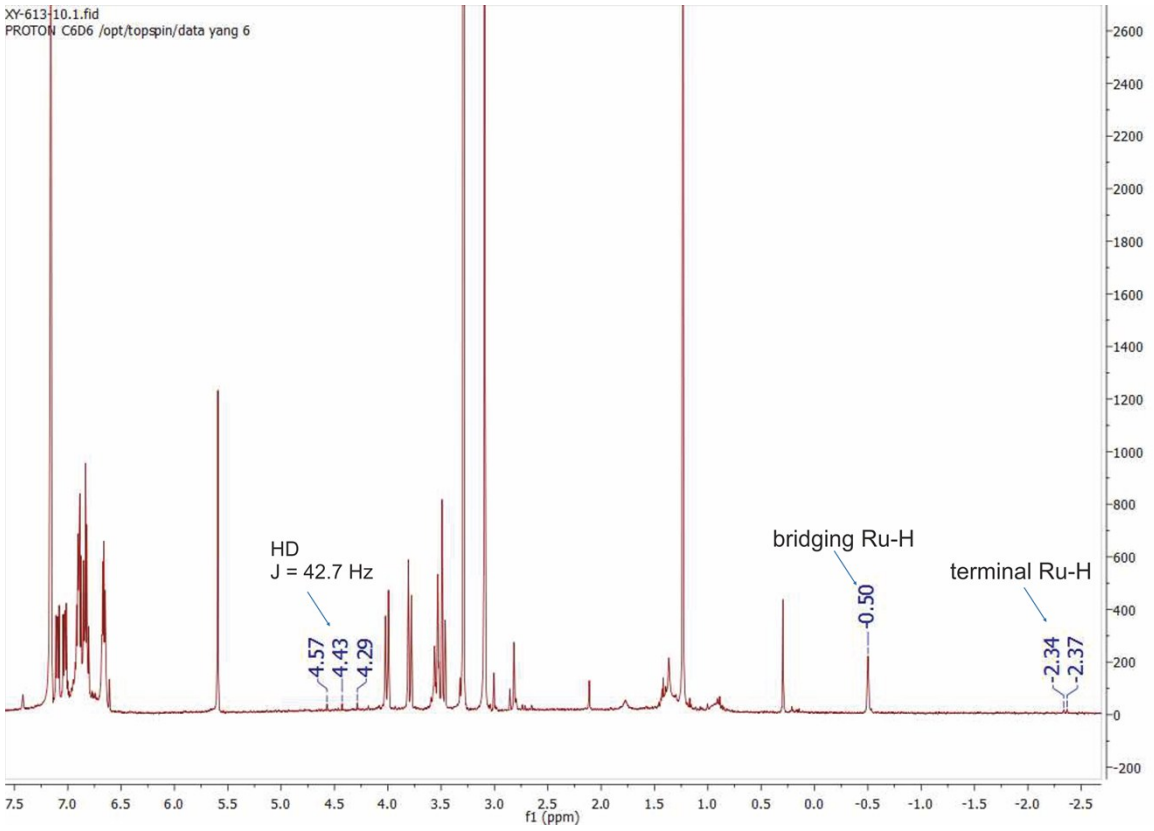


Supplementary Figure 7. The ^{31}P NMR spectrum of the reaction of **[3(μ-H)(PPh$_3$)][PF$_6$]** and P(OMe)$_3$ in THF-d_8.

D_2 experiment. No. 1: 5 mg **3(μ-H)H** dissolved in 0.4 mL of C_6D_6 was added to a J-Young NMR tube and 1 bar of D_2 was introduced at room temperature. After 14 h at room temperature, the ^1H NMR spectrum was recorded (See Supplementary Fig. 8).

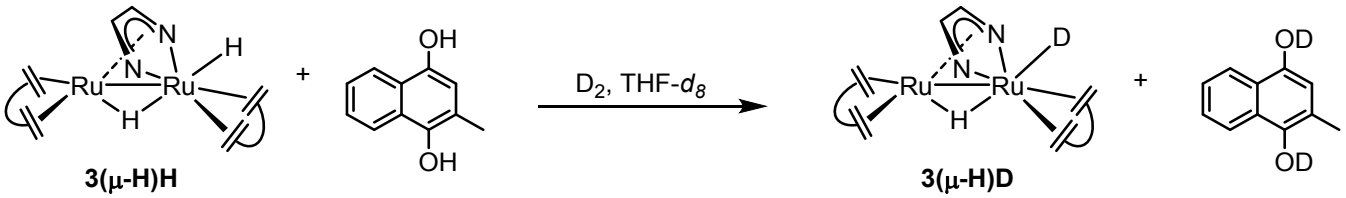


3(μ-H)H **3(μ-H)D**

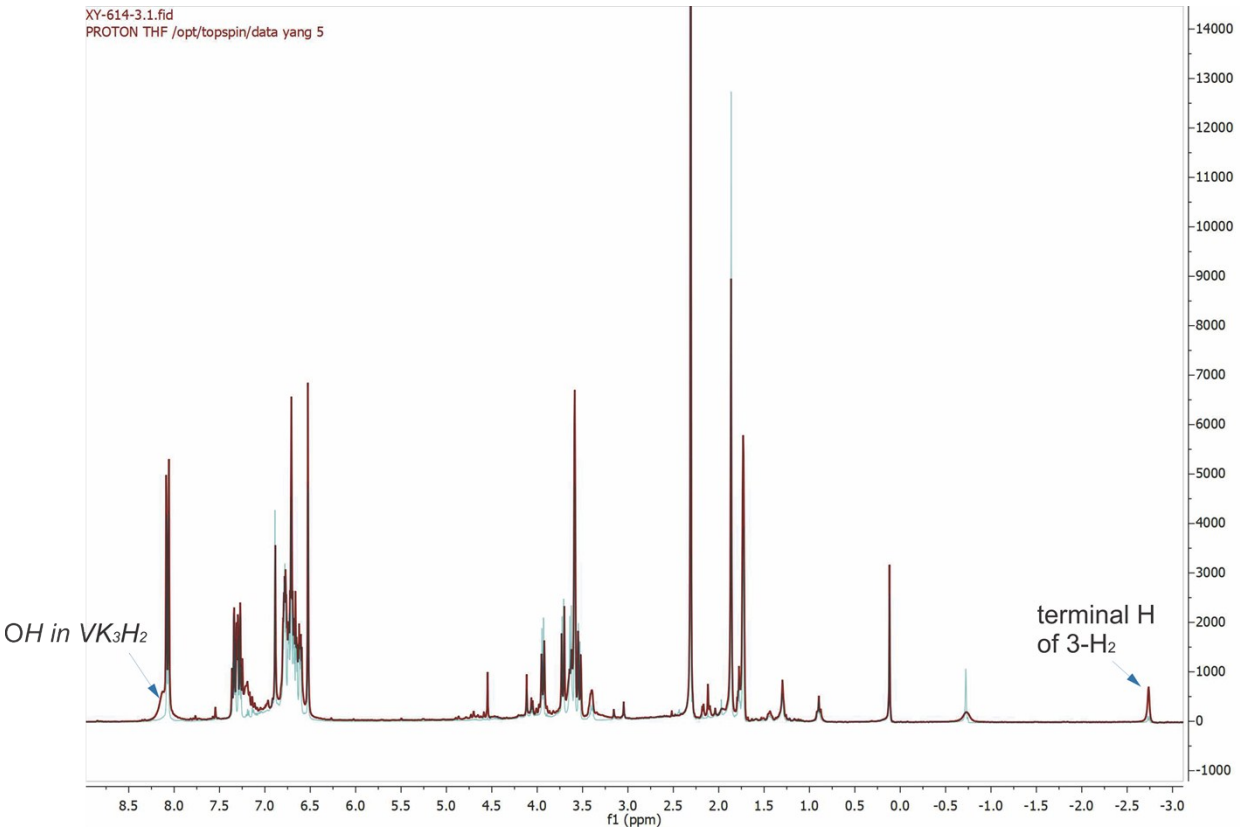


Supplementary Figure 8. ^1H NMR spectrum of $Ru_2D(\mu\text{-}H)(Me_2dad)(dbcot)_2$ in C_6D_6.

D_2 experiment. No. 2: 10 mg **3(μ-H)H** and 2.5 mg of VK_3H_2 were dissolved in 0.4 mL of THF-d_8 was added to a J-Young NMR tube and 1 bar of D_2 was introduced at room temperature. After 14 h at 40 °C, the ^{1}H NMR spectrum was recorded (See Supplementary Fig. 9).

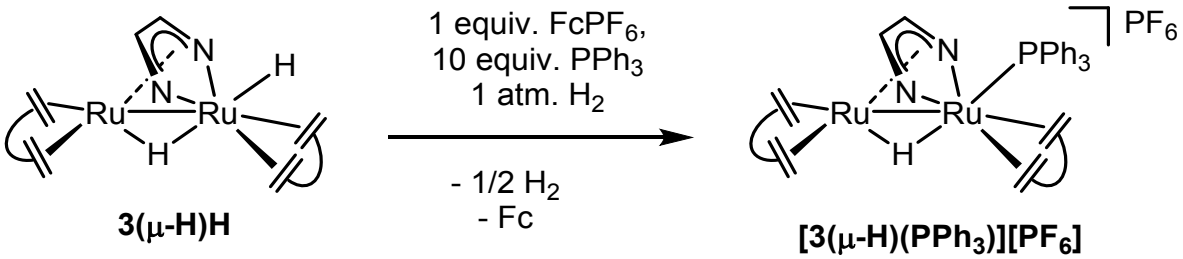


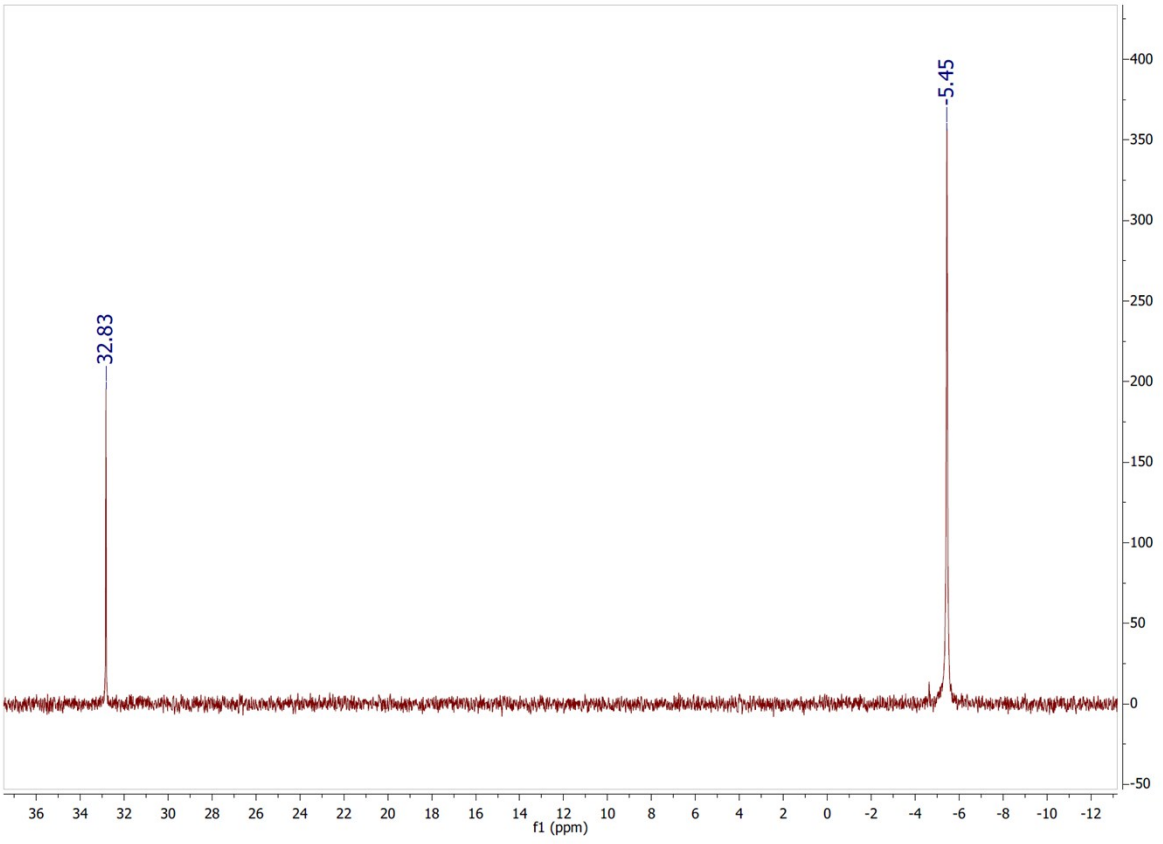
3(μ-H)H **3(μ-H)D**



Supplementary Figure 9. ^{1}H NMR spectra of **3(μ-H)H** and VK_3H_2 (red) vs $Ru_2D(\mu\text{-}H)(Me_2dad)(dbcot)_2$ and VK_3D_2 (green) in THF-d_8.

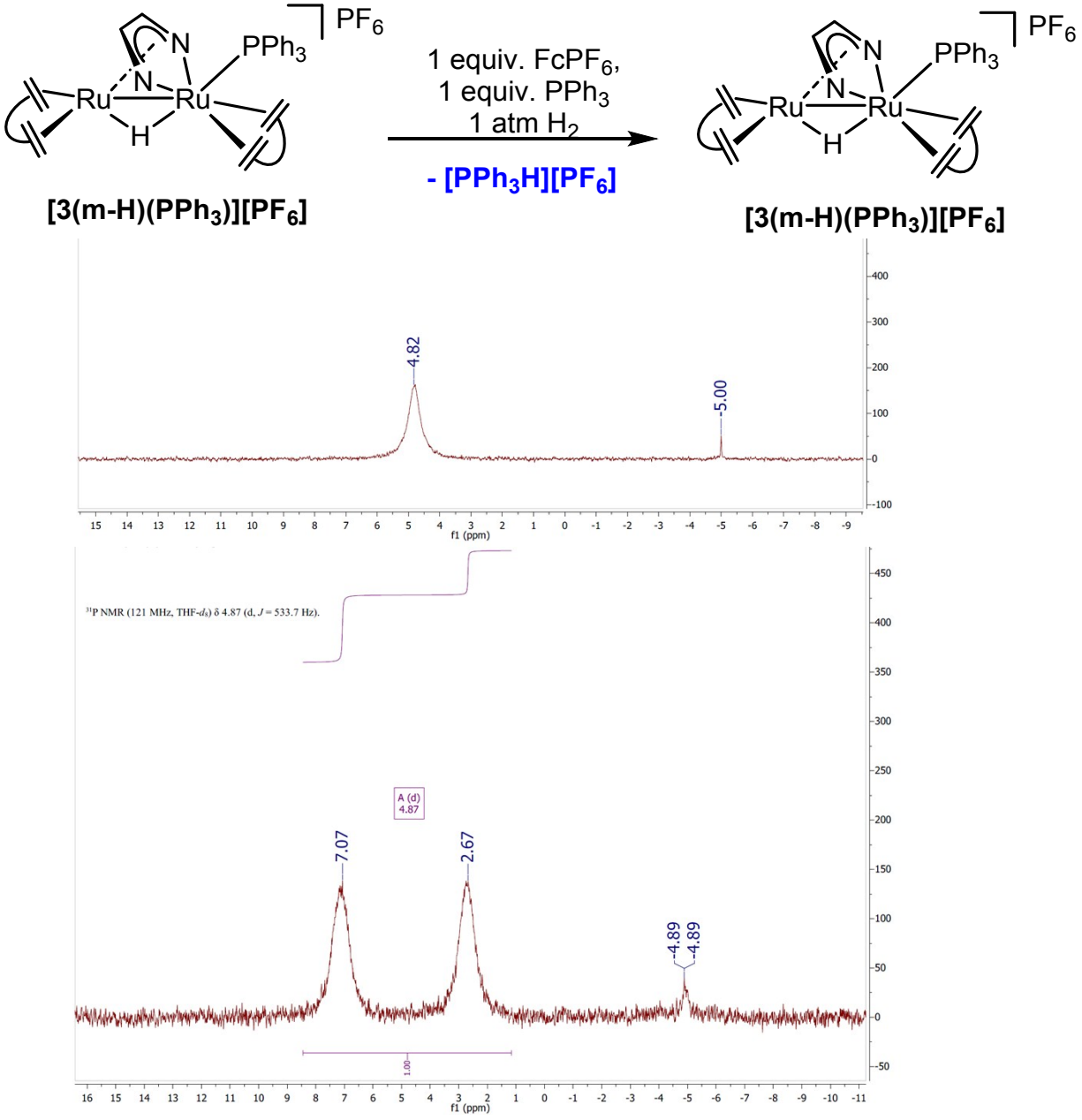
Reaction between 3(μ-H)H, 10 eq. of PPh_3 and 1 eq. of [Fc][PF_6] in the presence of H_2 . 5 mg of **3(μ-H)H,** 12 mg of PPh_3, and 1.5 mg of **[Fc][PF_6]** were mixed in 0.4 mL of THF-d_8 in a J-Young NMR tube. The tube was charged with 1 bar of H_2 and heated at 40 °C. After 2 h, a ^{31}P NMR spectrum was recorded showing the formation of **[3(μ-H)(PPh_3)][PF_6],** free PPh_3 and no [PPh_3H][PF_6] (See Supplementary Fig. 10).





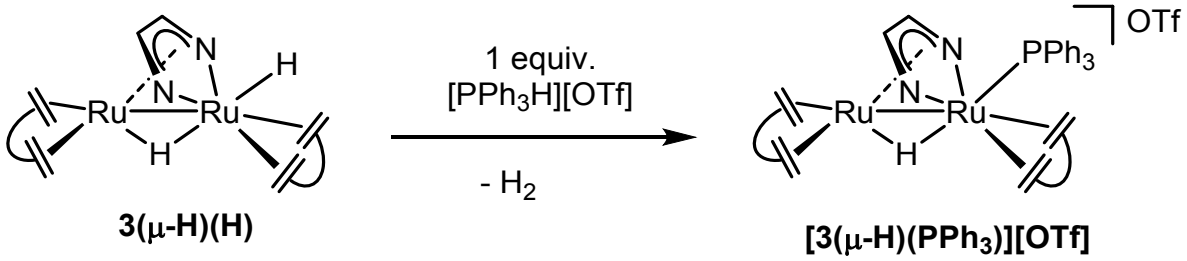
Supplementary Figure 10. The ^{31}P NMR spectrum of the reaction of **3(μ-H)H** with PPh_3 and [Fc][PF_6] (1:10:1) in THF-d_8.

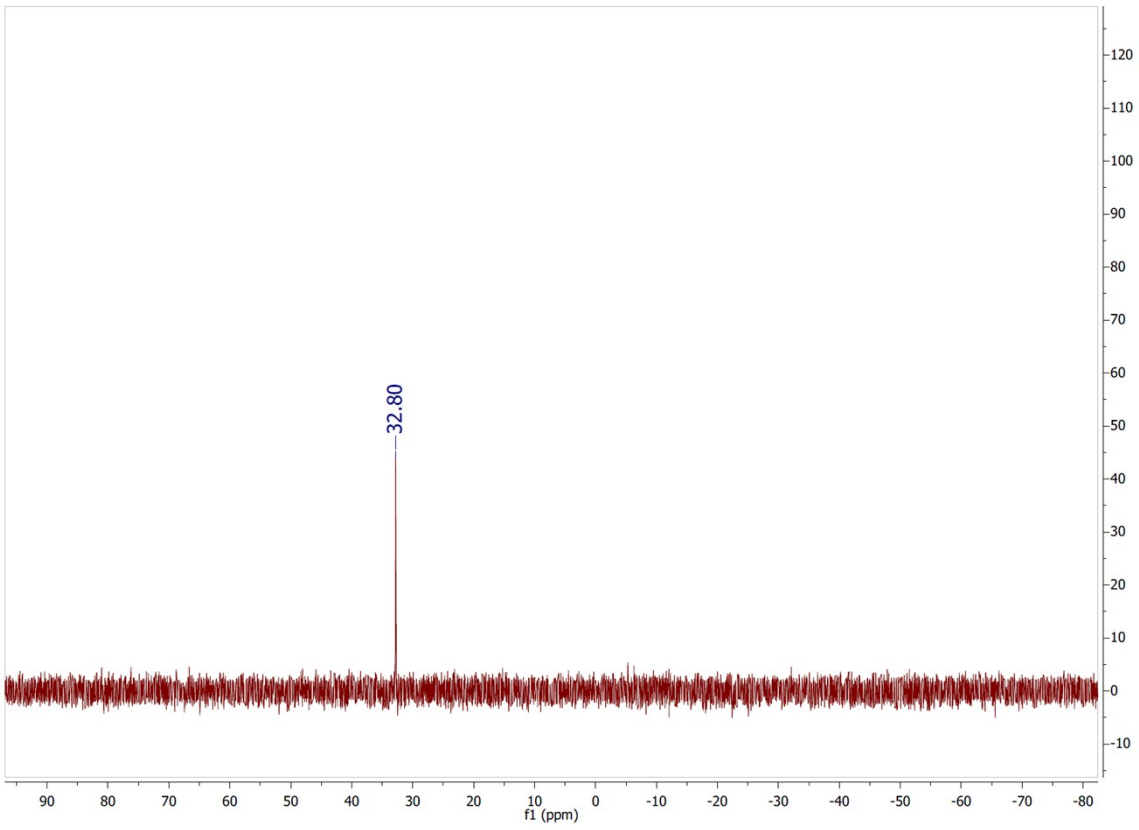
Reaction between [3(μ-H)(PPh$_3$)][PF$_6$], 1 eq. of PPh$_3$ and 1 eq. of [Fc][PF$_6$] in the presence of H$_2$. 5 mg of **[3(μ-H)(PPh$_3$)][PF$_6$],** 1.2 mg of PPh$_3$, and 1.5 mg of **[Fc][PF$_6$]** were mixed in 0.4 mL of THF-d_8 in a J-Young NMR tube. The tube was charged with 1 bar of H$_2$ and heated at 40 °C. After 2 h, a ^{31}P NMR spectrum was recorded showing **[PPh$_3$H]$^+$** (See Supplementary Fig. 11).



Supplementary Figure 11. The ^{31}P{^{1}H} NMR (top) and ^{31}P NMR (bottom) spectra of H$_2$ splitting by **[3(μ-H)(PPh$_3$)][PF$_6$]** in the presence of PPh$_3$ and 1 eq. of [Fc][PF$_6$] under H$_2$ in THF-d_8

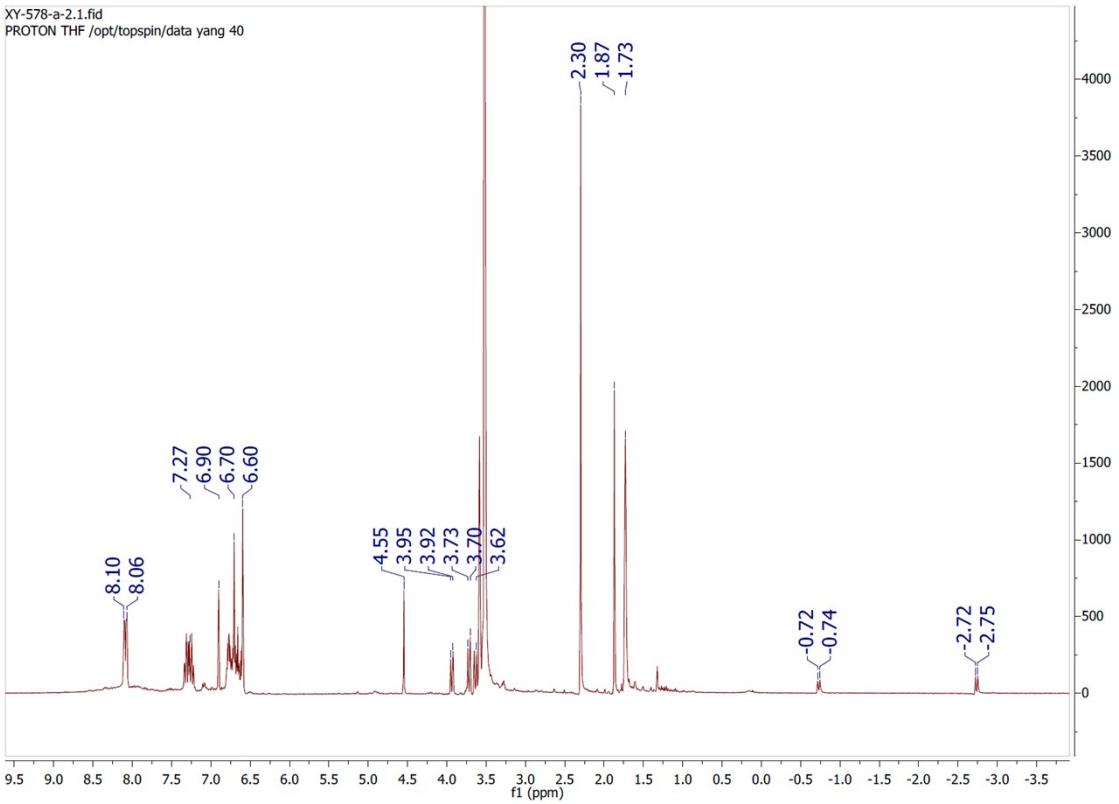
Reaction between 3(μ-H)H, 1 eq. of [PPh$_3$H][OTf]. 5 mg of **3(μ-H)H** and 3 mg of [PPh$_3$H][OTf] were mixed in 0.4 mL of THF in a J-Young NMR tube. The tube was heated at 40 °C. After 2 h, a ^{31}P NMR spectrum was recorded showing the formation of **[3(μ-H)(PPh$_3$)][OTf]** (See Supplementary Fig. 12).





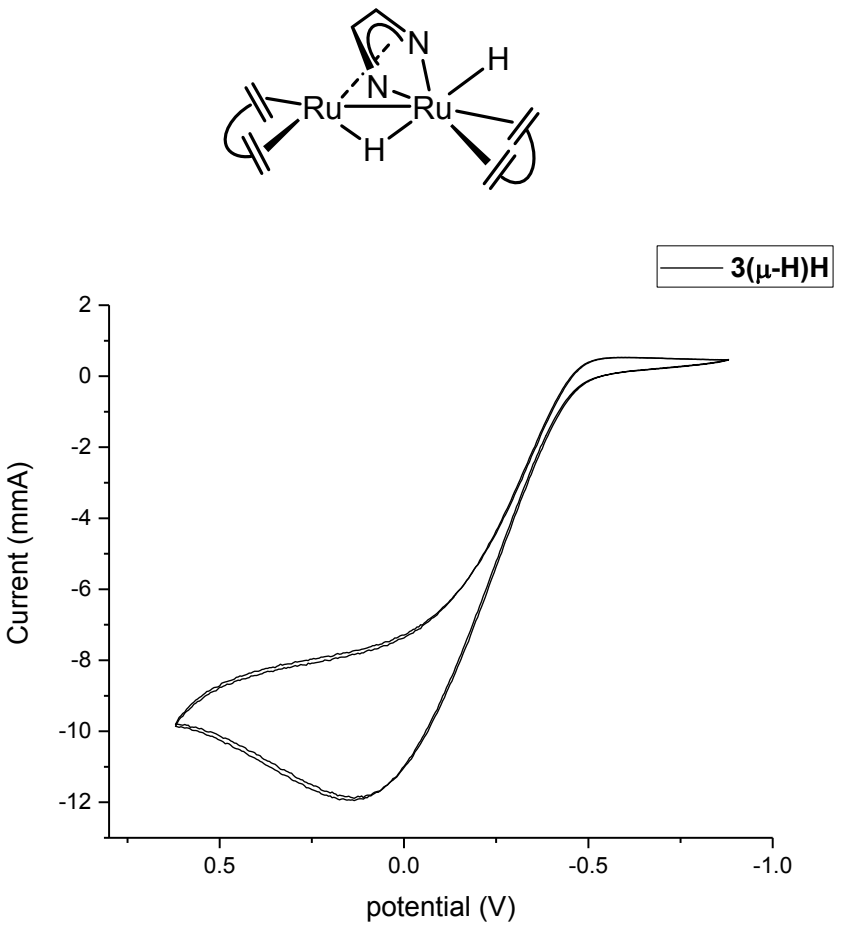
Supplementary Figure 12. The ^{31}P NMR spectrum of the reaction of **3(μ-H)H** with [PPh$_3$H][OTf] in THF.

Single turnover experiment for VK_3 . 4 mg of **3(μ-H)H,** and 1 mg of VK_3 were dissolved in 0.4 mL of THF-d_8 in a J-Young NMR tube. The tube was charged with 1 bar of H_2 and heated at 40 °C. After 2 h, one ^{1}H NMR spectrum was recorded showing the formation of VK_3H_2 and regeneration of **3(μ-H)H** as only organometallic species (See Supplementary Fig. 10).



Supplementary Figure 13. The ^{1}H NMR spectrum of hydrogenation of VK_3 by **3(μ-H)H** after the first turnover experiment in THF-d_8.

7.3 Cyclic voltammetry of 3(μ-H)H

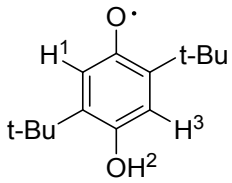


Supplementary Figure 14. Cyclic voltammetry of complex **3(μ-H)H** in 0.1 M solution of $[nBu_4N][PF_6]$ in THF vs. Fc/Fc+ at a scan rate of 50 mV/s; working electrode: glassy carbon; counter electrode: Pt; reference electrode: Ag. No other oxidation of reduction events were observed outside the [1,-1]V window.

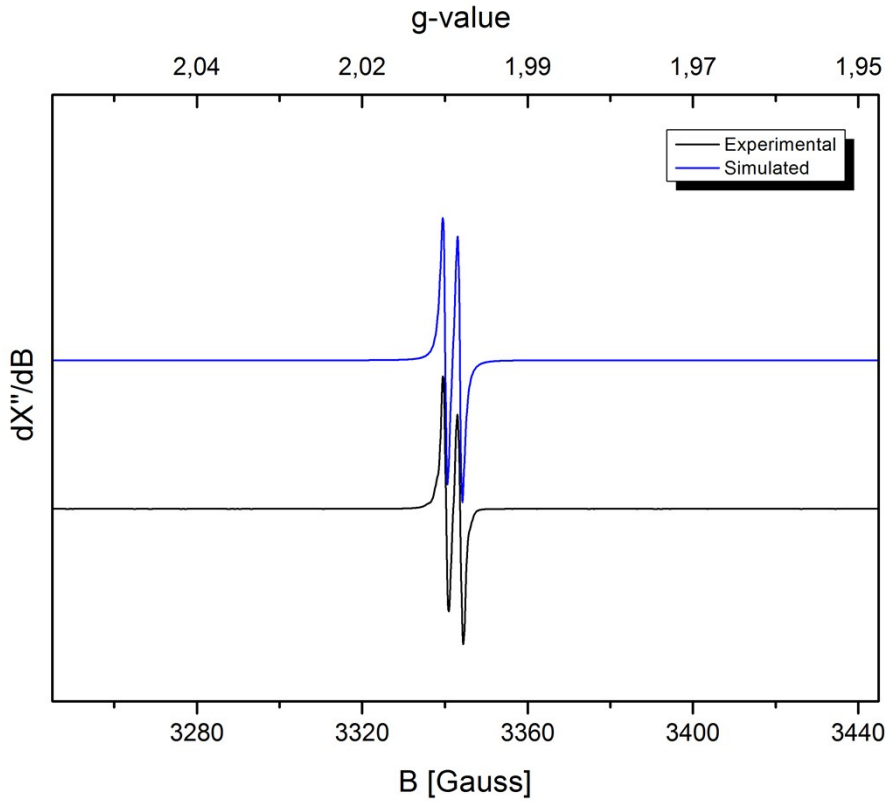
7.4 EPR data

In the protonated semiquinone, coupling with one aromatic proton (H^1) and the hydroxyl proton (H^2) is expected to be small (calculated: A^{H1}_{iso} = 4.6 Hz and A^{H2}_{iso} = 6.3 Hz), while coupling with the remaining aromatic proton (H^3) is expected to be significantly larger (calculated: A^{H3}_{iso} = –16.0 Hz at g_{iso} = 2.005). Hence, the observed and calculated g_{iso} and A_{iso} are in agreement with the formation of the neutral protonated semiquinone. Moreover, the formation of the anionic semiquinone would afford a triplet signal, due to coupling with the two symmetrical aromatic protons. EPR analysis of this reaction mixture at 20 K resulted in the loss of resolved hyperfine coupling. This can be a result of *g*-anisotropy or close-contact with a ruthenium centered radical in the frozen solution.

Supplementary Table 4. Experimental (simulated) and DFT calculated EPR parameters of the protonated semiquinone. [a] ORCA, B3LYP, TZVP.



	Simulated	DFT[a]
	g Tensor	
g_{iso}	2.005	2.005
	Hyperfine Coupling	
A^{H1}_{iso}	Not resolved	4.6
A^{H1}_{iso}	Not resolved	-6.3
A^{H1}_{iso}	-10.0	-16.0



Supplementary Figure 15. Experimental and simulated isotropic EPR spectrum of a mixture of 3(μ-H)H and 2,5-di-tertbutyl-p-benzoquinone in MeTHF at room temperature. Microwave frequency, 9.379153 GHz; microwave power: 0.6325 mW; modulation amplitude, 1.000 G.

XYZ coordinates of the optimised protonated semiquinone.

C	-0.0022550	-0.0028084	1.0126544
C	0.0000542	0.0005974	3.8343890
C	-0.0009336	-1.2831002	1.7392091
C	-0.0017925	1.2185042	1.8016126
C	-0.0004141	1.2723131	3.1801757
C	0.0001990	-1.2164603	3.1158266
H	-0.0023658	2.1251555	1.1990775
H	0.0009161	-2.1188825	3.7263972
O	-0.0035066	0.0792854	-0.2451285
O	0.0007597	-0.1590957	5.1884506

H	-0.0045522	0.7129522	5.6218670
C	-0.0009042	-2.6064228	0.9787675
C	0.0012500	2.6037420	3.9533998
C	-1.2670776	-2.6864571	0.0903481
H	-1.2872483	-1.8674316	-0.6367453
H	-2.1769481	-2.6367370	0.7066438
H	-1.2756152	-3.6434284	-0.4529607
C	1.2643147	-2.6853096	0.0891262
H	1.2823233	-1.8670923	-0.6391226
H	1.2741560	-3.6429621	-0.4530273
H	2.1749366	-2.6327954	0.7042487
C	-0.0000991	-3.8195205	1.9250269
H	0.8931920	-3.8412197	2.5670545
H	-0.0000872	-4.7427021	1.3284220
H	-0.8929453	-3.8415631	2.5676531
C	-0.0009658	3.8120998	2.9985599
H	0.8877483	3.8228924	2.3526242
H	0.0027784	4.7402195	3.5875142
H	-0.8945383	3.8253637	2.3593525
C	1.2780939	2.7197275	4.8228950
H	2.1748892	2.6734354	4.1898985
H	1.3837393	1.9268717	5.5783691
H	1.2824704	3.6796807	5.3593791
C	-1.2716723	2.7203916	4.8286573
H	-1.3663761	1.9373141	5.5960838
H	-2.1721360	2.6585016	4.2020660
H	-1.2803879	3.6869408	5.3532349

8 DFT calculations

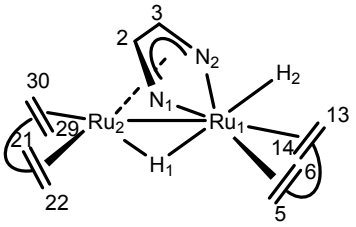
8.1 Computational details

All structures and energies were calculated using the Gaussian09 suite of programs.[S12] Self-consistent field computations were performed with tight convergence criteria on ultrafine grids, while geometry optimizations were converged to tight geometric convergence criteria for all compounds. Spin expectation values $<S>^2$ indicated that spin contamination was not significant in any result. Frequencies were calculated analytically at 298.15 K and 1 atm. Structures were considered true minima if they did not exhibit imaginary vibration modes.

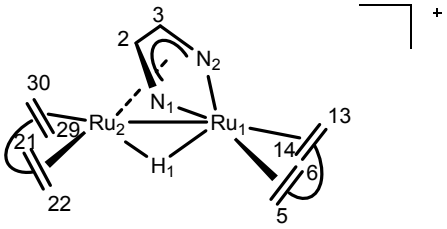
The geometry of all intermediates was optimized without structural simplification using the pure functional pure functionals PBE[S13], the light atoms (H, C, N, O and P) were treated with Pople's 6-31G(d) double-ζ split-valence basis,[S14] while the ruthenium atom was treated with a Stuttgart/Dresden ECPs pseudopotential (SDD).[S15] Frequency calculations of all species were also performed under the same conditions as described above. Thermochemical corrections were obtained at 298.15 K on the basis of frequency calculations. The influence of the solvent was taking in consideration through single-point calculation on the gas-phase optimized geometry using THF as conductor-like polarizable continuum solvent model (CPCM), employing larger basis sets (Def2-TZVP for H, C, N, O, P and SDD Def2-TZVP for Ru).[S16] Influence of the dispersion forces was considered by adding to the SCF-CPCM energy the D3(BJ) corrections as described by Grimme.[S17] The Gibbs free energies reported are obtained by summing the SCF-CPCM energy, the gas-phase Gibbs contribution at 298 K, and the D3(BJ) correction. (Free Gibbs energy = E(pcm+D3(bj)) + G(298 K) with E(pcm+D3(bj)) calculated using PBE/(6-311G++(2d,p) for H, C, N, O, P; SDD Def2-TZVP for Ru), G(298 K) using PBE/(6-31G(d,p) for H, C, N, O, P; SDD for Ru).

8.2 Results

8.2.1 Geometry comparison



3(μ-H)H



3(μ-H)$^+$

Supplementary Table 5. Metric Comparison between the X-ray structures and optimized structures for 3(μ-H)H and 3(μ-H)$^+$

	Distances in Å and angles in ^{o} for 3(μ-H)H	
	X-ray	PBE
Ru1-Ru2	2.739	2.77
Ru1-N1	2.088	2.12
Ru1-N2	2.095	2.12
Ru2-N1	2.182	2.23
Ru2-N2	2.171	2.23
Ru2-C2	2.224	2.26
Ru2-C3	2.229	2.26
Ru1-C5/14 av	2.153	2.15
Ru1-C6/13 av	2.141	2.15
Ru2-C22/29av	2.150	2.14
Ru2-C21/30av	2.147	2.14
C2-C3	1.400	1.41
N1-C2	1.379	1.39
C3-N2	1.371	1.39
C5-C6	1.426	1.44
C13-C14	1.420	1.44
C21-C22	1.427	1.45
C29-C30	1.430	1.45
N1-Ru1-N2	75.5	75.7
N1-Ru2-N2	72.0	71.3
C6-Ru1-C13	81.1	80.5
C21-Ru2-C30	81.3	80.9
Ru1-N1-Ru2	79.8	78.8
Ru1-N2-Ru2	79.9	78.8
Ru1-Ru2-N1	48.6	48.8
Ru2-Ru1-N1	51.3	52.4

	Distances in Å and angles in ^{o} for 3(μ-H)$^+$	
	X-ray	PBE
Ru1-Ru2	2.689	2.77
Ru1-N1	2.136	2.15
Ru1-N2	2.116	2.15
Ru2-N1	2.150	2.20
Ru2-N2	2.152	2.20
Ru2-C2	2.245	2.25
Ru2-C3	2.256	2.25
Ru1-C5/14 av	2.125	2.16
Ru1-C6/13 av	2.140	2.21
Ru2-C22/29av	2.114	2.14
Ru2-C21/30av	2.120	2.17
C2-C3	1.400	1.43
N1-C2	1.371	1.37
C3-N2	1.368	1.37
C5-C6	1.395	1.42
C13-C14	1.411	1.42
C21-C22	1.437	1.44
C29-C30	1.419	1.44
N1-Ru1-N2	75.3	76.1
N1-Ru2-N2	71.1	73.9
C6-Ru1-C13	80.8	80.5
C21-Ru2-C30	80.2	80.9
Ru1-N1-Ru2	77.9	79.0
Ru1-N2-Ru2	78.2	79.0
Ru1-Ru2-N1	49.0	49.6
Ru2-Ru1-N1	52.3	51.4

8.2.2 Activation of H_2 with PPh_3

Supplementary Table 6. The relative free energies of key transition states (kcal/mol) in figure 7 calculated in THF.

	PBE		
	G (298)	E (SCF)	G (TOT)
	Hartree	Hartree	Kcal/mol
$[3(\mu\text{-H})]^+$	0.50851	-1689.782515	-1060035.7
$[3(\mu\text{-H})(H_2)]^+$	0.526467	-1690.973671	-1060771.9
$[3(\mu\text{-H})(PPh_3)]^+$	0.7604	-2725.394137	-1709733.8
T.S-1	0.522495	-1690.9390594	-1060752.6
T.S-2	0.520829	-1690.889656	-1060722.7
T.S-3	0.525863	-1690.968122	-1060768.8
$[3(\mu\text{-H})(H_2]_a^+$	0.528962	-1690.950108	-1060755.5
$[3(\mu\text{-H})(H_2]_b^+$	0.52907	-1690.961340	-1060762.5
[3(μ-H)H]	0.518533	-1690.555699	-1060514.6
H_2	-0.001553	-1.166128	-732.7
PPh_3	0.219269	-1035.543479	-649675.9
$[PPh_3H]^+$	0.228573	-1035.9752614	-649941.0

8.2.3 Activation of H_2 with VK_3

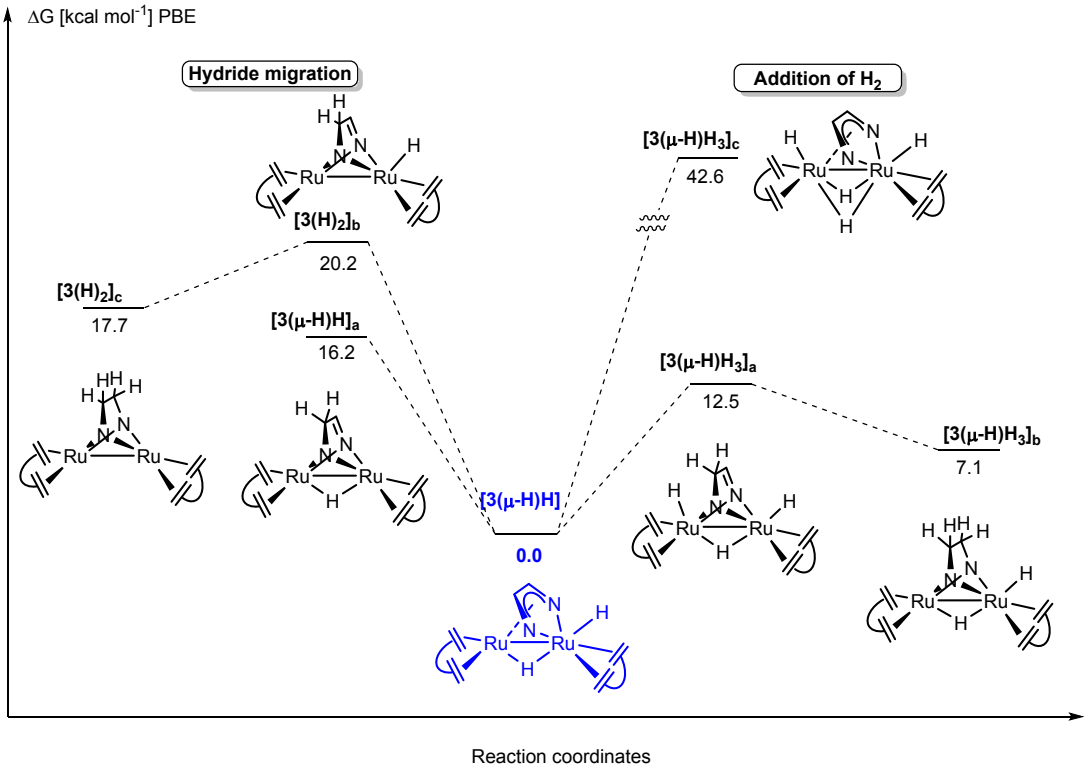
Supplementary Table 7. The relative free energies of key transition states (kcal/mol) in figure 8 calculated in THF.

	PBE		
	G (298)	E (SCF)	G (TOT)
	Hartree	Hartree	Kcal/mol
$[3(\mu\text{-H})]^+$	0.50851	-1689.782515	-1060035.7
$[3(\mu\text{-H})(VK_3H)]$	0.661747	-2264.58103	-1420631.1
T.S-4	0.671711	-2265.707863	-1421331.9
T.S-5	0.675675	-2265.695003	-1421321.4
$[3(\mu\text{-H})(H)_2(VK_3H)]$	0.683225	-2265.731501	-1421339.6
[3(μ-H)H]	0.518533	-1690.555699	-1060514.6
VK_3H_2	0.141608	-575.201262	-360855.4
VK_3H^-	0.127365	-574.710817	-360556.6
H_2	-0.001553	-1.166128	-732.7

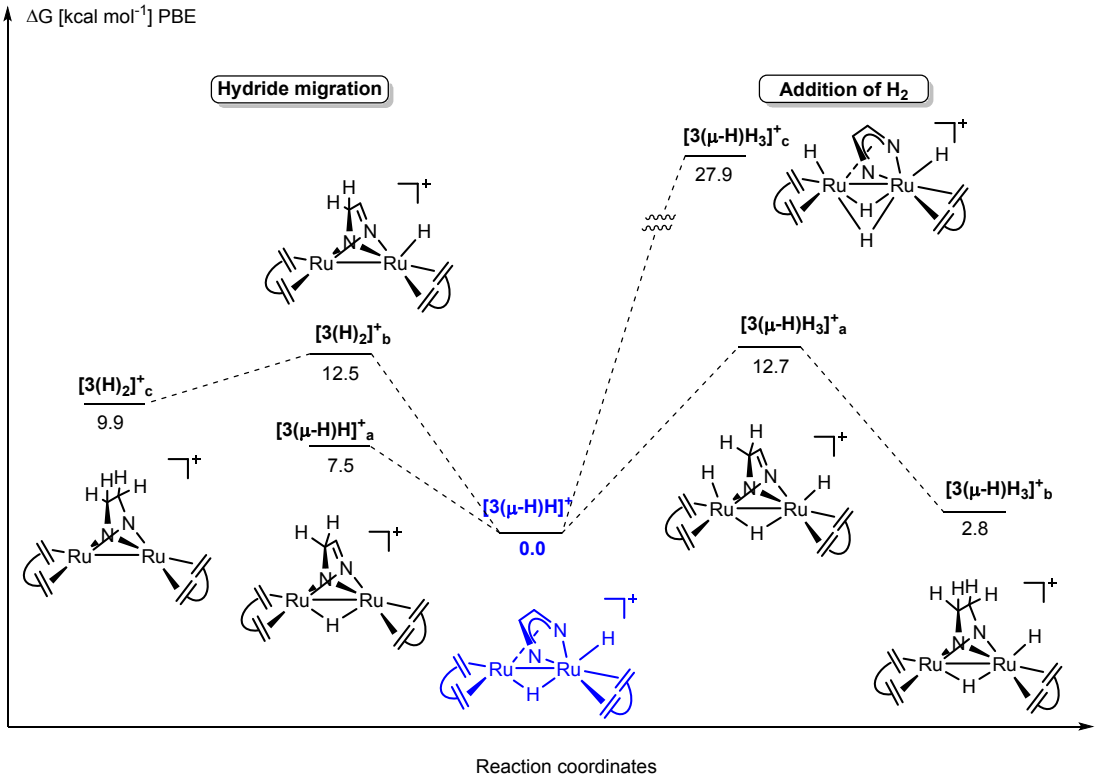
8.2.4 Ligand hydrogenation

Supplementary Table 8. The relative free energies of key transition states (kcal/mol) in supplementary figure 16 and 17 calculated in THF.

	PBE		
	G (298)	E (SCF)	G (TOT)
	Hartree	Hartree	Kcal/mol
[3(μ-H)H]	0.518533	-1690.555699	-1060514.6
$[3(\mu\text{-H})H]^+$	0.5157	-1690.363316	-1060395.7
$[3(\mu\text{-H})H]_a$	0.518636	-1690.530030	-1060498.4
$[3(\mu\text{-H})H]_a^+$	0.519264	-1690.355008	-1060388.2
$[3(H)_2]_b$	0.519664	-1690.524685	-1060494.4
$[3(H)_2]_b^+$	0.519686	-1690.347393	-1060383.1
$[3(H)_2]_c$	0.522292	-1690.531220	-1060496.8
$[3(H)_2]_c^+$	0.52342	-1690.355212	-1060385.7
$[3(\mu\text{-H})H_3]_a$	0.537918	-1691.722930	-1061234.8
$[3(\mu\text{-H})H_3]_a^+$	0.536317	-1691.531364	-1061115.6
$[3(\mu\text{-H})H_3]_b$	0.539016	-1691.732554	-1061240.2
$[3(\mu\text{-H})H_3]_b^+$	0.539526	-1691.550318	-1061125.5
$[3(\mu\text{-H})H_3]_c$	0.53	-1691.661257	-1061201.1
$[3(\mu\text{-H})H_3]_c^+$	0.528779	-1691.499649	-1061100.5
$[3(\mu\text{-H})]^+$	0.50851	-1689.782515	-1060035.7
H_2	-0.001553	-1.166128	-732.7

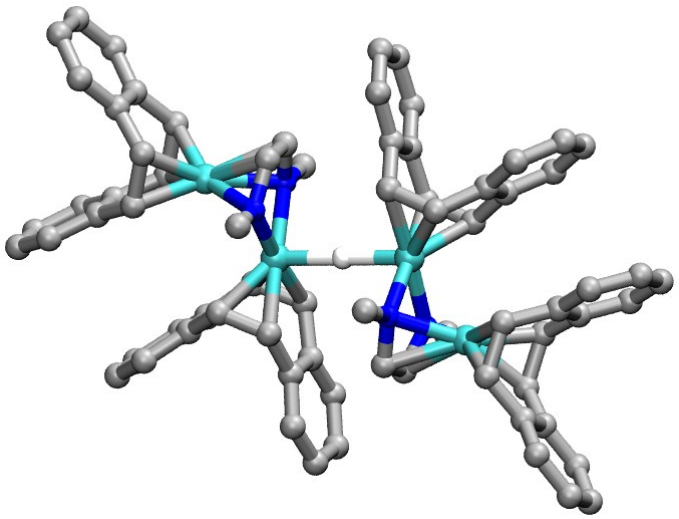


Supplementary Figure 16. Calculated energy profiles for the hydrogenation of **3(μ-H)H**.



Supplementary Figure 17. Calculated energy profiles for the hydrogenation of **[3(μ-H)H]**$^{+}$.

8.2.5 **Optimized Structure of** complex **[K][3$_2$(μ-H)]**



Supplementary Figure 18. Optimized structure of **[K][3$_2$(μ-H)]** supporting the presence of linear bridged hydride. All hydrogen atoms, but the bridged hydride, were omitted for clarity.

8.3 PBE/(6-31G(d,p)/SDD) optimized structures Cartesian coordinates in Angstrom

H_2

H	-5.51483000	0.14320600	-2.40173200
H	-6.26492200	0.14320600	-2.40173200

PPh_3

P	-3.56809400	0.02254400	-0.08791800
C	-2.68599700	-1.61083600	-0.12932000
C	-3.27072400	-2.67227700	0.59611300
C	-1.50264300	-1.85775700	-0.85552900
C	-2.67470600	-3.94156600	0.61593500
H	-4.20182100	-2.50053100	1.14797100
C	-0.91413700	-3.13275400	-0.84678600
H	-1.04013700	-1.05062900	-1.43219700
C	-1.49465800	-4.17598200	-0.10881900
H	-3.13906200	-4.75119500	1.18795700
H	0.00305300	-3.30890800	-1.41821000
H	-1.03411800	-5.16884500	-0.10371700
C	-2.74023800	0.94655000	-1.46964100
C	-1.63271800	1.80363800	-1.30359900
C	-3.28951200	0.79053800	-2.76144700
C	-1.08284100	2.47901800	-2.40527700
H	-1.19970100	1.94619400	-0.30854800
C	-2.73105700	1.45414700	-3.86336700
H	-4.16361600	0.14466700	-2.90206200
C	-1.62638300	2.30351400	-3.68732200
H	-0.22419200	3.14250100	-2.25931700
H	-3.16688800	1.31740900	-4.85820300
H	-1.19608700	2.83104900	-4.54432600
C	-2.83108700	0.82631700	1.41485300
C	-3.43344500	2.02395400	1.86142200
C	-1.75248900	0.29628500	2.15239600
C	-2.95362800	2.68768300	2.99930400
H	-4.28638800	2.43784400	1.31156900
C	-1.28327200	0.95332200	3.30180300
H	-1.27694200	-0.63503100	1.82975500
C	-1.87764100	2.15142500	3.72607200
H	-3.42928900	3.61783600	3.32630900
H	-0.44662700	0.52638300	3.86443400
H	-1.50983200	2.66183100	4.62163200

$[PPh_3H]^+$

C	-2.53971600	-1.67307500	-0.11501300
C	-3.16082200	-2.62562800	0.72312200
C	-1.46607500	-2.04052600	-0.95214100
C	-2.69848200	-3.94723700	0.71960500
H	-3.99607900	-2.34351200	1.37280500

C	-1.01214300	-3.36736100	-0.94197600
H	-0.99439800	-1.30362200	-1.60912900
C	-1.62605100	-4.31658300	-0.11033600
H	-3.17926800	-4.68998800	1.36203900
H	-0.18094700	-3.65857000	-1.58994300
H	-1.27135900	-5.35116800	-0.11111300
C	-2.57716800	0.97740400	-1.52364300
C	-1.51056700	1.89320400	-1.40934000
C	-3.21443300	0.76218300	-2.76559400
C	-1.08016300	2.58926100	-2.54781600
H	-1.02810900	2.06867600	-0.44302600
C	-2.77569600	1.46763500	-3.89301100
H	-4.04529600	0.05457100	-2.85608200
C	-1.71061800	2.37783700	-3.78406000
H	-0.25530700	3.30224700	-2.46532100
H	-3.26980900	1.31025400	-4.85563200
H	-1.37488300	2.92885700	-4.66715800
C	-2.71212300	0.86741200	1.47044400
C	-3.45385300	2.00721100	1.85214600
C	-1.64447300	0.40208800	2.26609800
C	-3.11834500	2.68048800	3.03310400
H	-4.28532200	2.36903800	1.23805400
C	-1.31856900	1.08882100	3.44457700
H	-1.08054700	-0.48947400	1.97550300
C	-2.05226400	2.22293100	3.82615800
H	-3.69311700	3.55966600	3.33678600
H	-0.49333300	0.73188200	4.06680300
H	-1.79650600	2.75075200	4.74929800
P	-3.12677400	0.03704000	-0.08077900
H	-4.54409400	-0.00917200	-0.14890900

VK_3H^-

C	-1.82723400	7.99907900	4.66771400
C	-0.43683800	7.99129300	4.70477100
C	0.31099400	9.20945700	4.63873400
C	-0.41383000	10.45867100	4.53619900
C	-1.82598500	10.42348500	4.50115000
C	-2.53754900	9.22482100	4.56382500
H	-2.37623500	7.05035400	4.72076900
H	0.11102200	7.04698300	4.78594800
C	1.72973600	9.23699700	4.66834900
C	0.28420700	11.76758100	4.47246900
H	-2.32966600	11.39410300	4.42255400
H	-3.63377300	9.22571500	4.53449100
C	1.71529900	11.67571800	4.51613500
C	2.42258200	10.45366200	4.60375200
H	2.27748800	12.61702300	4.47217300
C	3.93907100	10.45884400	4.63122100
H	4.31946300	11.49126900	4.57239300
H	4.35406200	10.02097500	5.56403000
H	4.37889300	9.89635400	3.78334900
O	2.39942700	7.99489000	4.74413100

H	3.32211800	8.18530000	4.98779300
O	-0.35872700	12.87131900	4.38673000

VK_3H_2

C	-1.81677400	8.01305000	4.66881300
C	-0.42953700	8.00648900	4.70336800
C	0.30467700	9.22590600	4.64848500
C	-0.41804200	10.46794900	4.55626700
C	-1.84087800	10.44283300	4.52270400
C	-2.52783800	9.23848600	4.57801000
H	-2.36631500	7.06753200	4.71205300
H	0.12311000	7.06643000	4.77324000
C	1.73449400	9.25013000	4.68202500
C	0.32491100	11.68867700	4.50030300
H	-2.37863900	11.39157300	4.45201300
H	-3.62185700	9.23277600	4.55145500
C	1.71110800	11.66896300	4.53512700
C	2.44243900	10.45000800	4.62644100
H	2.27065100	12.61185200	4.49083600
C	3.95368900	10.46051000	4.66226300
H	4.34099200	11.48870000	4.59682400
H	4.35461100	10.02793300	5.59915000
H	4.39750800	9.89930100	3.81742500
O	2.36142800	8.02245400	4.77165500
H	3.32572000	8.16178800	4.78385200
O	-0.40994200	12.85374700	4.41108000
H	0.20554700	13.60837400	4.37673600

$[3(\mu\text{-}H)]^+$

Ru	1.45880500	-0.95237300	0.00000600
Ru	-1.30541600	-0.87609900	0.00000100
C	2.14766800	0.60391200	1.40800500
H	1.44609700	0.70089200	2.24870000
N	0.09126300	-1.94590200	1.32393200
C	2.69670700	3.07555000	1.40609400
H	2.68010000	3.07833600	2.50104500
C	-4.29080300	-0.68105500	-0.70318200
N	0.09126700	-1.94591200	-1.32391700
C	3.01446800	-0.52526400	1.43788900
H	2.92456400	-1.18668900	2.31359800
C	-2.95953200	-0.65391500	-1.38029200
H	-2.86201400	-1.34285900	-2.23401700
C	2.45746700	1.87926100	-0.70454400
C	-2.46463200	1.78589600	-0.70684900
C	-2.73875300	2.97520300	-1.40565900
H	-2.72406200	2.97785900	-2.50083600
C	-5.50616300	-0.72722200	1.40790000
H	-5.50522000	-0.73808000	2.50310900
C	-2.11702700	0.51360500	-1.41476200
H	-1.47398800	0.63395000	-2.29962200

C	5.52321000	-0.82251500	1.40454500
H	5.51896800	-0.84557300	2.49930800
C	2.69671300	3.07553800	-1.40610900
H	2.68011100	3.07831500	-2.50106100
C	-2.11703000	0.51361700	1.41474900
H	-1.47399300	0.63397200	2.29961000
C	-5.50615900	-0.72723500	-1.40790900
H	-5.50521400	-0.73810200	-2.50311800
C	-3.02781700	4.15472000	0.70255800
H	-3.24345000	5.07643100	1.25082400
C	-2.95953500	-0.65390200	1.38028800
H	-2.86201900	-1.34283900	2.23401900
C	3.01447500	-0.52527500	-1.43787400
H	2.92457400	-1.18670700	-2.31357800
C	-3.02781600	4.15471400	-0.70260600
H	-3.24344700	5.07641900	-1.25088100
C	-2.46463400	1.78590300	0.70682300
C	-0.66872400	-2.91295400	-0.71260100
H	-1.26824100	-3.62364900	-1.29321900
C	2.14767400	0.60390100	-1.40800300
H	1.44610600	0.70087300	-2.24870100
C	-4.29080500	-0.68104900	0.70317500
C	2.45746400	1.87926700	0.70453800
C	5.52321600	-0.82252600	-1.40451600
H	5.51897900	-0.84559200	-2.49927900
C	-6.71950700	-0.76862500	0.70245700
H	-7.66562500	-0.81263400	1.24974900
C	4.31324900	-0.62806100	0.70934500
C	6.72625400	-0.97759100	0.70338000
H	7.66303100	-1.11238400	1.25172300
C	4.31325200	-0.62806600	-0.70932300
C	-2.73875600	2.97521600	1.40562200
H	-2.72406700	2.97788200	2.50080000
C	0.12592500	-1.95140400	-2.79264000
H	0.34219800	-0.93909500	-3.16068100
H	-0.83269900	-2.29042900	-3.22086100
H	0.92671400	-2.62668300	-3.13997800
C	-0.66872600	-2.91294900	0.71262000
H	-1.26824500	-3.62364000	1.29324100
C	6.72625800	-0.97759700	-0.70334500
H	7.66303600	-1.11239400	-1.25168200
C	2.95260700	4.26145900	-0.70282200
H	3.13934400	5.18953500	-1.25075400
C	2.95260400	4.26146500	0.70279800
H	3.13933900	5.18954500	1.25072300
C	-6.71950500	-0.76863200	-0.70246900
H	-7.66562200	-0.81264500	-1.24976200
C	0.12591600	-1.95138400	2.79265400
H	0.92670400	-2.62666100	3.14000000
H	-0.83270900	-2.29040700	3.22087500
H	0.34218800	-0.93907200	3.16068900
H	0.26655800	0.20560000	-0.00000100

[3(μ-H)(H$_2$)]$^+$

Ru	1.44027300	-1.19749000	0.00133800
Ru	-1.27397900	-0.93058300	0.00015100
C	2.03297600	0.43387100	1.41029300
H	1.32808200	0.44409200	2.25209000
N	0.03377200	-2.12192600	1.30665000
C	2.29315500	2.95281400	1.39193900
H	2.27394500	2.95999300	2.48690300
C	-4.21359500	-0.52922100	-0.70858500
N	0.03598100	-2.11448900	-1.30702400
C	3.05269600	-0.55290300	1.44194600
H	3.07210100	-1.21194100	2.32143700
C	-2.88083300	-0.57238700	-1.38799400
H	-2.82479200	-1.24773500	-2.25573800
C	2.18638500	1.73022000	-0.71128800
C	-2.28578000	1.83656100	-0.69643100
C	-2.55452600	3.02667300	-1.39387200
H	-2.54380700	3.03236000	-2.48924200
C	-5.43430700	-0.51160400	1.39970900
H	-5.43634700	-0.52511100	2.49499300
C	-1.97059500	0.54820300	-1.39157900
H	-1.30577700	0.63894100	-2.26367800
C	5.56651000	-0.28110800	1.40863300
H	5.56912700	-0.28383700	2.50378400
C	2.30136100	2.93798800	-1.42026800
H	2.28817500	2.93377200	-2.51533500
C	-1.97587400	0.53796200	1.39960900
H	-1.31528300	0.62173200	2.27563000
C	-5.42818700	-0.50251700	-1.41473100
H	-5.42534700	-0.50886900	-2.51008000
C	-2.83143300	4.20275300	0.71831200
H	-3.03703200	5.12505700	1.26959200
C	-2.88673500	-0.58200500	1.38374000
H	-2.83492800	-1.26379000	2.24670700
C	3.04845700	-0.57748500	-1.42511800
H	3.06788700	-1.25068500	-2.29345400
C	-2.82870500	4.20798800	-0.68592500
H	-3.03210600	5.13441400	-1.23107000
C	-2.28826500	1.83140000	0.71301100
C	-0.80648700	-3.03406300	-0.70951600
H	-1.44103100	-3.69523300	-1.30813000
C	2.03564200	0.41832700	-1.41169700
H	1.33598300	0.42464900	-2.25785300
C	-4.21660400	-0.53379200	0.69876300
C	2.18251800	1.73801800	0.69440600
C	5.56371800	-0.31032800	-1.40017500
H	5.56465600	-0.33525400	-2.49502700
C	-6.64731900	-0.48367900	0.69205000
H	-7.59543400	-0.47678100	1.23766800
C	4.35184700	-0.40769300	0.71177300
C	6.77382500	-0.15673300	0.70362700
H	7.71579000	-0.06137000	1.25114800
C	4.34950000	-0.42238400	-0.69995100

C	-2.55982000	3.01618400	1.41836700
H	-2.55339100	3.01350400	2.51379100
C	0.10416600	-2.14165100	-2.77516000
H	0.35797700	-1.14433900	-3.15817200
H	-0.85969200	-2.45121000	-3.21294900
H	0.88507700	-2.85164800	-3.09693900
C	-0.80691800	-3.03864600	0.70412800
H	-1.44335400	-3.70297700	1.29741900
C	6.77229400	-0.17183200	-0.69985000
H	7.71333400	-0.08833400	-1.25094900
C	2.42185400	4.14994700	-0.72198000
H	2.50467000	5.08978400	-1.27524100
C	2.41757500	4.15740200	0.68169700
H	2.49704500	5.10293200	1.22565200
C	-6.64428200	-0.47914800	-0.71225000
H	-7.59000600	-0.46868600	-1.26194600
C	0.09805200	-2.15119100	2.77483200
H	0.87213000	-2.86806400	3.09825800
H	-0.86908200	-2.45273800	3.21116200
H	0.35989600	-1.15603100	3.15863600
H	0.13425100	0.09922600	-0.00214600
H	2.45423500	-2.55687800	-0.38617700
H	2.55425900	-2.44446100	0.47357000

[3(μ-H)(PPh_3)]$^+$

Ru	-0.49913900	0.22770000	-0.04436300
Ru	2.05773800	-0.83206600	-0.09822600
C	-0.02578500	1.93357300	-1.34643400
H	0.57083500	1.58971000	-2.20149000
N	0.35024700	-1.20384100	-1.43595100
C	1.18853200	4.16190900	-1.19680200
H	1.24461900	4.20797600	-2.28978600
C	4.84289700	-1.87729200	0.59574800
N	0.36833600	-1.31500700	1.19268400
C	-1.43677900	1.73250800	-1.39810900
H	-1.83702700	1.28974300	-2.32141000
C	3.64278900	-1.30651800	1.28304800
H	3.28148200	-1.89162100	2.14255900
C	0.52239100	2.99273000	0.83351400
C	4.26786800	1.11195400	0.65568600
C	5.07749400	2.00295700	1.38057200
H	5.07064500	1.97964900	2.47584000
C	5.94256800	-2.36507800	-1.52253800
H	5.94491800	-2.34145500	-2.61782000
C	3.37101500	0.11138800	1.31704900
H	2.83427700	0.48831200	2.20049000
C	-3.12669100	3.62834500	-1.33312000
H	-3.05895600	3.72299200	-2.42275800
C	1.07833500	4.02279400	1.61029800
H	1.04805400	3.96171500	2.70364100
C	3.37493300	0.18041900	-1.46201200
H	2.84189500	0.58914200	-2.33370400

C	5.92341300	-2.44845900	1.28952800
H	5.91122200	-2.48837000	2.38426800
C	5.88462700	2.96583900	-0.70341900
H	6.50885000	3.69195100	-1.23278900
C	3.65621100	-1.23598100	-1.48203400
H	3.30864900	-1.79395000	-2.36606600
C	-1.52803400	1.56327300	1.40814700
H	-1.95553500	1.01914600	2.26008600
C	5.88662600	2.92739500	0.70041600
H	6.51224300	3.62370200	1.26686600
C	4.26665800	1.15016700	-0.75243800
C	0.67253100	-2.49263200	0.53165200
H	0.94413200	-3.39912900	1.08148400
C	-0.11690100	1.78526300	1.44717300
H	0.42696100	1.36267800	2.30134300
C	4.85219900	-1.83611700	-0.81102300
C	0.57715300	3.06366200	-0.57038700
C	-3.31308200	3.36914100	1.45730900
H	-3.38488900	3.26889900	2.54590200
C	7.02230200	-2.93420200	-0.82722200
H	7.86637700	-3.35446500	-1.38205200
C	-2.35397800	2.66166100	-0.66627700
C	-3.99448400	4.45880700	-0.60778100
H	-4.59903000	5.20582500	-1.13076900
C	-2.43117600	2.54592400	0.73494600
C	5.07396600	2.07917200	-1.43038300
H	5.06522300	2.11371800	-2.52538600
C	0.43162000	-1.36044200	2.65989100
H	0.88831300	-0.43805800	3.04512300
H	1.03229400	-2.21786800	3.00617100
H	-0.58388600	-1.44884800	3.07414300
C	0.66826200	-2.43087400	-0.88263700
H	0.93888200	-3.28657600	-1.51027100
C	-4.09608000	4.32114900	0.78620300
H	-4.78389700	4.95681300	1.35159200
C	1.68293200	5.12386500	0.98256800
H	2.12355700	5.92101200	1.58838300
C	1.73918100	5.19261500	-0.41835900
H	2.22435900	6.04284800	-0.90648900
C	7.01249300	-2.97625000	0.57643800
H	7.84904900	-3.42922800	1.11675100
C	0.45006900	-1.13091700	-2.90654100
H	-0.15880200	-1.92335300	-3.37011900
H	1.49454800	-1.24924400	-3.23974800
H	0.08545600	-0.15606600	-3.25699200
H	1.32990000	0.70498200	-0.02532300
C	-2.28918100	-3.35303000	1.45831300
C	-2.70191900	-2.00459800	1.54915800
C	-3.01874100	-1.48987100	2.82889000
C	-2.97645500	-2.31006100	3.96828900
C	-2.58623000	-3.65324400	3.85832000
C	-2.23061400	-4.16640800	2.60119700
H	-2.02421000	-3.78134500	0.48804800
H	-3.30883700	-0.44288600	2.94934300

H	-3.24672400	-1.89155800	4.94246400
H	-2.55769500	-4.29384100	4.74448200
H	-1.91840600	-5.21075300	2.50243200
P	-2.70767200	-0.90907100	0.05325600
C	-3.11124000	-2.05375900	-1.35815100
C	-2.73529200	-1.68805700	-2.66383100
C	-3.97461500	-3.15853500	-1.18519900
C	-3.17331500	-2.42821800	-3.77404700
H	-2.11842700	-0.80059900	-2.81624700
C	-4.39950700	-3.90622200	-2.29242200
H	-4.33600300	-3.42944600	-0.18968100
C	-3.99656900	-3.54809100	-3.58950200
H	-2.87693500	-2.12266900	-4.78245100
H	-5.06215200	-4.76348100	-2.14000400
H	-4.33756700	-4.12933200	-4.45118000
C	-4.37410800	-0.06597000	0.09231900
C	-5.34662000	-0.29187700	1.08782500
C	-4.73391700	0.69885600	-1.03817200
C	-6.62956500	0.26803700	0.97172300
H	-5.13729100	-0.92792300	1.94860100
C	-6.01369200	1.25541000	-1.15087500
H	-4.02300100	0.84937500	-1.85325500
C	-6.96622500	1.04946200	-0.14116400
H	-7.36833600	0.07647300	1.75581100
H	-6.26553900	1.84890700	-2.03462200
H	-7.96658500	1.48314500	-0.22950200

[3(μ-H)(VK_3H)]

Ru	-0.49972700	-0.05082400	0.00887700
Ru	2.11331800	-0.95277600	0.00232500
C	-0.40411400	1.59591100	-1.38727800
H	0.22631300	1.36210700	-2.25724200
N	0.44344200	-1.47597200	-1.31197600
C	0.22645400	4.06679600	-1.43219100
H	0.22614300	4.05326200	-2.52797600
C	4.94344900	-1.81840300	0.70276800
N	0.45155500	-1.45804900	1.33023600
C	-1.72952700	1.03873900	-1.37794200
H	-2.01125100	0.41395800	-2.23661600
C	3.71120600	-1.30421000	1.38040100
H	3.39660500	-1.88448400	2.26186700
C	-0.06879800	2.90541000	0.68820000
C	4.19701700	1.12908700	0.68948700
C	4.94883500	2.09436500	1.38090100
H	4.93994200	2.10703300	2.47659700
C	6.05278900	-2.32032900	-1.40753900
H	6.04355800	-2.33359100	-2.50333400
C	3.35581200	0.10126500	1.38081400
H	2.80527400	0.46992700	2.25917300
C	-3.95895000	2.27202100	-1.37171500
H	-3.97664400	2.24797500	-2.46709900
C	0.25091600	4.08780600	1.37709300

H	0.26963000	4.09077300	2.47278200
C	3.34716900	0.08584200	-1.39539900
H	2.79111900	0.44511500	-2.27428200
C	6.06155600	-2.30446500	1.40232300
H	6.05919500	-2.30534000	2.49822700
C	5.68889100	3.04272500	-0.73352900
H	6.25840800	3.79473400	-1.28863200
C	3.70286000	-1.31945900	-1.38234300
H	3.38386800	-1.90863600	-2.25626000
C	-1.70104700	1.05330600	1.40642400
H	-1.96147000	0.44059300	2.28021300
C	5.69331400	3.05069100	0.67072800
H	6.26634900	3.80894200	1.21358500
C	4.19251500	1.12121900	-0.72080800
C	0.76124700	-2.65387700	0.72272800
H	1.04317000	-3.53659900	1.30746000
C	-0.37651300	1.61479200	1.37912600
H	0.27357600	1.39430000	2.23812800
C	4.93910000	-1.82626000	-0.70653600
C	-0.08137300	2.89517600	-0.71999100
C	-3.93336500	2.27933500	1.43549900
H	-3.93202300	2.25890200	2.53093500
C	7.16654500	-2.81161900	-0.70540800
H	8.02595100	-3.20894300	-1.25461300
C	-2.87293500	1.70527000	-0.68186600
C	-5.02689300	2.84385200	-0.66212800
H	-5.87525700	3.27270800	-1.20505000
C	-2.85955500	1.71023100	0.72863200
C	4.93986100	2.07849200	-1.42800100
H	4.92390300	2.07862100	-2.52369300
C	0.41040900	-1.45731900	2.79226800
H	0.60664200	-0.44507600	3.17262500
H	1.15476700	-2.14976500	3.22527800
H	-0.59600200	-1.76610600	3.12647800
C	0.76025100	-2.66215800	-0.69178700
H	1.04096300	-3.55238700	-1.26586800
C	-5.01430000	2.84677400	0.74251100
H	-5.85317900	3.27747600	1.29847000
C	0.56046900	5.25703700	0.66302800
H	0.82201600	6.17267400	1.20269500
C	0.54853500	5.24650400	-0.74127300
H	0.80066100	6.15383900	-1.29913000
C	7.17096900	-2.80360100	0.69882400
H	8.03386000	-3.19461400	1.24708600
C	0.40359000	-1.48705800	-2.77383700
H	-0.61064800	-1.77003300	-3.10680500
H	1.12903700	-2.20285600	-3.20096500
H	0.62708300	-0.48364400	-3.16291000
H	1.23702200	0.56160800	-0.00335400
C	-5.73644000	-1.51561800	0.39106400
C	-4.34160300	-1.52178500	0.76141600
C	-3.31619400	-1.52618100	-0.26465600
C	-3.74066300	-1.59515300	-1.60440500
C	-5.10019300	-1.58502500	-1.99230100

C	-6.08165500	-1.51608800	-0.99774200
H	-2.97308900	-1.65586600	-2.38359900
O	-2.03019400	-1.55641700	0.07213700
O	-7.39330600	-1.47749100	-1.42633900
H	-7.97417500	-1.33846700	-0.65663500
C	-4.00168100	-1.56431600	2.13883500
C	-4.97467300	-1.57199400	3.12987100
H	-4.68857300	-1.60788800	4.18601600
C	-6.34665200	-1.54534800	2.77033900
H	-7.11816400	-1.55691000	3.54650400
C	-6.71324800	-1.52502900	1.43128900
C	-5.50477700	-1.63154800	-3.44543700
H	-6.07647700	-0.73058000	-3.72999000
H	-4.62052000	-1.70185600	-4.09823700
H	-6.16099800	-2.49418900	-3.65464400
H	-7.78504100	-1.53647600	1.19357700
H	-2.93820600	-1.60721400	2.38939600

$[3(\mu\text{-}H)(H)_2]_a^+$

Ru	-1.30969300	-0.86150100	-0.01357000
Ru	1.42687200	-0.95450000	0.07239100
C	-2.09822300	0.48391900	-1.50821200
H	-1.47241800	0.50250300	-2.41292600
N	-0.19196700	-2.42761900	-1.28382600
C	-2.76416400	2.93210800	-1.72022800
H	-2.78669800	2.83869900	-2.81137100
C	4.44089500	-0.70449000	0.53503400
N	0.06375700	-1.93207800	1.41900500
C	-2.98218000	-0.64383900	-1.35920700
H	-2.97434900	-1.38331700	-2.17365100
C	3.17263000	-0.77516000	1.32458500
H	3.17510600	-1.50203300	2.14977500
C	-2.38265100	1.94718800	0.47467800
C	2.55824400	1.70174300	0.85827200
C	2.84451700	2.83957900	1.63533100
H	2.91374800	2.75264400	2.72504000
C	5.47935200	-0.49382500	-1.65678000
H	5.39024400	-0.39955400	-2.74434600
C	2.30484600	0.36913500	1.48084600
H	1.72555300	0.41404000	2.41553600
C	-5.52351600	-0.66686100	-1.24137100
H	-5.57614200	-0.75747700	-2.33173800
C	-2.68067200	3.17859200	1.08174800
H	-2.63566500	3.27809600	2.17155400
C	2.07690700	0.59486600	-1.32036000
H	1.34370700	0.74928900	-2.12516200
C	5.71010900	-0.76820700	1.13502900
H	5.79945700	-0.88595200	2.22029900
C	2.92927600	4.19667200	-0.38124300
H	3.06835200	5.16845200	-0.86381000
C	2.94146700	-0.53832500	-1.43664900
H	2.79207800	-1.17368700	-2.32426200

C	-2.85197700	-0.40435300	1.42394500
H	-2.72678100	-0.98390000	2.35094500
C	3.04099500	4.08207800	1.01478600
H	3.26804700	4.96368900	1.62116100
C	2.44410200	1.81653400	-0.54501400
C	-0.86194800	-2.86201600	0.99260100
H	-1.48132200	-3.38774200	1.72933700
C	-1.98971300	0.73754900	1.26453700
H	-1.27018700	0.92608900	2.07463400
C	4.32356200	-0.56995200	-0.86125900
C	-2.42531000	1.82340100	-0.92678400
C	-5.38923900	-0.46915600	1.56216300
H	-5.33565600	-0.40321800	2.65418500
C	6.74728400	-0.55154300	-1.05600300
H	7.64623400	-0.50066300	-1.67718300
C	-4.27405600	-0.58627500	-0.60308200
C	-6.70283000	-0.64104800	-0.47904800
H	-7.67403500	-0.70987500	-0.97760300
C	-4.20822500	-0.48451500	0.80023600
C	2.62286400	3.06922000	-1.15818600
H	2.51766100	3.16269000	-2.24425800
C	0.15009900	-1.77513700	2.88412600
H	-0.66107900	-2.31247300	3.40293900
H	0.09294800	-0.71132600	3.15729300
H	1.11507900	-2.17446600	3.23562400
C	-1.11586300	-3.04577000	-0.38135400
H	-1.86144000	-3.74464100	-0.76679300
C	-6.63595700	-0.54377300	0.92027400
H	-7.55476700	-0.53667200	1.51372900
C	-3.02319300	4.28437100	0.28664400
H	-3.24695300	5.24515000	0.75924800
C	-3.06350300	4.16179400	-1.11147900
H	-3.31869700	5.02704500	-1.73021300
C	6.86249800	-0.68926000	0.33700000
H	7.85090400	-0.74640800	0.80209100
C	-0.36915700	-2.62386600	-2.74054300
H	-1.38453100	-2.32716800	-3.03332100
H	-0.20000900	-3.67861800	-3.01462200
H	0.35484600	-1.98794100	-3.26835500
H	-0.14914200	0.32139600	-0.15862300
H	2.35994800	-2.23102000	-0.00388800
H	0.79392000	-2.67796300	-1.00587500

$[3(\mu\text{-}H)(H)_2]_b^+$

Ru	1.34487700	-0.79642600	0.03624200
Ru	-1.39853400	-1.10410800	-0.00570100
C	2.04576200	0.77578800	-1.37443800
H	1.32506300	0.90921300	-2.19381400
N	0.09371200	-1.93573400	-1.26186900
C	2.85227000	-0.38701200	-1.46611300
H	2.71862400	-1.00804000	-2.36300500

C	2.43631900	2.03182600	-0.67536800
C	2.09941300	0.77918500	1.44459600
H	1.41252900	0.91231500	2.29244300
N	0.09975600	-1.89981700	1.37198100
C	-3.05924000	-0.65877200	1.39706100
H	-3.04971400	-1.33928100	2.26028000
C	-2.36846600	2.91764100	1.36200500
H	-2.39759300	2.91991600	2.45685600
C	4.11477100	-0.65074000	-0.72356500
C	-4.36484400	-0.48638700	-0.71562200
C	5.27190900	-1.04105300	-1.43370300
H	5.23994100	-1.07310300	-2.52771400
C	-2.06404900	0.40208500	-1.47140600
H	-1.40420400	0.42003900	-2.34846500
C	-2.23650700	2.91746600	-1.44284000
H	-2.17185800	2.91616500	-2.53617700
C	2.78228100	3.21486300	1.42482500
H	2.78591800	3.21933400	2.51994100
C	2.90606900	-0.38465000	1.49242900
H	2.80457500	-1.01764000	2.38644200
C	4.14384500	-0.64255700	0.70374700
C	-2.10759400	0.40348400	1.41309600
H	-1.44833100	0.46700700	2.28926100
C	6.45327900	-1.36417400	-0.75849500
H	7.34804800	-1.63820400	-1.32472600
C	-3.05239900	-0.62060600	-1.41959900
H	-3.03996600	-1.33827500	-2.25211000
C	2.45998800	2.03415600	0.73004400
C	3.09360200	4.38361200	0.71451400
H	3.34293900	5.30009400	1.25715700
C	-2.20164200	1.69718100	-0.74147600
C	2.73616300	3.20908500	-1.38548700
H	2.70305500	3.20958500	-2.48012500
C	-2.36074600	4.12866700	-0.74737700
H	-2.39434700	5.07249800	-1.29909800
C	6.48267300	-1.35385500	0.64879200
H	7.40054700	-1.61976600	1.18094100
C	0.15375400	-1.96129800	-2.72256400
H	0.16143400	-0.93810400	-3.12701600
H	-0.71805900	-2.49730800	-3.14244600
H	1.06662600	-2.48077400	-3.07257900
C	-0.00335500	-1.83254600	2.83398700
H	0.83576400	-2.39698000	3.27569600
H	-0.94981900	-2.27168300	3.19340500
H	0.06619200	-0.78940300	3.17097600
C	5.33008600	-1.02178000	1.36882100
H	5.34388600	-1.04127100	2.46353400
C	-5.57228900	-0.35810100	-1.42386500
H	-5.56532500	-0.33308700	-2.51872000
C	-2.26236700	1.69527400	0.67353500
C	-6.79651100	-0.33460000	0.67770000
H	-7.74442000	-0.28706100	1.22154600
C	-6.78718800	-0.27787200	-0.72540000
H	-7.72690200	-0.18610000	-1.27754200

C	-0.46432900	-2.95886500	0.71809400
H	-1.04890200	-3.69130700	1.28990100
C	-5.59152300	-0.46438800	1.38593800
H	-5.60015500	-0.51459400	2.47990100
C	-2.42948700	4.12833700	0.65590100
H	-2.51646600	5.07260400	1.20115000
C	3.07097400	4.38065300	-0.69040200
H	3.30267800	5.29482800	-1.24461500
C	-4.37110300	-0.53660200	0.69146700
C	0.10261400	-3.28864700	-0.64719500
H	1.10927700	-3.76530700	-0.61644200
H	-0.57734000	-3.97247800	-1.18904100
H	-2.49251200	-2.23024000	-0.20110700
H	0.23265400	0.34000700	0.03093100

[3(μ-H)(H)$_2$(VK$_3$H)]

Ru	-0.58243700	-0.11732900	-0.11166300
Ru	2.18154000	-1.26520900	-0.09500000
C	-0.50021100	1.51164800	-1.55587700
H	-0.06036700	1.19240700	-2.51268800
N	1.20030200	-2.58818200	-1.56863800
C	0.38961800	3.89574600	-1.73059500
H	0.21472300	3.89094900	-2.81236900
C	4.98529800	-1.53372800	1.06517600
N	0.43110000	-1.77628200	0.99468400
C	-1.86226100	1.14021700	-1.31509000
H	-2.35935000	0.55232700	-2.09747000
C	3.61355100	-1.14365800	1.52317800
H	3.26605200	-1.65241200	2.43348800
C	0.31963200	2.75315300	0.41928400
C	3.84617500	1.22384200	0.53938200
C	4.36132600	2.36771700	1.17449800
H	4.22431700	2.49472200	2.25448000
C	6.46224100	-2.04124000	-0.80337300
H	6.62039900	-2.15935400	-1.88147300
C	3.08566100	0.16583200	1.27309100
H	2.38838700	0.54385400	2.03081000
C	-3.89957600	2.62295100	-0.93696200
H	-4.09208900	2.63766400	-2.01548200
C	0.85673800	3.89328500	1.04083000
H	1.05300700	3.88482100	2.11880400
C	3.44451000	-0.17195400	-1.47578000
H	2.98011300	-0.02493000	-2.46271000
C	6.04604500	-1.75980800	1.95911700
H	5.87855100	-1.65767300	3.03730800
C	5.18597100	3.19655000	-0.95689000
H	5.69519400	3.96847400	-1.54266200
C	4.00926300	-1.47170600	-1.21638200
H	3.93621800	-2.20543000	-2.03704000
C	-1.37662300	1.09134000	1.42192200
H	-1.54507400	0.51188400	2.34217100
C	5.03120700	3.35177300	0.43003800

H	5.41915900	4.24497400	0.92999800
C	4.00921100	1.06399600	-0.85315600
C	-0.14657800	-2.92260900	0.40369800
H	-0.93163200	-3.44646800	0.96205300
C	-0.00929200	1.49486800	1.15541400
H	0.71889900	1.21512500	1.92586900
C	5.19223500	-1.67699500	-0.32298400
C	0.08408100	2.75575000	-0.96848800
C	-3.43667600	2.52418100	1.83228300
H	-3.26878300	2.46147600	2.91307400
C	7.52045800	-2.26760600	0.09223500
H	8.50406200	-2.56146200	-0.28773200
C	-2.78690900	1.92185500	-0.44053300
C	-4.77072300	3.28184000	-0.05507500
H	-5.64093200	3.81825600	-0.44627400
C	-2.55350900	1.87716600	0.95013000
C	4.67683900	2.05414000	-1.59544000
H	4.79076500	1.93368500	-2.67882200
C	0.34398200	-1.79141900	2.46121500
H	0.72498400	-0.84203300	2.86595300
H	0.94385800	-2.61571800	2.89028100
H	-0.70573300	-1.91594900	2.78912100
C	0.16723200	-3.31961300	-0.84872500
H	-0.35848000	-4.12683500	-1.36926700
C	-4.53970000	3.23133600	1.32976200
H	-5.22996300	3.72651000	2.01976000
C	1.15723200	5.03315100	0.27846700
H	1.58743700	5.91523400	0.76303500
C	0.92612600	5.03385400	-1.10679100
H	1.17365500	5.91740200	-1.70354100
C	7.31193900	-2.12803300	1.47411700
H	8.13206100	-2.31342500	2.17493900
C	0.72529800	-2.04272400	-2.86804500
H	0.27076300	-2.83293900	-3.49411700
H	1.57331000	-1.59209100	-3.40577900
H	-0.02740400	-1.26252600	-2.67161900
H	1.04163200	0.19435000	-0.55173600
C	-5.95024700	-1.26443700	0.43689900
C	-4.56070300	-1.25240100	0.81161800
C	-3.53801300	-1.29088800	-0.21400300
C	-3.94936200	-1.39822700	-1.55173100
C	-5.31276100	-1.42464000	-1.94018000
C	-6.29517400	-1.33785400	-0.94882400
H	-3.17693400	-1.49581400	-2.32245900
O	-2.25034200	-1.33264200	0.13409600
H	2.75147800	-2.70252000	0.28220700
H	1.97287300	-3.23610700	-1.77441000
C	-4.22921700	-1.22337300	2.19278100
C	-5.21645600	-1.19367200	3.16919900
H	-4.93991500	-1.17730700	4.22853800
C	-6.58596200	-1.18503900	2.79653300
H	-7.36161800	-1.15658300	3.56845300
C	-6.94553400	-1.22122400	1.45608300
C	-5.70051100	-1.54811800	-3.39733100

H	-6.27755500	-0.67315800	-3.75546300
H	-4.80564400	-1.61811200	-4.03486900
H	-6.30674300	-2.45282500	-3.59751800
O	-7.64344100	-1.34258100	-1.24470100
H	-7.75092900	-1.39063200	-2.21196800
H	-7.99809100	-1.22391900	1.16134000
H	-3.16992200	-1.23457400	2.46334800

T.S-1 (ν= -1204 cm^{-1})

Ru	-1.29363700	-0.86402000	0.03718800
Ru	1.40589200	-1.01762500	0.06927800
C	-2.01779900	0.53218100	-1.43154100
H	-1.33826300	0.60635000	-2.29391000
N	0.03514900	-2.25085500	-1.20320700
C	-2.71321100	2.97842400	-1.56388400
H	-2.67889900	2.93579800	-2.65787800
C	4.40136200	-0.63439300	0.54977900
N	0.04703800	-1.94631700	1.44599400
C	-2.88716500	-0.61763300	-1.39571800
H	-2.80855700	-1.31774900	-2.24185600
C	3.13798900	-0.71696800	1.34761400
H	3.14734600	-1.43811800	2.17695600
C	-2.43381400	1.89564200	0.60002400
C	2.47873800	1.72534200	0.81990100
C	2.78349400	2.87480200	1.56942000
H	2.87999100	2.80723100	2.65838100
C	5.45131200	-0.42429700	-1.63851200
H	5.36690500	-0.34165100	-2.72738200
C	2.24273500	0.39848300	1.46902700
H	1.63452900	0.44143200	2.38347000
C	-5.43175100	-0.66626000	-1.44275000
H	-5.41569200	-0.71139200	-2.53707100
C	-2.77745300	3.09468700	1.24678900
H	-2.79083400	3.14266700	2.34095900
C	2.00324000	0.56711800	-1.33149500
H	1.24781900	0.67461200	-2.12318600
C	5.66951700	-0.67189200	1.15462200
H	5.75464500	-0.77917800	2.24124700
C	2.80657700	4.19928600	-0.47104500
H	2.92436500	5.16380600	-0.97326500
C	2.92009600	-0.51904300	-1.44989800
H	2.80603300	-1.16369400	-2.33397200
C	-2.92827100	-0.50760500	1.38862500
H	-2.85273600	-1.14058400	2.28618700
C	2.95337700	4.10899200	0.92259700
H	3.18660400	5.00258800	1.50873700
C	2.33606700	1.81522600	-0.57914500
C	-0.80291500	-2.90476400	0.93461700
H	-1.43577300	-3.50490500	1.59752800
C	-2.07191200	0.65212800	1.35085200
H	-1.41593300	0.80890500	2.21986600
C	4.29125900	-0.51229300	-0.84964700

C	-2.40119400	1.83703100	-0.80629500
C	-5.47188600	-0.57962900	1.36979900
H	-5.48664800	-0.55652800	2.46477300
C	6.71669600	-0.45289400	-1.03092800
H	7.61778800	-0.38987700	-1.64774300
C	-4.22516000	-0.60758800	-0.72463600
C	-6.65596900	-0.67625600	-0.75454400
H	-7.59424800	-0.72896700	-1.31438600
C	-4.24605100	-0.56208400	0.68257300
C	2.49438600	3.05505800	-1.22205000
H	2.36837600	3.12807000	-2.30750400
C	0.10719600	-1.84479900	2.91277500
H	-0.76181900	-2.32968400	3.38799500
H	0.12978400	-0.78881100	3.21629100
H	1.02650200	-2.33348700	3.27612200
C	-0.87970500	-3.02818900	-0.46883600
H	-1.51710300	-3.75645800	-0.97703300
C	-6.67597800	-0.63396300	0.64901600
H	-7.62976400	-0.65429500	1.18417900
C	-3.09206700	4.23303000	0.48706600
H	-3.35204900	5.16837500	0.99116700
C	-3.05951100	4.17507700	-0.91555300
H	-3.29450700	5.06540100	-1.50611200
C	6.82547200	-0.57867800	0.36335900
H	7.81159100	-0.61494000	0.83527200
C	0.03922000	-2.38541100	-2.67465800
H	-0.99493400	-2.40620300	-3.05010100
H	0.55157200	-3.31306000	-2.98004700
H	0.56003700	-1.52387100	-3.11356400
H	-0.05885100	0.29810800	0.07019100
H	2.27153300	-2.42044900	-0.12496400
H	1.30512700	-2.56402900	-0.71727200

T.S-2 (ν= -1378 cm^{-1})

Ru	-1.22852300	-0.68588700	0.06345300
Ru	1.38758200	-0.74912000	0.05920700
C	-2.25768300	0.76453700	1.35768000
H	-1.58872000	1.03208200	2.18843800
N	0.02275100	-1.73257100	1.39724700
C	-2.90576100	-0.51410700	1.43458200
H	-2.72369800	-1.10816500	2.34116300
C	-2.80092000	1.91048100	0.57670800
C	-2.21717900	0.56091400	-1.42715500
H	-1.56894600	0.73005400	-2.29889700
N	0.00422400	-1.65592900	-1.31556900
C	2.88003600	-0.37169000	-1.47786500
H	2.69841300	-0.93529000	-2.40188100
C	3.00088100	3.21448200	-1.20374700
H	2.88490300	3.29524800	-2.28961600
C	-4.20271100	-0.80271400	0.74337400
C	4.27157800	-0.80875600	0.59505700
C	-5.40349600	-0.98754600	1.44897300

H	-5.41426000	-0.91083700	2.54146800
C	2.36983100	0.65414700	1.50623300
H	1.69040700	0.77654000	2.36205300
C	3.25713100	3.02110100	1.59057900
H	3.33966800	2.95038700	2.68019700
C	-3.26452700	2.86986800	-1.61287400
H	-3.24251500	2.79577900	-2.70536700
C	-2.87805900	-0.72015900	-1.35860500
H	-2.68828800	-1.42314000	-2.18140200
C	-4.18493700	-0.91637300	-0.66060600
C	2.14269600	0.83329600	-1.29264400
H	1.40226600	1.06715600	-2.07007700
C	-6.58678600	-1.28162800	0.75148500
H	-7.51972600	-1.43114300	1.30261500
C	3.07211700	-0.57573000	1.45379900
H	2.96522500	-1.26324700	2.30300800
C	-2.78978000	1.80393500	-0.82950500
C	-3.75740100	4.03087600	-0.99596000
H	-4.12299700	4.85933400	-1.60970400
C	2.79271200	1.92034200	0.84736300
C	-3.28461300	3.07884100	1.19205400
H	-3.27996000	3.16394200	2.28380900
C	3.60763600	4.20965000	0.93280300
H	3.96873000	5.06503500	1.51091400
C	-6.56928100	-1.39827800	-0.64765800
H	-7.48878300	-1.63922400	-1.18896400
C	0.00747900	-1.75690600	2.86210500
H	0.82210200	-2.40561300	3.22777500
H	-0.94745500	-2.15124200	3.24896800
H	0.16055100	-0.74148400	3.25547100
C	0.09069500	-1.65587500	-2.76727000
H	-0.82796100	-2.07744000	-3.21384300
H	0.94349600	-2.28033100	-3.09307000
H	0.23384600	-0.63214600	-3.13966100
C	-5.36930800	-1.21969800	-1.35469500
H	-5.35313600	-1.32110700	-2.44509900
C	5.47880600	-1.23733600	1.18107400
H	5.53684600	-1.35413300	2.26814100
C	2.66426400	2.01603600	-0.54961900
C	6.51645900	-1.37876600	-1.01324500
H	7.38912400	-1.59331500	-1.63668100
C	6.60245800	-1.49739200	0.38641900
H	7.54221200	-1.80323900	0.85496700
C	-0.17714700	-2.94089400	-0.66932100
H	-0.63212400	-3.74221400	-1.27215800
C	5.30722900	-1.00271600	-1.61062800
H	5.23084900	-0.94081500	-2.70112800
C	3.47756100	4.30672000	-0.46286900
H	3.73636500	5.23863400	-0.97373800
C	-3.76765100	4.13540300	0.40487400
H	-4.14128800	5.04479600	0.88424800
C	4.18170000	-0.69143000	-0.82108500
C	-0.67323200	-2.72278600	0.69101800
H	-1.23909700	-3.49124000	1.22783100

H	1.19716700	-3.08166100	-0.40993200
H	1.96625000	-2.45270100	-0.16617600
H	0.09832800	0.52143400	0.14255900

T.S-3 (ν= -675 cm^{-1})

Ru	-1.43206900	-1.21235200	-0.02108500
Ru	1.27821600	-0.90319400	-0.00666900
C	-2.04538900	0.38827500	-1.40968200
H	-1.37971400	0.41522800	-2.28248100
N	-0.02855000	-2.13007100	-1.31482800
C	-2.33224200	2.90636500	-1.39832100
H	-2.30267300	2.91431500	-2.49306600
C	4.20619600	-0.52873100	0.72988300
N	-0.06026300	-2.09720600	1.28781700
C	-3.10215000	-0.59695600	-1.45192400
H	-3.18115300	-1.15628400	-2.39826900
C	2.86781800	-0.54843800	1.40044500
H	2.79739600	-1.21420800	2.27428000
C	-2.22811400	1.68380600	0.70763200
C	2.31479400	1.86459800	0.69177600
C	2.59961100	3.05090300	1.38905100
H	2.57857100	3.05977800	2.48426100
C	5.44828200	-0.53777600	-1.36608800
H	5.46100000	-0.55517800	-2.46127100
C	1.97157500	0.58273900	1.38505100
H	1.29406500	0.68354800	2.24596100
C	-5.60810400	-0.20726700	-1.37381300
H	-5.63151800	-0.17651100	-2.46828300
C	-2.36362800	2.88983700	1.41477100
H	-2.35652300	2.88616300	2.50984400
C	2.00453700	0.56396800	-1.40109400
H	1.34912700	0.65418800	-2.28018400
C	5.41441500	-0.51951400	1.44737400
H	5.40046700	-0.52266300	2.54267900
C	2.91987400	4.21533500	-0.72355600
H	3.14818800	5.13206000	-1.27522600
C	2.90089200	-0.56716800	-1.38005400
H	2.85030200	-1.24592700	-2.24526300
C	-3.03881600	-0.65216700	1.40516700
H	-3.04991300	-1.33908200	2.26122700
C	2.90211200	4.22507700	0.68050400
H	3.11646900	5.14939100	1.22505700
C	2.33204000	1.85492200	-0.71697400
C	0.81567600	-3.00691700	0.70663100
H	1.45182900	-3.64560200	1.32579400
C	-2.04860400	0.37125100	1.40048400
H	-1.34374000	0.39086400	2.24159100
C	4.22304800	-0.53801400	-0.67793400
C	-2.21485100	1.69332700	-0.69920000
C	-5.55036200	-0.33033000	1.43420100
H	-5.53206400	-0.38716300	2.52752400
C	6.65470900	-0.52670400	-0.64673100

H	7.60807800	-0.53657600	-1.18308400
C	-4.39179000	-0.40650100	-0.70093300
C	-6.79494900	-0.05711800	-0.63963200
H	-7.74274900	0.09472200	-1.16352500
C	-4.35425100	-0.46758300	0.70801600
C	2.63476200	3.03147900	-1.42315200
H	2.64122300	3.02521100	-2.51857600
C	-0.14647400	-2.13019800	2.75561100
H	-0.43180700	-1.14358800	3.14280200
H	0.82280400	-2.41153700	3.20000000
H	-0.90777700	-2.86635000	3.06428300
C	0.82749700	-3.02946300	-0.70136700
H	1.48090100	-3.68419900	-1.28594000
C	-6.76536300	-0.12349200	0.76201000
H	-7.69189900	-0.02402600	1.33464300
C	-2.49283500	4.10066100	0.71502000
H	-2.59034800	5.03945900	1.26764800
C	-2.47583600	4.10932900	-0.68842800
H	-2.55991600	5.05434700	-1.23248900
C	6.63785700	-0.51763400	0.75735200
H	7.57803000	-0.52041900	1.31659500
C	-0.08342500	-2.16764900	-2.78270100
H	-0.84413600	-2.89739800	-3.10966600
H	0.89062300	-2.45782900	-3.21146500
H	-0.35199500	-1.17685200	-3.17467200
H	0.01480100	0.18915900	-0.01652900
H	-2.31424200	-2.56253600	0.17584400
H	-2.71158800	-1.92305200	-0.78614800

T.S-4 (ν= -276 cm^{-1})

Ru	0.32099500	0.77590800	-0.73286000
Ru	-1.90730700	-0.83991800	-0.50166300
C	0.58823000	1.66685500	1.22731900
H	0.38672600	0.95054100	2.03530900
N	0.22657700	-1.24465700	-0.01270200
C	-0.32243700	3.62738400	2.57229100
H	0.10798700	3.20290100	3.48618400
C	-4.61448100	-2.19450100	-0.80141200
N	-0.73869500	-0.28376400	-2.26601600
C	1.84894100	1.54813700	0.55093700
H	2.51489000	0.72975700	0.86619800
C	-3.79838000	-1.11924300	-1.44955400
H	-3.71659000	-1.20451100	-2.54466400
C	-0.71433800	3.49634600	0.17066300
C	-4.41208100	0.61098400	0.35753800
C	-5.50043600	1.49992000	0.38783000
H	-5.87368400	1.93322800	-0.54706800
C	-4.80223200	-3.77478800	1.04450400
H	-4.40208200	-4.20139700	1.97124400
C	-3.70709700	0.22376900	-0.90508000
H	-3.57539800	1.03999000	-1.63181500
C	3.72385700	3.26750200	0.44463500

H	4.15710700	2.84447300	1.35787300
C	-1.45503700	4.68987100	0.23275800
H	-1.90999700	5.09376300	-0.67863200
C	-2.72804500	-0.83831100	1.46434000
H	-1.96793400	-0.68524400	2.24530800
C	-5.81152900	-2.69217900	-1.34475300
H	-6.19856800	-2.27519000	-2.28146600
C	-5.60614700	1.30104400	2.80998100
H	-6.06208500	1.57760100	3.76587100
C	-2.81799400	-2.17157500	0.89999300
H	-2.10944200	-2.91483700	1.29708300
C	0.72708100	2.62256900	-1.77678300
H	0.68580600	2.50100700	-2.86936000
C	-6.09628400	1.84580400	1.61203200
H	-6.93553000	2.54825500	1.63115900
C	-3.91794100	0.06560000	1.56154600
C	-0.61634200	-1.65839100	-2.18694400
H	-0.93348500	-2.30787000	-3.00956800
C	-0.53540900	2.72689900	-1.09850500
H	-1.43772200	2.67634900	-1.72589400
C	-4.10921000	-2.73679000	0.39819600
C	-0.14549300	2.96203100	1.34598500
C	2.61742300	4.32517900	-1.90867000
H	2.18863500	4.73029500	-2.83209300
C	-5.99491200	-4.27473600	0.49498400
H	-6.52469300	-5.09265800	0.99342900
C	2.53561000	2.72147200	-0.07432200
C	4.35613900	4.33853500	-0.20804500
H	5.28245800	4.75659900	0.19922200
C	1.97595000	3.25726100	-1.25511900
C	-4.51936200	0.41137300	2.78396600
H	-4.12617900	-0.00425100	3.71860000
C	-1.21643000	0.26948400	-3.53413600
H	-1.70371900	1.23894200	-3.35541200
H	-1.93836300	-0.40446800	-4.02919400
H	-0.35928100	0.42887800	-4.21258400
C	-0.09426800	-2.16784000	-0.97599300
H	0.01281400	-3.24165200	-0.79241300
C	3.80434800	4.86533300	-1.38758400
H	4.30068300	5.69257400	-1.90469800
C	-1.62614700	5.35233200	1.45860400
H	-2.21335300	6.27488200	1.50286600
C	-1.05974100	4.82060700	2.62886400
H	-1.20326600	5.32829900	3.58781500
C	-6.49967200	-3.73314700	-0.69857800
H	-7.42395900	-4.12768300	-1.13239200
C	0.74893300	-1.75444500	1.25753800
H	1.84852000	-1.68779400	1.24990900
H	0.46223000	-2.80890900	1.41520700
H	0.35538400	-1.15471800	2.09090200
H	-1.27367500	0.77438100	-0.01896600
C	6.06090800	-0.49311100	0.34614200
C	4.82570700	-0.40002400	-0.32169400
C	3.92400900	-1.50174000	-0.46575500

C	4.35832000	-2.78516000	0.11199100
C	5.61621400	-2.88821500	0.79975100
C	6.44481900	-1.72662300	0.90563900
H	4.52981200	0.55502500	-0.76775300
O	2.78543500	-1.38565400	-1.06084800
H	1.86723400	0.45819400	-2.77595600
H	2.23403900	-0.08032700	-2.36012200
C	6.00841400	-4.14431800	1.34625300
C	3.55951100	-3.94535300	-0.02418400
C	3.96150800	-5.16655000	0.51177200
H	3.33297400	-6.05493600	0.39114800
C	5.19304000	-5.26185500	1.20736500
H	5.50866900	-6.22115700	1.62986200
C	6.97228500	0.70937400	0.46099500
H	7.94464400	0.54674800	-0.04299100
H	6.51037200	1.59030900	-0.00976900
H	7.18143100	0.98042300	1.51438800
O	7.63692800	-1.88375000	1.57587400
H	8.11400500	-1.03331600	1.56970200
H	6.96482200	-4.21555900	1.87087900
H	2.62261800	-3.84694100	-0.58133400

T.S-5(ν= -912 cm^{-1})

Ru	-0.51810500	0.02069500	0.16663700
Ru	2.04138000	-1.35182700	0.21243900
C	-0.31352500	1.52286300	-1.36545700
H	0.17870300	1.12822100	-2.26738600
N	0.71456600	-2.81234000	-0.73557200
C	0.57213000	3.90423800	-1.66986800
H	0.47683000	3.81662200	-2.75799700
C	5.00364800	-1.38674900	0.93274600
N	0.41523700	-1.55039500	1.58889800
C	-1.70194400	1.18001300	-1.18305300
H	-2.15898100	0.54644300	-1.95507200
C	3.71422000	-0.91772100	1.53077800
H	3.52055000	-1.25369300	2.55932500
C	0.36513300	2.92335100	0.54873600
C	3.71663800	1.22820800	0.10543000
C	4.29971900	2.46113100	0.44447400
H	4.33999500	2.77141200	1.49435500
C	6.20496900	-2.17774400	-1.03373100
H	6.20653600	-2.46105000	-2.09226400
C	3.11161900	0.31765700	1.12901400
H	2.50698200	0.83012700	1.88653100
C	-3.72881400	2.73049600	-1.05376600
H	-3.85345700	2.67037300	-2.14077800
C	0.83505900	4.11770600	1.12111800
H	0.94437300	4.19490800	2.20909600
C	3.04035100	-0.49484200	-1.55078000
H	2.39246300	-0.53942300	-2.43783700
C	6.18719000	-1.48437200	1.68561000
H	6.17541300	-1.22130500	2.74924100

C	4.71916000	2.92035800	-1.90623900
H	5.09522600	3.58422800	-2.69100900
C	3.71238300	-1.69844600	-1.17712100
H	3.52547400	-2.58216900	-1.80398700
C	-1.38991400	1.32403200	1.55364100
H	-1.61811300	0.81519600	2.50356500
C	4.80235000	3.30481000	-0.55864800
H	5.23997200	4.27098300	-0.28906900
C	3.64173100	0.83923100	-1.24650000
C	-0.25499000	-2.77177800	1.40045800
H	-0.88286900	-3.16688300	2.20398000
C	-0.00086900	1.70900200	1.34108200
H	0.67927300	1.48981800	2.17578100
C	5.01078900	-1.73845500	-0.43461100
C	0.22890100	2.81790300	-0.84803100
C	-3.43700300	2.83354100	1.73955700
H	-3.33260900	2.85479500	2.83023600
C	7.38602000	-2.26844000	-0.27959400
H	8.30941800	-2.61840400	-0.75155400
C	-2.66776200	2.04575800	-0.43710500
C	-4.63862100	3.46797900	-0.27822700
H	-5.47136100	3.98843600	-0.76182100
C	-2.52298700	2.09970800	0.96470400
C	4.14025500	1.68807400	-2.24959800
H	4.06904300	1.38685800	-3.30087000
C	0.54078800	-1.21028100	3.01401400
H	1.03803800	-0.23895100	3.13696000
H	1.13367900	-1.97341400	3.55163300
H	-0.45661700	-1.15256100	3.48995200
C	-0.17925500	-3.35842600	0.16788700
H	-0.76627800	-4.23899700	-0.11493500
C	-4.49265900	3.51989400	1.11779700
H	-5.21125400	4.08003800	1.72433900
C	1.17431300	5.20415300	0.29815800
H	1.54946900	6.13093900	0.74400700
C	1.04667200	5.09549300	-1.09640000
H	1.32433300	5.93692100	-1.73920000
C	7.37614900	-1.92470200	1.08190100
H	8.29176600	-2.00627000	1.67594600
C	0.67764000	-3.27900800	-2.11740900
H	-0.19131700	-2.84691200	-2.64856000
H	0.60420100	-4.38272200	-2.17887100
H	1.58627300	-2.96338800	-2.65151500
H	1.16225500	0.19349100	-0.18154700
C	-5.80720000	-1.36601500	0.04110500
C	-4.48326400	-1.25281000	0.59371700
C	-3.33148300	-1.35105200	-0.27756500
C	-3.55033400	-1.59571900	-1.64185400
C	-4.84611000	-1.72462500	-2.20308300
C	-5.95671400	-1.59494900	-1.36291900
H	-2.67623700	-1.72049000	-2.29083900
O	-2.09952000	-1.29723600	0.23724700
H	2.64811200	-2.90567600	0.66910900
H	1.99999700	-3.11333300	-0.01973400

C	-4.34206000	-1.05422300	1.99307000
C	-5.45450500	-0.96321100	2.81979400
H	-5.32642500	-0.81384400	3.89688100
C	-6.75980000	-1.06108000	2.27127800
H	-7.63374800	-0.98283700	2.92580200
C	-6.93300200	-1.25946500	0.90799200
C	-5.02633000	-1.99856900	-3.67994500
H	-5.58251500	-1.19040800	-4.19404000
H	-4.05051800	-2.07872700	-4.18320600
H	-5.56354200	-2.94781000	-3.87063800
O	-7.25036300	-1.69770500	-1.83150300
H	-7.22376600	-1.84062100	-2.79509200
H	-7.93518800	-1.33958300	0.47918800
H	-3.32934900	-0.97937900	2.39800000

[3(μ-H)H]

Ru	-1.45127400	-1.04112400	0.00000700
Ru	1.30888000	-0.84738300	-0.00000700
C	-2.13472800	0.45500900	-1.39168200
H	-1.47354000	0.55306200	-2.26614800
N	-0.08415400	-2.01056600	-1.30205900
C	-2.69505200	2.94277200	-1.40327400
H	-2.68284000	2.94250300	-2.49921300
C	4.25344300	-0.63272000	0.70488100
N	-0.08414700	-2.01060100	1.30203300
C	-3.04839600	-0.65989900	-1.39184200
H	-3.01906400	-1.32357900	-2.26840800
C	2.91870900	-0.60000800	1.38493500
H	2.83933400	-1.25208900	2.26844700
C	-2.44557600	1.74808500	0.70539600
C	2.50630100	1.84779500	0.70474800
C	2.87473600	3.00941600	1.40452400
H	2.86246500	3.01042100	2.50028900
C	5.47126900	-0.68510000	-1.40464200
H	5.46812000	-0.69290000	-2.50057500
C	2.08114600	0.58363500	1.38591800
H	1.43013900	0.72558800	2.26109600
C	-5.59704600	-0.54146600	-1.40356600
H	-5.59440700	-0.54882500	-2.49954900
C	-2.69503700	2.94272200	1.40342400
H	-2.68281600	2.94241300	2.49936300
C	2.08115400	0.58358900	-1.38597100
H	1.43017700	0.72549600	-2.26117800
C	5.47123700	-0.68510800	1.40472800
H	5.46806400	-0.69291200	2.50066100
C	3.23827000	4.17040600	-0.70219900
H	3.50978300	5.07763600	-1.25112800
C	2.91874000	-0.60004000	-1.38490900
H	2.83940500	-1.25215900	-2.26839800
C	-3.04842600	-0.65994600	1.39182400
H	-3.01912600	-1.32365700	2.26836800
C	3.23828800	4.17042100	0.70203600
H	3.50981600	5.07766300	1.25093800
C	2.50628800	1.84777700	-0.70484400
C	0.76660700	-2.92730000	0.70577200
H	1.40976400	-3.58263300	1.30177400

C	-2.13474400	0.45495400	1.39173800
H	-1.47359700	0.55296700	2.26623800
C	4.25345800	-0.63271900	-0.70482200
C	-2.44558000	1.74811100	-0.70529100
C	-5.59707500	-0.54149900	1.40349600
H	-5.59445900	-0.54888400	2.49947800
C	6.68702500	-0.74429700	-0.70205000
H	7.63244300	-0.79945500	-1.25096300
C	-4.37762100	-0.58666100	-0.70565500
C	-6.81369700	-0.50125600	-0.70224400
H	-7.76031900	-0.47783600	-1.25158900
C	-4.37763500	-0.58667800	0.70560900
C	2.87470400	3.00938500	-1.40465400
H	2.86241000	3.01036700	-2.50041900
C	-0.11773600	-2.01582700	2.76771200
H	-0.40318100	-1.02035700	3.13604800
H	0.86246900	-2.28447700	3.20108500
H	-0.87189700	-2.74317200	3.11625600
C	0.76660200	-2.92728100	-0.70582300
H	1.40977500	-3.58258100	-1.30184500
C	-6.81371100	-0.50127200	0.70214900
H	-7.76034500	-0.47786600	1.25147500
C	-2.94003100	4.13507300	0.70221800
H	-3.11936600	5.06474200	1.25163300
C	-2.94004000	4.13509700	-0.70202300
H	-3.11938400	5.06478600	-1.25140200
C	6.68700900	-0.74430300	0.70216300
H	7.63241500	-0.79946700	1.25109800
C	-0.11774900	-2.01578800	-2.76773800
H	-0.87173400	-2.74331500	-3.11628400
H	0.86252100	-2.28419200	-3.20111600
H	-0.40343700	-1.02038400	-3.13606200
H	-2.37178500	-2.33390300	-0.00002700
H	0.10501700	0.30897000	0.00000900

[3(μ-H)H]$^{+}$

Ru	1.44334200	-0.98548800	0.00000700
Ru	-1.28474400	-0.80380100	0.00000200
C	2.12251500	0.50960100	1.39239200
H	1.48295100	0.59354000	2.28316400
N	0.09637800	-1.98347200	1.30522700
C	2.61113300	3.00371900	1.40903100
H	2.59667000	3.00610100	2.50405900
C	-4.20561800	-0.68998500	-0.70837200
N	0.09638000	-1.98348500	-1.30520700
C	3.03577700	-0.61463600	1.40554800
H	2.99370900	-1.24487200	2.30438100
C	-2.88992100	-0.57541100	-1.40193000
H	-2.79190200	-1.19702700	-2.30368900
C	2.40210000	1.80288000	-0.70761300
C	-2.49914400	1.88429500	-0.70554700
C	-2.87137600	3.04240600	-1.40929000
H	-2.86069600	3.04543600	-2.50442200
C	-5.41452900	-0.85031200	1.40863800
H	-5.41204500	-0.86790200	2.50364100
C	-2.06931800	0.62422200	-1.38093700
H	-1.42982000	0.76509200	-2.26494600

C	5.57150900	-0.65974400	1.40936000
H	5.57067100	-0.67839100	2.50415800
C	2.61113600	3.00370300	-1.40906000
H	2.59667500	3.00607300	-2.50408700
C	-2.06932700	0.62422400	1.38093400
H	-1.42983400	0.76509500	2.26494700
C	-5.41451900	-0.85031400	-1.40866000
H	-5.41202900	-0.86790600	-2.50366300
C	-3.24728800	4.19567700	0.70328100
H	-3.53253900	5.09949400	1.24952700
C	-2.88993000	-0.57540800	1.40192300
H	-2.79191600	-1.19702400	2.30368400
C	3.03577900	-0.61465100	-1.40553700
H	2.99371300	-1.24489700	-2.30436300
C	-3.24728400	4.19567600	-0.70329600
H	-3.53253100	5.09949200	-1.24954500
C	-2.49914900	1.88429600	0.70554000
C	-0.74725100	-2.90345700	-0.70510500
H	-1.37947400	-3.56907700	-1.30036000
C	2.12251800	0.50958500	-1.39239400
H	1.48295400	0.59351500	-2.28316600
C	-4.20562300	-0.68998400	0.70835700
C	2.40209800	1.80288800	0.70759700
C	5.57151100	-0.65975900	-1.40934300
H	5.57067500	-0.67841800	-2.50414200
C	-6.61924100	-0.99194900	0.70360700
H	-7.55896100	-1.11371100	1.25001600
C	4.35253900	-0.60916500	0.70957800
C	6.78283300	-0.68730500	0.70430700
H	7.73022700	-0.71887100	1.25009100
C	4.35254000	-0.60917300	-0.70956400
C	-2.87138500	3.04240900	1.40927900
H	-2.86071100	3.04544000	2.50441100
C	0.15111800	-2.00883900	-2.77351300
H	0.42671200	-1.01623500	-3.15609700
H	-0.81979600	-2.29770600	-3.21089500
H	0.91448200	-2.73546900	-3.09953000
C	-0.74725200	-2.90345000	0.70513300
H	-1.37947600	-3.56906400	1.30039300
C	6.78283500	-0.68731300	-0.70428800
H	7.73023000	-0.71888400	-1.25007000
C	2.83138800	4.19591900	-0.70383900
H	2.99458200	5.12956700	-1.24992000
C	2.83138700	4.19592700	0.70379800
H	2.99457900	5.12958100	1.24986800
C	-6.61923700	-0.99195000	-0.70363600
H	-7.55895300	-1.11371300	-1.25005200
C	0.15111300	-2.00881200	2.77353300
H	0.91447900	-2.73543500	3.09955900
H	-0.81980100	-2.29767800	3.21091600
H	0.42670200	-1.01620200	3.15610800
H	2.35149100	-2.28294000	0.00001500
H	-0.09526000	0.36557200	0.00000100

[3(μ-H)H]$_a$

Ru	-1.43781900	-0.92199500	0.02116300
Ru	1.33873500	-0.76941800	0.04337000

C	-2.20783900	0.63569600	1.32411900
H	-1.53855800	0.83658600	2.17309100
N	-0.01781800	-1.75653100	1.36064400
C	-3.02529200	-0.54096700	1.40860500
H	-2.91308700	-1.14437400	2.32352800
C	-2.59595200	1.84900700	0.54904800
C	-2.21887700	0.45881600	-1.47811700
H	-1.55979500	0.53902000	-2.35393300
N	0.00785100	-1.86971400	-1.23521600
C	2.88966100	-0.48947200	-1.43391300
H	2.72090700	-1.08466300	-2.34468000
C	2.75824400	3.14801400	-1.10449500
H	2.65838100	3.25422600	-2.19063800
C	-4.34978500	-0.66971900	0.72407400
C	4.36821000	-0.76388900	0.52964600
C	-5.56206800	-0.76561400	1.43250600
H	-5.55276500	-0.71531500	2.52704700
C	2.30574000	0.43715400	1.52122200
H	1.77327100	0.50872400	2.48153600
C	2.96088100	2.88112600	1.67645500
H	3.02136700	2.77737300	2.76581700
C	-2.89644800	2.90218100	-1.62955500
H	-2.88198200	2.83546100	-2.72313100
C	-3.03698700	-0.71669900	-1.39341500
H	-2.93654300	-1.43580900	-2.22261400
C	-4.35610100	-0.75273000	-0.68746200
C	2.10221400	0.70954300	-1.32383400
H	1.43360000	0.95203100	-2.16369400
C	-6.77474900	-0.93386800	0.74558400
H	-7.71263600	-1.01180400	1.30451900
C	3.08760400	-0.75854500	1.29578100
H	3.02285900	-1.52264800	2.08853600
C	-2.59738500	1.76114600	-0.86141000
C	-3.20076300	4.12001900	-1.00283800
H	-3.42579100	5.00413400	-1.60756900
C	2.63439500	1.75471100	0.89663800
C	-2.89389800	3.07570100	1.17127900
H	-2.87442000	3.14517000	2.26453200
C	3.19680100	4.12712200	1.07558800
H	3.44765900	4.99392900	1.69536400
C	-6.78117200	-1.01448700	-0.65711400
H	-7.72401800	-1.15490500	-1.19513300
C	-0.07803300	-1.68512700	2.81584400
H	-0.28186500	-0.65445800	3.14162200
H	0.88119900	-2.00525500	3.27043400
H	-0.87555300	-2.34268800	3.21816200
C	0.03820500	-1.89700200	-2.69735300
H	-0.78037100	-2.53383300	-3.07984500
H	0.99416600	-2.30337700	-3.07318500
H	-0.09581600	-0.88235500	-3.10146100
C	-5.57452100	-0.92808300	-1.36930800
H	-5.57467700	-1.00462300	-2.46243400
C	5.63045500	-0.93797200	1.12621800
H	5.70545600	-1.05889800	2.21285400
C	2.52991200	1.89087700	-0.51285300
C	6.68747300	-0.82261700	-1.06238400
H	7.58806600	-0.85456800	-1.68398000
C	6.78818000	-0.96907100	0.33142400
H	7.76744400	-1.11522800	0.79855000

C	0.80474200	-2.76725800	-0.53528900
H	1.45512700	-3.45289900	-1.09590300
C	5.42863600	-0.64685700	-1.66038000
H	5.34613200	-0.54222600	-2.74826800
C	3.09557100	4.26094100	-0.31901900
H	3.26608200	5.23294600	-0.79266500
C	-3.19978500	4.20685000	0.39965300
H	-3.42341300	5.15873100	0.89141600
C	4.26663500	-0.61957000	-0.86822800
C	0.30752600	-3.11886900	0.85091000
H	-0.55387800	-3.82713500	0.88502000
H	1.12811600	-3.57046000	1.44342500
H	-0.26377000	0.26214600	-0.02951600

$[3(\mu\text{-}H)H]_a^+$

Ru	-1.41940000	-0.62623300	0.00226400
Ru	1.27936600	-0.45408800	0.03387300
C	-2.39978500	0.90602600	1.29380400
H	-1.71377800	1.22597400	2.09060500
N	-0.02802500	-1.40787600	1.38592200
C	-2.99671000	-0.36909300	1.47612900
H	-2.75508600	-0.89773000	2.40869000
C	-2.99721800	2.01310800	0.49540700
C	-2.47097100	0.65599800	-1.52516400
H	-1.81364700	0.83004200	-2.38854800
N	-0.03108000	-1.61423800	-1.25449300
C	2.87035500	-0.37110800	-1.49191800
H	2.56844800	-0.89736000	-2.40680200
C	3.46472300	3.18998300	-1.08290100
H	3.36580500	3.34401600	-2.16260700
C	-4.21564200	-0.87529100	0.78414200
C	4.19573700	-1.09007600	0.51095800
C	-5.31056500	-1.34472200	1.54048100
H	-5.27991600	-1.26597300	2.63212100
C	2.48941500	0.57875200	1.48955900
H	1.91379200	0.75047100	2.41199800
C	3.68369900	2.80746600	1.69240900
H	3.75089200	2.66667700	2.77636900
C	-3.56091100	2.93004300	-1.69105400
H	-3.57626200	2.83679500	-2.78205800
C	-3.05240200	-0.63286900	-1.45174100
H	-2.83222000	-1.32260600	-2.27877900
C	-4.24072900	-1.00869500	-0.63375700
C	2.33664400	0.93598100	-1.31606300
H	1.64963900	1.28510800	-2.10127600
C	-6.43282000	-1.89287500	0.90890100
H	-7.28403700	-2.23085700	1.50680700
C	3.00734800	-0.75501700	1.33844400
H	2.79520300	-1.46149300	2.15390700
C	-3.03669900	1.88614600	-0.90598700
C	-4.05768100	4.08894100	-1.07654400
H	-4.46407900	4.89841700	-1.68973000
C	3.09563400	1.80844100	0.89495300
C	-3.48176300	3.18426900	1.10696800
H	-3.43537400	3.28999600	2.19589700
C	4.17488500	3.98268900	1.10388700
H	4.63294300	4.75442600	1.72938300

C	-6.45641200	-2.02578600	-0.49175800
H	-7.32576500	-2.46767300	-0.98696500
C	-0.08824400	-1.29927400	2.84036700
H	-0.32628600	-0.26809400	3.13924900
H	0.87738100	-1.58254100	3.30056200
H	-0.86019700	-1.97649900	3.25349100
C	-0.00619300	-1.68387300	-2.71723700
H	-0.83541600	-2.32067400	-3.07319300
H	0.93573000	-2.12436500	-3.08572000
H	-0.12622500	-0.67901500	-3.14990700
C	-5.35791600	-1.60837400	-1.25210200
H	-5.36421500	-1.73438100	-2.33971700
C	5.34971600	-1.66075900	1.08375500
H	5.38292000	-1.84925000	2.16194500
C	2.98918700	2.00015600	-0.50056300
C	6.40332500	-1.74655200	-1.10632800
H	7.26152200	-1.99991600	-1.73540100
C	6.45439200	-1.97422500	0.28011800
H	7.35233800	-2.40481600	0.73254200
C	0.79998000	-2.44961400	-0.50866700
H	1.48794500	-3.12299500	-1.03573300
C	5.24525300	-1.21060600	-1.68862900
H	5.19657600	-1.05697800	-2.77180700
C	4.06315500	4.17501500	-0.28340500
H	4.43293700	5.09709700	-0.74118000
C	-4.01754500	4.21610200	0.32207600
H	-4.39212000	5.12535200	0.80099400
C	4.14080400	-0.86852500	-0.88647500
C	0.30260000	-2.78083500	0.88715300
H	-0.55908000	-3.48300100	0.92828900
H	1.12201000	-3.21944000	1.48781800
H	-0.52700100	0.68454000	-0.12656900

$[3(H)_2]_b$

Ru	-1.53162400	-0.89126400	0.05267500
Ru	1.29633200	-0.41573300	0.04406700
C	-2.36677800	0.63179600	1.31055000
H	-1.71588000	0.86947000	2.16665100
N	-0.02849300	-1.49541000	1.39047100
C	-3.16860400	-0.55550000	1.43047600
H	-3.06378200	-1.12512100	2.36529600
C	-2.76714200	1.82464300	0.50291500
C	-2.37913100	0.37341200	-1.48084000
H	-1.74789800	0.43930200	-2.38042300
N	-0.02402900	-1.69624000	-1.17891600
C	2.83730200	-0.35930800	-1.48820100
H	2.53614400	-0.86768800	-2.41447000
C	3.51902100	3.18424500	-1.09891300
H	3.41358700	3.33064600	-2.17959800
C	-4.49546200	-0.69325700	0.75694100
C	4.19314800	-1.05304300	0.49209500
C	-5.70974000	-0.73944000	1.46615000
H	-5.70051300	-0.65377800	2.55867800
C	2.49193500	0.61344400	1.48485300
H	1.93593200	0.79037300	2.41970500
C	3.74927200	2.82044800	1.67471000
H	3.82192900	2.68405600	2.75943400

C	-3.06845000	2.81388300	-1.70555900
H	-3.05474000	2.71438100	-2.79695600
C	-3.18215400	-0.81068400	-1.35114200
H	-3.08554500	-1.55651900	-2.15423000
C	-4.50243100	-0.81721700	-0.65078900
C	2.30959700	0.95483000	-1.28866100
H	1.61504600	1.31706400	-2.06397500
C	-6.92523800	-0.90719600	0.78348000
H	-7.86485500	-0.95158500	1.34348600
C	2.99987000	-0.72740400	1.31964900
H	2.81363600	-1.42596700	2.14862500
C	-2.76793900	1.69586100	-0.90496100
C	-3.37308700	4.05076600	-1.11527200
H	-3.59935500	4.91640600	-1.74602800
C	3.12660800	1.83000500	0.89244200
C	-3.06857000	3.06857700	1.08818000
H	-3.05220800	3.16908500	2.17934700
C	4.26051200	3.98225600	1.07516100
H	4.73809200	4.75009400	1.69200000
C	-6.93229500	-1.02950100	-0.61614800
H	-7.87733200	-1.16928800	-1.15075100
C	-0.10524300	-1.41028300	2.84540300
H	-0.47157100	-0.42077400	3.15919500
H	0.88376900	-1.57814600	3.31802900
H	-0.79855200	-2.17837300	3.24251400
C	-0.03847100	-1.82501300	-2.63846800
H	-0.80380300	-2.56594500	-2.93277500
H	0.93502000	-2.16614700	-3.03331400
H	-0.29258600	-0.86495600	-3.11206700
C	-5.72351800	-0.98477800	-1.32925200
H	-5.72503100	-1.09104700	-2.42004000
C	5.35925900	-1.60919100	1.05438900
H	5.40500200	-1.78288900	2.13520500
C	3.01370100	2.01310400	-0.50437200
C	6.38452300	-1.73066800	-1.14614900
H	7.23281200	-1.99619100	-1.78472500
C	6.45404800	-1.93860800	0.24208100
H	7.35655600	-2.36681500	0.68926300
C	0.94413200	-2.41897000	-0.47033700
H	1.67119800	-3.02142900	-1.03140000
C	5.21911500	-1.19706100	-1.71647600
H	5.15484900	-1.05319100	-2.80078300
C	4.14373200	4.16519000	-0.31287400
H	4.52871400	5.07638600	-0.78137100
C	-3.37385800	4.17816300	0.28391100
H	-3.60018200	5.14348400	0.74782000
C	4.12081800	-0.84756200	-0.90745900
C	0.52478900	-2.80151400	0.92627200
H	-0.22018700	-3.62533700	0.98205000
H	1.41307600	-3.09322400	1.52112200
H	-2.28048500	-2.26347900	0.19419900

$[3(H)_2]_b^+$

Ru	-1.41909900	-0.72340200	0.01112500
Ru	1.30964600	-0.46243100	0.01987600
C	-2.39265100	0.74149500	1.31927100
H	-1.70554900	1.00309400	2.13840000

N	0.00880400	-1.44346100	1.38349800
C	-3.06581700	-0.50600800	1.45615000
H	-2.87330400	-1.08007800	2.37170800
C	-2.89749900	1.90323900	0.53187700
C	-2.44152400	0.53378400	-1.49863600
H	-1.76238100	0.66440900	-2.35509200
N	0.01200000	-1.63492200	-1.24011600
C	2.92831500	-0.38965500	-1.49625500
H	2.64466000	-0.94586300	-2.39918200
C	3.35639100	3.21465100	-1.15558600
H	3.27184800	3.33123500	-2.24104600
C	-4.34063800	-0.84436700	0.75994100
C	4.23572000	-1.02720400	0.55059900
C	-5.50688300	-1.13520200	1.49421700
H	-5.48587900	-1.07487500	2.58731700
C	2.49173600	0.62875600	1.49010600
H	1.89300700	0.79880500	2.39782800
C	3.52616600	2.93011200	1.63346200
H	3.57153100	2.82722500	2.72268600
C	-3.33285700	2.89880100	-1.65202500
H	-3.33756200	2.82139000	-2.74438900
C	-3.10472200	-0.71952600	-1.42748500
H	-2.92300400	-1.43061200	-2.24399900
C	-4.35980600	-0.95116900	-0.65481300
C	2.36065800	0.90281300	-1.35530700
H	1.66431800	1.20720400	-2.15186100
C	-6.68875800	-1.49567200	0.83331800
H	-7.59316000	-1.70699700	1.41104500
C	3.04798300	-0.68166300	1.37047600
H	2.83198700	-1.38049100	2.19090500
C	-2.92377100	1.79853800	-0.87517100
C	-3.73268800	4.09003800	-1.02904700
H	-4.05411800	4.94090600	-1.63669200
C	3.02996600	1.86723500	0.85450800
C	-3.28023300	3.10830100	1.15047000
H	-3.24342200	3.19479300	2.24146700
C	3.95989300	4.11457400	1.02094600
H	4.35277200	4.93154300	1.63307000
C	-6.70718200	-1.60139200	-0.56905200
H	-7.62595600	-1.89468400	-1.08500200
C	-0.06884700	-1.34125100	2.83800800
H	-0.35113600	-0.32263800	3.14194800
H	0.90117100	-1.59045300	3.30883900
H	-0.82037000	-2.04986200	3.23499300
C	0.00563200	-1.73704600	-2.70253600
H	-0.78574100	-2.43911500	-3.01788500
H	0.96725700	-2.11587600	-3.08841500
H	-0.19697400	-0.75429000	-3.15423800
C	-5.54345400	-1.34641800	-1.30706200
H	-5.55103800	-1.44942800	-2.39714600
C	5.38676000	-1.57884600	1.14939000
H	5.41250000	-1.73014100	2.23355800
C	2.94583900	2.01125400	-0.55039100
C	6.45372500	-1.74351200	-1.02845900
H	7.31513900	-2.01993300	-1.64319100
C	6.49717600	-1.91885100	0.36577700
H	7.39227200	-2.33169400	0.83969900
C	0.88447200	-2.44728600	-0.50160400
H	1.59515300	-3.08565300	-1.04200000

C	5.29834200	-1.23246800	-1.63617700
H	5.25479100	-1.12165700	-2.72471000
C	3.87381300	4.25748600	-0.37454800
H	4.19849600	5.18625000	-0.85242500
C	-3.70589300	4.19480300	0.37230200
H	-4.00620100	5.12769100	0.85814800
C	4.18880200	-0.85670700	-0.85471900
C	0.43280600	-2.79752300	0.89963500
H	-0.37792800	-3.55289200	0.96328500
H	1.29688800	-3.16415700	1.48617000
H	-2.06561400	-2.13250500	0.11902800

$[3(H)_2]_c$

Ru	1.34519600	-1.12480000	0.00016600
Ru	-1.34529200	-1.12470900	-0.00015100
C	1.79950700	0.46354200	-1.39004900
H	1.12935800	0.47370700	-2.26107800
N	0.00007600	-2.15154400	-1.25708900
C	2.84082700	-0.53570400	-1.39695000
H	2.86855000	-1.19083300	-2.28306100
C	1.94951800	1.77590000	-0.70515200
C	1.80054600	0.46239700	1.39144600
H	1.13102600	0.47182800	2.26297200
N	-0.00009300	-2.15152900	1.25712100
C	-2.84099600	-0.53554800	1.39690800
H	-2.86873100	-1.19079400	2.28293100
C	-2.03742900	2.99569100	1.40207800
H	-2.02061900	2.99443300	2.49772200
C	4.15584200	-0.34173600	-0.70786800
C	-4.15647200	-0.34217000	-0.70699500
C	5.37273800	-0.22216100	-1.40394600
H	5.37076800	-0.23448000	-2.49980300
C	-1.80062800	0.46246400	-1.39153200
H	-1.13117100	0.47184700	-2.26310300
C	-2.03864800	2.99447700	-1.40547500
H	-2.02281100	2.99224700	-2.50113400
C	2.03917900	2.99438900	1.40549900
H	2.02336000	2.99218200	2.50115700
C	2.84177900	-0.53694400	1.39680300
H	2.87003400	-1.19280400	2.28235900
C	4.15633900	-0.34242500	0.70697000
C	-1.79961100	0.46361100	1.39015400
H	-1.12954100	0.47370100	2.26124100
C	6.58393500	-0.10078500	-0.70355500
H	7.52669400	-0.01514800	-1.25335100
C	-2.84191200	-0.53680400	-1.39677800
H	-2.87015200	-1.19276200	-2.28226000
C	1.95011400	1.77530800	0.70757100
C	2.13746700	4.20526200	0.70500100
H	2.20182700	5.15005500	1.25402100
C	-1.94994400	1.77535100	-0.70755700
C	2.03794100	2.99559500	-1.40208600
H	2.02113300	2.99435200	-2.49773000
C	-2.13658300	4.20538500	-0.70500000
H	-2.20063900	5.15019100	-1.25403200
C	6.58442700	-0.10147200	0.70117500
H	7.52757300	-0.01636800	1.25039100

C	0.00053900	-2.12906300	-2.72076100
H	0.00076500	-1.09418100	-3.09366600
H	-0.89422900	-2.64287600	-3.12586900
H	0.89549100	-2.64298600	-3.12535300
C	-0.00090200	-2.12904400	2.72079400
H	0.89299800	-2.64418000	3.12614500
H	-0.89672100	-2.64164200	3.12514100
H	0.00032800	-1.09416300	3.09369900
C	5.37372400	-0.22353000	1.40230700
H	5.37253100	-0.23689800	2.49815200
C	-5.37382800	-0.22314100	-1.40235200
H	-5.37262400	-0.23652200	-2.49819700
C	-1.94935800	1.77595000	0.70516300
C	-6.58405000	-0.10022000	0.70349400
H	-7.52680400	-0.01446000	1.25328000
C	-6.58452600	-0.10093600	-0.70123500
H	-7.52765400	-0.01573300	-1.25046600
C	-0.00222300	-3.55379200	0.77468500
H	-0.89393100	-4.08389900	1.17221900
H	0.88490400	-4.08834300	1.17640700
C	-5.37287400	-0.22172000	1.40390400
H	-5.37091800	-0.23401300	2.49976100
C	-2.13593500	4.20598900	0.70062500
H	-2.19947300	5.15126800	1.24890400
C	2.13681200	4.20586100	-0.70062100
H	2.20064600	5.15112400	-1.24889400
C	-4.15599200	-0.34145900	0.70784000
C	0.00154700	-3.55380100	-0.77464400
H	0.89299500	-4.08435300	-1.17217500
H	-0.88584300	-4.08791500	-1.17636000

$[3(H)_2]_c^+$

Ru	1.24569900	-0.85341300	-0.00001100
Ru	-1.24567800	-0.85343400	0.00002800
C	1.83261100	0.78991000	-1.40158400
H	1.10871400	0.87989400	-2.22325900
N	0.00000000	-1.97448200	-1.27601000
C	2.69911500	-0.32758000	-1.51531700
H	2.61299000	-0.93384000	-2.42726700
C	2.14398400	2.06446600	-0.70200900
C	1.83266100	0.78992800	1.40152400
H	1.10879800	0.87991900	2.22322700
N	0.00004000	-1.97445300	1.27605300
C	-2.69911400	-0.32758800	1.51531300
H	-2.61298400	-0.93383600	2.42727200
C	-2.39088500	3.25806200	1.40587200
H	-2.37620900	3.25950200	2.50093300
C	3.92184600	-0.61098900	-0.71858700
C	-3.92188500	-0.61102100	-0.71844600
C	5.07844900	-1.06138400	-1.39914900
H	5.06722000	-1.08866900	-2.49358500
C	-1.83267400	0.78986400	-1.40154300
H	-1.10881300	0.87984300	-2.22324900
C	-2.39094200	3.25801900	-1.40590000
H	-2.37631100	3.25942400	-2.50096200
C	2.39091200	3.25808700	1.40583100
H	2.37627500	3.25951700	2.50089300

C	2.69917200	-0.32755900	1.51523300
H	2.61308300	-0.93381100	2.42719300
C	3.92187300	-0.61097700	0.71846000
C	-1.83261800	0.78990700	1.40156900
H	-1.10872400	0.87991100	2.22324300
C	6.22946400	-1.43819900	-0.70450900
H	7.12363400	-1.74473200	-1.25477400
C	-2.69917400	-0.32763600	-1.51521700
H	-2.61308000	-0.93391100	-2.42716100
C	2.14400500	2.06447600	0.70192200
C	2.64830800	4.44408700	0.70258500
H	2.83753200	5.37160900	1.25073600
C	-2.14402600	2.06442400	-0.70196600
C	2.39087100	3.25806700	-1.40594200
H	2.37620100	3.25948200	-2.50100300
C	-2.64834000	4.44403300	-0.70268000
H	-2.83757200	5.37154200	-1.25085200
C	6.22949200	-1.43818600	0.70430800
H	7.12368300	-1.74470900	1.25454300
C	-0.00002500	-1.94299700	-2.73777700
H	-0.00002800	-0.90527700	-3.10358500
H	-0.89208900	-2.45815600	-3.14345800
H	0.89202200	-2.45816100	-3.14348900
C	0.00006000	-1.94293400	2.73781900
H	0.89212000	-2.45809000	3.14351500
H	-0.89199100	-2.45808200	3.14354000
H	0.00007000	-0.90520500	3.10360300
C	5.07850300	-1.06136000	1.39898500
H	5.06731700	-1.08862700	2.49342200
C	-5.07852300	-1.06139200	-1.39896200
H	-5.06733700	-1.08868600	-2.49339900
C	-2.14399700	2.06444600	0.70196500
C	-6.22949200	-1.43815500	0.70454200
H	-7.12366800	-1.74465500	1.25481400
C	-6.22951900	-1.43817700	-0.70427400
H	-7.12371700	-1.74469600	-1.25450100
C	0.00003100	-3.37468800	0.77405900
H	-0.88952300	-3.90410400	1.17021800
H	0.88959200	-3.90410700	1.17019700
C	-5.07846900	-1.06134700	1.39917400
H	-5.06724000	-1.08860600	2.49361100
C	-2.64831100	4.44405500	0.70262500
H	-2.83752100	5.37158100	1.25077600
C	2.64828700	4.44407700	-0.70272000
H	2.83749600	5.37159100	-1.25089100
C	-3.92185700	-0.61099800	0.71859800
C	0.00001300	-3.37470500	-0.77398500
H	0.88956800	-3.90412800	-1.17013300
H	-0.88954700	-3.90413600	-1.17011100

$[3(\mu\text{-H})(H)_2]_a$

Ru	2.46920200	12.23245200	9.50253500
Ru	1.45669600	10.22708400	7.88990700
C	3.41840800	13.66729800	8.20450300
H	3.89616500	13.20096500	7.33042500
N	3.41149000	10.47326800	8.74381400
C	4.13981800	13.59093000	9.44895800

H	5.10988700	13.07450100	9.42667300
C	2.49787700	14.80178000	7.87551000
C	1.00527500	13.82251300	9.60668200
H	-0.03505200	13.46488300	9.62382200
N	1.17333300	10.62350500	10.05421100
C	-0.51335900	9.45867500	7.37565800
H	-1.03990600	9.02736300	8.23916000
C	-1.53137300	12.32351100	5.42315700
H	-2.47829600	12.35011300	5.97382000
C	4.01845000	14.66054200	10.49115700
C	0.71359100	8.56818500	5.40067000
C	5.06168200	15.55248300	10.79424200
H	6.01006800	15.48257700	10.24925700
C	1.91761100	10.80477700	5.83115700
H	2.90667000	11.27570100	5.75881900
C	0.90903100	12.28884000	4.03822500
H	1.86757800	12.28469900	3.50749600
C	0.35853800	15.89611900	8.27499200
H	-0.59428100	15.94416100	8.81470900
C	1.73506100	13.74819200	10.84628600
H	1.19952200	13.32341100	11.70826100
C	2.79961300	14.74102200	11.19801600
C	-0.51742300	10.89194700	7.26479500
H	-1.03103300	11.45291900	8.05737700
C	4.89785600	16.51879700	11.80111900
H	5.71869000	17.20217500	12.04130400
C	1.87332700	9.37574800	5.90009300
H	2.84154200	8.85752100	5.88491900
C	1.27691400	14.87618800	8.57999200
C	0.64934100	16.83900900	7.27508100
H	-0.07651300	17.62269600	7.03545900
C	0.78003400	11.58516200	5.24749900
C	2.78663100	15.74967400	6.87823000
H	3.73047400	15.68217900	6.32497100
C	-0.18004500	13.00924100	3.52116100
H	-0.06977000	13.56832500	2.58687500
C	3.68513400	16.59928700	12.50460200
H	3.55686300	17.34584400	13.29502600
C	4.69337800	10.42800100	8.05189500
H	4.74020700	11.20793200	7.27665700
H	4.85545100	9.44317100	7.56842200
H	5.52731900	10.60032000	8.76111600
C	-0.14945300	10.69023200	10.68049000
H	-0.01480700	10.87985200	11.75946300
H	-0.71299600	9.74904700	10.55068600
H	-0.72773400	11.52220200	10.25584800
C	2.63793400	15.71339900	12.20032700
H	1.69308000	15.76932200	12.75305100
C	0.79696800	7.77906200	4.24121500
H	1.72623200	7.76132600	3.66082500
C	-0.44406400	11.60418900	5.94842900
C	-1.48331300	7.01252300	4.59418600
H	-2.33627400	6.39846200	4.28851100
C	-0.30067300	7.00085100	3.83754700
H	-0.22748200	6.37842400	2.94033300
C	1.76743500	9.40270600	9.93294700
H	1.22763400	8.50790100	10.26994500
C	-1.57091300	7.80704000	5.74920600
H	-2.49271500	7.81549000	6.34157900

C	-1.40126500	13.02414000	4.21278600
H	-2.24847400	13.59432400	3.81911300
C	1.86550000	16.76688800	6.57701000
H	2.09235300	17.49392500	5.79065000
C	-0.47589900	8.58799600	6.15850000
C	3.26911500	9.41732800	9.77047500
H	3.80682600	9.65329600	10.71565800
H	3.61578700	8.43623400	9.38833300
H	3.30926000	12.03448600	10.85916500
H	1.69988200	8.61507200	7.85029500
H	1.58014100	12.01062900	7.88475200

$[3(\mu\text{-}H)H_3]_a^+$

Ru	1.43023500	-0.97441100	0.01302300
Ru	-1.32604900	-1.08019800	-0.01646200
C	2.01857200	0.52549900	-1.39412700
H	1.41100100	0.57180100	-2.30829800
N	0.12097300	-2.10258400	-1.23360100
C	2.99923100	-0.55226000	-1.38483900
H	2.99024300	-1.17288400	-2.29039700
C	2.18641600	1.83122000	-0.70499200
C	2.01890100	0.54894900	1.42553300
H	1.45313000	0.61198500	2.36468800
N	0.11290000	-2.02827900	1.34513100
C	-2.94580900	-0.64580400	1.37884800
H	-2.93009000	-1.31196200	2.25288000
C	-2.40822400	2.94175100	1.37364300
H	-2.41573100	2.94028300	2.46895700
C	4.31790100	-0.45139900	-0.70461700
C	-4.28625300	-0.47638400	-0.71631200
C	5.53686500	-0.42464100	-1.40458900
H	5.53923500	-0.44929800	-2.49918900
C	-1.99786200	0.44291900	-1.45643900
H	-1.33074400	0.47749700	-2.32830700
C	-2.36017200	2.94827100	-1.43673000
H	-2.33140600	2.95197100	-2.53167100
C	2.21668400	3.06936300	1.40923600
H	2.18304700	3.07758700	2.50366600
C	2.99770100	-0.53960300	1.39239100
H	2.99883700	-1.14835800	2.30735800
C	4.31641900	-0.44373100	0.71462400
C	-2.00162700	0.43839800	1.38913000
H	-1.34463000	0.50840000	2.26695800
C	6.74568400	-0.37216600	-0.69638100
H	7.69441300	-0.34692900	-1.24020400
C	-2.98259000	-0.59112200	-1.44055800
H	-2.97832600	-1.27572100	-2.29909400
C	2.17199900	1.84133800	0.71980000
C	2.30772000	4.27101600	0.69734200
H	2.35624000	5.22182800	1.23586200
C	-2.20413900	1.73991900	-0.73665900
C	2.25459000	3.04633300	-1.40978100
H	2.24429900	3.04019400	-2.50467500
C	-2.54695100	4.14920000	-0.73380600
H	-2.66653400	5.08792100	-1.28257400
C	6.74471000	-0.36518300	0.71323800
H	7.69241600	-0.33496300	1.25850700

C	0.23255300	-2.15447300	-2.69081200
H	0.34404000	-1.14301100	-3.10873500
H	-0.67124800	-2.61624700	-3.13169200
H	1.10613300	-2.76039800	-2.99835100
C	0.04717900	-1.92948300	2.80863600
H	0.88358700	-2.50640500	3.23809800
H	-0.89990600	-2.34149300	3.19637400
H	0.14121000	-0.88275300	3.12838700
C	5.53461600	-0.41036100	1.41803700
H	5.53318000	-0.42349900	2.51289600
C	-5.50490600	-0.36021000	-1.40560200
H	-5.51522400	-0.33449200	-2.50041500
C	-2.22633500	1.73374200	0.67706400
C	-6.69669600	-0.34875900	0.71570700
H	-7.63680100	-0.30972500	1.27359600
C	-6.70951700	-0.29097100	-0.68798300
H	-7.65849300	-0.20618600	-1.22517800
C	-0.59311600	-3.02583800	0.73289800
H	-1.22628400	-3.68152500	1.34285000
C	-5.48009700	-0.46832800	1.40529400
H	-5.47146400	-0.52062300	2.49917000
C	-2.57253200	4.14533500	0.67093200
H	-2.71306700	5.08145700	1.21926900
C	2.32851100	4.25966200	-0.71259700
H	2.39230800	5.20196600	-1.26437800
C	-4.26917800	-0.52828700	0.69348100
C	-0.07795700	-3.43815900	-0.62280700
H	0.85331400	-4.04323000	-0.57417900
H	-0.85202100	-4.00666400	-1.17127200
H	2.39277300	-2.25890100	-0.02709800
H	-2.42593700	-2.23034200	-0.33569400
H	-0.03657700	0.15702000	-0.05473900

[3(μ-H)H$_3$]$_b$

Ru	2.41264700	12.24057200	9.39885000
Ru	1.39080100	10.23381300	7.81569500
C	3.39163900	13.73905900	8.11938800
H	3.84338300	13.27319700	7.23268700
N	3.31877000	10.46557700	8.64741100
C	4.09807100	13.59239400	9.35202700
H	5.04684700	13.03485400	9.30148700
C	2.46338700	14.86883300	7.82989000
C	0.94689300	13.87014400	9.54049900
H	-0.08300300	13.48793300	9.51770100
N	1.16636600	10.58623900	9.88865300
C	-0.57081400	9.48867700	7.28811400
H	-1.10877100	9.07350000	8.15305200
C	-1.52389900	12.38763300	5.32229900
H	-2.46896900	12.45540500	5.87333200
C	3.99342400	14.56064500	10.48751400
C	0.70301800	8.51342700	5.38969500
C	5.08451300	15.34719900	10.90308000
H	6.03403800	15.28061200	10.36045300
C	1.86928600	10.76902000	5.77880800
H	2.86176500	11.23380800	5.67843100
C	0.90774100	12.23513500	3.93277600
H	1.86322300	12.18264400	3.39832200

C	0.31469600	15.94869300	8.23856200
H	-0.63961700	15.98311500	8.77549400
C	1.65550600	13.72852100	10.77251100
H	1.09882800	13.25567000	11.59706800
C	2.77148300	14.62954500	11.19712300
C	-0.56060100	10.92083700	7.16818600
H	-1.10010100	11.48256200	7.94562100
C	4.96343400	16.20529400	12.00681700
H	5.81775500	16.81181700	12.32335700
C	1.84362900	9.33655800	5.90102800
H	2.81799600	8.82584300	5.89394000
C	1.24153900	14.93273900	8.53867800
C	0.60196900	16.90373000	7.25261500
H	-0.12717900	17.68667600	7.02229400
C	0.75788800	11.54817500	5.15126000
C	2.73847300	15.82285000	6.83180000
H	3.67599300	15.75878500	6.26869600
C	-0.15080400	12.99528200	3.40965900
H	-0.02193900	13.53571400	2.46638700
C	3.74954400	16.27437500	12.71117000
H	3.65431000	16.93478700	13.57877800
C	4.56830400	10.43452100	7.88881000
H	4.48581000	11.05735200	6.98632200
H	4.80475600	9.39976200	7.57173300
H	5.42145600	10.80557900	8.49323100
C	-0.11558600	10.69585000	10.58227800
H	0.00980100	11.09594900	11.60924100
H	-0.59922800	9.70272600	10.66579200
H	-0.79524100	11.36191800	10.03074000
C	2.66109000	15.48466900	12.31007900
H	1.71810400	15.52577800	12.86646700
C	0.81532100	7.65901400	4.27833700
H	1.76844200	7.59288900	3.74122300
C	-0.46701700	11.62423900	5.85094000
C	-1.49690200	6.96069000	4.56361900
H	-2.35014800	6.35056300	4.25016600
C	-0.28015600	6.88228700	3.86624900
H	-0.18145900	6.21100000	3.00706500
C	2.10694700	9.74080900	10.66227800
H	1.67298100	8.73059000	10.79469900
H	2.24963200	10.16253700	11.68205100
C	-1.61516400	7.81495100	5.67241200
H	-2.56040800	7.87132000	6.22431800
C	-1.36847500	13.07158200	4.10553200
H	-2.19279600	13.67157300	3.70684000
C	1.81631100	16.84094000	6.54843100
H	2.03706700	17.57474600	5.76708300
C	-0.52005700	8.59099500	6.09176600
C	3.45047400	9.67642000	9.89532000
H	4.28339900	10.07869200	10.51413400
H	3.71837200	8.63123900	9.64563800
H	1.59180700	12.24033200	8.00176200
H	1.41299900	8.66370200	8.03283800

$[3(\mu\text{-}H)H_3]_b^+$

Ru	-1.32092700	-0.67308100	-0.00001100
Ru	1.31779200	-0.85793300	-0.00003200

C	-2.17699900	0.87442700	1.42272400
H	-1.48325100	1.05740500	2.25511700
N	-0.06279600	-1.81113900	1.26661200
C	-2.88974000	-0.34447200	1.48891700
H	-2.72049900	-0.96421900	2.38045500
C	-2.62905700	2.09599200	0.70326300
C	-2.17703200	0.87443800	-1.42273000
H	-1.48329700	1.05741600	-2.25513400
N	-0.06280300	-1.81114400	-1.26665100
C	2.95777000	-0.57079100	-1.44518800
H	2.84019100	-1.22254700	-2.32049700
C	2.90461700	3.04671800	-1.40553000
H	2.89323300	3.04870900	-2.50065700
C	-4.10824400	-0.70977900	0.71414600
C	4.24813100	-0.73028900	0.71003100
C	-5.24329400	-1.19417300	1.40143100
H	-5.23212000	-1.21893500	2.49598600
C	2.17409600	0.61789300	1.40616800
H	1.47999000	0.75496300	2.24822700
C	2.90450200	3.04676200	1.40547200
H	2.89303200	3.04878800	2.50059800
C	-3.01262200	3.25457100	-1.40473500
H	-2.99533400	3.25906300	-2.49960500
C	-2.88977500	-0.34445800	-1.48891200
H	-2.72054900	-0.96420500	-2.38045400
C	-4.10826200	-0.70977000	-0.71411500
C	2.17417800	0.61785900	-1.40621000
H	1.48010400	0.75492300	-2.24829800
C	-6.37831400	-1.61958400	0.70382500
H	-7.25848600	-1.96528300	1.25338600
C	2.95770200	-0.57074700	1.44518700
H	2.84008800	-1.22249900	2.32049300
C	-2.62907100	2.09599800	-0.70324800
C	-3.41099000	4.40131100	-0.70242200
H	-3.70817900	5.29949600	-1.25134100
C	2.57500100	1.87234300	0.70440500
C	-3.01259600	3.25455900	1.40476600
H	-2.99528600	3.25904100	2.49963600
C	3.24196100	4.21336200	0.70242300
H	3.49539800	5.12529400	1.25084800
C	-6.37833200	-1.61957300	-0.70375100
H	-7.25851800	-1.96526500	-1.25329500
C	-0.03552400	-1.75968700	2.72828600
H	0.07216900	-0.72121000	3.07325000
H	0.81163900	-2.35194700	3.12205600
H	-0.96361000	-2.18015700	3.16055200
C	-0.03554400	-1.75968400	-2.72832600
H	-0.96364200	-2.18013300	-3.16058700
H	0.81160400	-2.35195800	-3.12210600
H	0.07216600	-0.72120700	-3.07328200
C	-5.24332900	-1.19415400	-1.40137900
H	-5.23218200	-1.21890000	-2.49593500
C	5.45215900	-0.95037500	1.40530200
H	5.44805000	-0.97116300	2.50009700
C	2.57505700	1.87232200	-0.70445300
C	6.65083700	-1.13793300	-0.70327000
H	7.58424500	-1.29509500	-1.25141800
C	6.65080700	-1.13789300	0.70345800
H	7.58419200	-1.29502300	1.25165500

C	-0.30219900	-3.19839700	-0.77577300
H	0.48505000	-3.86673700	-1.17186800
H	-1.26967400	-3.56773300	-1.17384900
C	5.45222000	-0.95045200	-1.40517500
H	5.44815800	-0.97129700	-2.49997000
C	3.24202100	4.21334000	-0.70249000
H	3.49550400	5.12525400	-1.25092300
C	-3.41097800	4.40130500	0.70247100
H	-3.70815700	5.29948400	1.25140400
C	4.24816200	-0.73032500	-0.70996800
C	-0.30216600	-3.19840200	0.77573600
H	-1.26961100	-3.56777100	1.17385000
H	0.48512600	-3.86671100	1.17179600
H	-0.29171200	0.54344600	-0.00003900
H	2.14040200	-2.19625800	-0.00000200

$[3(\mu\text{-}H)H_3]_c$

Ru	1.37468100	-0.93985800	-0.00042200
Ru	-1.37447100	-0.93965600	-0.00040500
C	2.13108000	0.56670600	-1.41722300
H	1.48863500	0.68073700	-2.30313400
N	0.00009700	-2.10279900	-1.24058100
C	2.98901100	-0.58224300	-1.39572900
H	2.92289400	-1.26043300	-2.25835100
C	2.46796300	1.84106300	-0.70730200
C	2.12977000	0.56723500	1.41643800
H	1.48640700	0.68156100	2.30165700
N	0.00017300	-2.10326200	1.23910500
C	-2.98769200	-0.58195100	1.39613000
H	-2.92080000	-1.25994600	2.25884300
C	-2.74185500	3.03272900	1.40211400
H	-2.72902100	3.03278800	2.49782300
C	4.31735600	-0.56117200	-0.70388100
C	-4.31711600	-0.56141800	-0.70409800
C	5.53670200	-0.56317900	-1.40276100
H	5.53410500	-0.57288900	-2.49848300
C	-2.13101900	0.56701800	-1.41701800
C	-2.74318900	3.03261600	-1.40210300
H	-2.73137600	3.03259200	-2.49782300
C	2.74123800	3.03300200	1.40153900
H	2.72838800	3.03322900	2.49724800
C	2.98776600	-0.58168800	1.39623700
H	2.92089600	-1.25949100	2.25910100
C	4.31672200	-0.56089000	0.70558800
C	-2.12984100	0.56708100	1.41662700
H	-1.48660600	0.68141300	2.30193300
C	6.75304300	-0.56667500	-0.70021300
H	7.70002100	-0.57909700	-1.24897700
C	-2.98872200	-0.58210700	-1.39585100
H	-2.92235600	-1.26013000	-2.25858300
C	2.46728900	1.84133600	0.70634700
C	3.01439800	4.21918000	0.70121700
H	3.21469500	5.14387900	1.25140400
C	-2.46825100	1.84118300	-0.70689800
C	2.74258900	3.03247000	-1.40267100
H	2.73078700	3.03228300	-2.49839100
C	-3.01598900	4.21887900	-0.70179100

H	-3.21706800	5.14339900	-1.25199300
C	6.75241400	-0.56639700	0.70411100
H	7.69889900	-0.57860100	1.25373000
C	0.00028900	-2.08268500	-2.70091100
H	-0.00010000	-1.04386600	-3.06500600
H	-0.89529300	-2.59032300	-3.11153700
H	0.89639600	-2.58958200	-3.11130400
C	0.00024100	-2.08402700	2.69944600
H	0.89586200	-2.59197700	3.10959000
H	-0.89581100	-2.59113600	3.10969600
H	0.00075300	-1.04545100	3.06420500
C	5.53544100	-0.56262900	1.40556200
H	5.53186000	-0.57190300	2.50128600
C	-5.53640700	-0.56359700	-1.40307700
H	-5.53372600	-0.57324600	-2.49880000
C	-2.46759100	1.84124000	0.70673900
C	-6.75228900	-0.56710500	0.70369800
H	-7.69881500	-0.57947600	1.25324300
C	-6.75280300	-0.56732700	-0.70062600
H	-7.69973300	-0.57988800	-1.24947000
C	-0.00003400	-3.43657000	0.67072800
H	-0.00034400	-4.30975900	1.32724300
C	-5.53537200	-0.56317900	1.40524600
H	-5.53187200	-0.57251000	2.50097000
C	-3.01532000	4.21893600	0.70196500
H	-3.21586500	5.14350300	1.25228400
C	3.01507500	4.21891200	-0.70253600
H	3.21590900	5.14340000	-1.25288200
C	-4.31660000	-0.56123000	0.70536900
C	-0.00004500	-3.43628700	-0.67280100
H	-0.00033000	-4.30923700	-1.32964400
H	2.31103500	-2.20653300	0.00008900
H	-2.31061200	-2.20648700	-0.00011700
H	-0.00011900	0.39960700	-0.43797000
H	-1.48855200	0.68139900	-2.30287100
H	0.00019900	0.39982100	0.43600900

$[3(\mu\text{-}H)H_3]_c^+$

Ru	-1.37132300	-0.89588700	0.00001800
Ru	1.37130300	-0.89587200	0.00003400
C	-2.19247600	0.58138600	1.41769300
H	-1.53084600	0.70081400	2.28888000
N	-0.00000200	-2.05132700	1.31344600
C	-3.01536900	-0.58806300	1.39953900
H	-2.91559700	-1.27376400	2.25267800
C	-2.54875000	1.84597000	0.70637800
C	-2.19231700	0.58153600	-1.41760100
H	-1.53059700	0.70105800	-2.28870800
N	0.00002300	-2.05136100	-1.31334600
C	3.01523600	-0.58797200	-1.39960900
H	2.91538500	-1.27361900	-2.25278100
C	2.84047000	3.03117500	-1.40530000
H	2.82783600	3.03410800	-2.50039000
C	-4.34038000	-0.61646400	0.70350000
C	4.34034500	-0.61645600	0.70359300
C	-5.55608700	-0.65333700	1.40688500
H	-5.55559000	-0.66543500	2.50198700

C	2.19244900	0.58146600	1.41767900
C	2.84057100	3.03115300	1.40534800
H	2.82801400	3.03407000	2.50043800
C	-2.84039900	3.03123500	-1.40518500
H	-2.82774000	3.03421800	-2.50027400
C	-3.01521200	-0.58791500	-1.39966100
H	-2.91534300	-1.27352400	-2.25286100
C	-4.34030200	-0.61639000	-0.70377400
C	2.19235700	0.58148700	-1.41762300
H	1.53065900	0.70097800	-2.28875000
C	-6.76996100	-0.68423400	0.70181700
H	-7.71595100	-0.72027100	1.24975100
C	3.01531600	-0.58799900	1.39959900
H	2.91550700	-1.27365900	2.25276500
C	-2.54866900	1.84604600	-0.70619100
C	-3.14448100	4.20691800	-0.70204800
H	-3.37025300	5.12584200	-1.25068400
C	2.54875800	1.84601100	0.70630900
C	-2.84056200	3.03108500	1.40546400
H	-2.82802800	3.03395200	2.50055500
C	3.14460600	4.20687500	0.70225400
H	3.37044300	5.12576100	1.25092600
C	-6.76988300	-0.68416100	-0.70237000
H	-7.71581200	-0.72014100	-1.25041200
C	-0.00000800	-2.05243400	2.77912600
H	0.00004500	-1.01793600	3.14944000
H	0.89596500	-2.56507900	3.17307300
H	-0.89603700	-2.56498500	3.17306800
C	0.00003800	-2.05252200	-2.77902700
H	-0.89593000	-2.56518500	-3.17296100
H	0.89607100	-2.56508600	-3.17294200
H	-0.00001500	-1.01803900	-3.14937900
C	-5.55593000	-0.65319000	-1.40729900
H	-5.55531100	-0.66517300	-2.50240100
C	5.55603100	-0.65332200	1.40701300
H	5.55550500	-0.66537600	2.50211400
C	2.54870700	1.84602200	-0.70625900
C	6.76988500	-0.68424700	-0.70220800
H	7.71582800	-0.72026200	-1.25022300
C	6.76992500	-0.68426600	0.70197900
H	7.71589900	-0.72029600	1.24994000
C	-0.00001600	-3.29511000	-0.69512400
H	-0.00004900	-4.21655300	-1.28839300
C	5.55595100	-0.65328400	-1.40717100
H	5.55536200	-0.66531000	-2.50227300
C	3.14455500	4.20688600	-0.70221000
H	3.37035300	5.12578100	-1.25088300
C	-3.14456200	4.20684300	0.70241700
H	-3.37039800	5.12570800	1.25112500
C	4.34030500	-0.61643800	-0.70368100
C	-0.00003000	-3.29509400	0.69525800
H	-0.00007200	-4.21652200	1.28855000
H	-2.31423000	-2.15071300	-0.00009300
H	2.31419600	-2.15071200	0.00000200
H	0.00004600	0.49268500	0.42762000
H	1.53080100	0.70094700	2.28884500
H	-0.00000100	0.49273000	-0.42739800

[3(μ-H)]$^+$

Ru	1.45880500	-0.95237300	0.00000600
Ru	-1.30541600	-0.87609900	0.00000100
C	2.14766800	0.60391200	1.40800500
H	1.44609700	0.70089200	2.24870000
N	0.09126300	-1.94590200	1.32393200
C	2.69670700	3.07555000	1.40609400
H	2.68010000	3.07833600	2.50104500
C	-4.29080300	-0.68105500	-0.70318200
N	0.09126700	-1.94591200	-1.32391700
C	3.01446800	-0.52526400	1.43788900
H	2.92456400	-1.18668900	2.31359800
C	-2.95953200	-0.65391500	-1.38029200
H	-2.86201400	-1.34285900	-2.23401700
C	2.45746700	1.87926100	-0.70454400
C	-2.46463200	1.78589600	-0.70684900
C	-2.73875300	2.97520300	-1.40565900
H	-2.72406200	2.97785900	-2.50083600
C	-5.50616300	-0.72722200	1.40790000
H	-5.50522000	-0.73808000	2.50310900
C	-2.11702700	0.51360500	-1.41476200
H	-1.47398800	0.63395000	-2.29962200
C	5.52321000	-0.82251500	1.40454500
H	5.51896800	-0.84557300	2.49930800
C	2.69671300	3.07553800	-1.40610900
H	2.68011100	3.07831500	-2.50106100
C	-2.11703000	0.51361700	1.41474900
H	-1.47399300	0.63397200	2.29961000
C	-5.50615900	-0.72723500	-1.40790900
H	-5.50521400	-0.73810200	-2.50311800
C	-3.02781700	4.15472000	0.70255800
H	-3.24345000	5.07643100	1.25082400
C	-2.95953500	-0.65390200	1.38028800
H	-2.86201900	-1.34283900	2.23401900
C	3.01447500	-0.52527500	-1.43787400
H	2.92457400	-1.18670700	-2.31357800
C	-3.02781600	4.15471400	-0.70260600
H	-3.24344700	5.07641900	-1.25088100
C	-2.46463400	1.78590300	0.70682300
C	-0.66872400	-2.91295400	-0.71260100
H	-1.26824100	-3.62364900	-1.29321900
C	2.14767400	0.60390100	-1.40800300
H	1.44610600	0.70087300	-2.24870100
C	-4.29080500	-0.68104900	0.70317500
C	2.45746400	1.87926700	0.70453800
C	5.52321600	-0.82252600	-1.40451600
H	5.51897900	-0.84559200	-2.49927900
C	-6.71950700	-0.76862500	0.70245700
H	-7.66562500	-0.81263400	1.24974900
C	4.31324900	-0.62806100	0.70934500
C	6.72625400	-0.97759100	0.70338000
H	7.66303100	-1.11238400	1.25172300
C	4.31325200	-0.62806600	-0.70932300
C	-2.73875600	2.97521600	1.40562200
H	-2.72406700	2.97788200	2.50080000
C	0.12592500	-1.95140400	-2.79264000
H	0.34219800	-0.93909500	-3.16068100
H	-0.83269900	-2.29042900	-3.22086100

H	0.92671400	-2.62668300	-3.13997800
C	-0.66872600	-2.91294900	0.71262000
H	-1.26824500	-3.62364000	1.29324100
C	6.72625800	-0.97759700	-0.70334500
H	7.66303600	-1.11239400	-1.25168200
C	2.95260700	4.26145900	-0.70282200
H	3.13934400	5.18953500	-1.25075400
C	2.95260400	4.26146500	0.70279800
H	3.13933900	5.18954500	1.25072300
C	-6.71950500	-0.76863200	-0.70246900
H	-7.66562200	-0.81264500	-1.24976200
C	0.12591600	-1.95138400	2.79265400
H	0.92670400	-2.62666100	3.14000000
H	-0.83270900	-2.29040700	3.22087500
H	0.34218800	-0.93907200	3.16068900
H	0.26655800	0.20560000	-0.00000100

$[3(\mu\text{-}H)(H)_2]_a^+$

Ru	1.34487700	-0.79642600	0.03624200
Ru	-1.39853400	-1.10410800	-0.00570100
C	2.04576200	0.77578800	-1.37443800
H	1.32506300	0.90921300	-2.19381400
N	0.09371200	-1.93573400	-1.26186900
C	2.85227000	-0.38701200	-1.46611300
H	2.71862400	-1.00804000	-2.36300500
C	2.43631900	2.03182600	-0.67536800
C	2.09941300	0.77918500	1.44459600
H	1.41252900	0.91231500	2.29244300
N	0.09975600	-1.89981700	1.37198100
C	-3.05924000	-0.65877200	1.39706100
H	-3.04971400	-1.33928100	2.26028000
C	-2.36846600	2.91764100	1.36200500
H	-2.39759300	2.91991600	2.45685600
C	4.11477100	-0.65074000	-0.72356500
C	-4.36484400	-0.48638700	-0.71562200
C	5.27190900	-1.04105300	-1.43370300
H	5.23994100	-1.07310300	-2.52771400
C	-2.06404900	0.40208500	-1.47140600
H	-1.40420400	0.42003900	-2.34846500
C	-2.23650700	2.91746600	-1.44284000
H	-2.17185800	2.91616500	-2.53617700
C	2.78228100	3.21486300	1.42482500
H	2.78591800	3.21933400	2.51994100
C	2.90606900	-0.38465000	1.49242900
H	2.80457500	-1.01764000	2.38644200
C	4.14384500	-0.64255700	0.70374700
C	-2.10759400	0.40348400	1.41309600
H	-1.44833100	0.46700700	2.28926100
C	6.45327900	-1.36417400	-0.75849500
H	7.34804800	-1.63820400	-1.32472600
C	-3.05239900	-0.62060600	-1.41959900
H	-3.03996600	-1.33827500	-2.25211000
C	2.45998800	2.03415600	0.73004400
C	3.09360200	4.38361200	0.71451400
H	3.34293900	5.30009400	1.25715700
C	-2.20164200	1.69718100	-0.74147600
C	2.73616300	3.20908500	-1.38548700

H	2.70305500	3.20958500	-2.48012500
C	-2.36074600	4.12866700	-0.74737700
H	-2.39434700	5.07249800	-1.29909800
C	6.48267300	-1.35385500	0.64879200
H	7.40054700	-1.61976600	1.18094100
C	0.15375400	-1.96129800	-2.72256400
H	0.16143400	-0.93810400	-3.12701600
H	-0.71805900	-2.49730800	-3.14244600
H	1.06662600	-2.48077400	-3.07257900
C	-0.00335500	-1.83254600	2.83398700
H	0.83576400	-2.39698000	3.27569600
H	-0.94981900	-2.27168300	3.19340500
H	0.06619200	-0.78940300	3.17097600
C	5.33008600	-1.02178000	1.36882100
H	5.34388600	-1.04127100	2.46353400
C	-5.57228900	-0.35810100	-1.42386500
H	-5.56532500	-0.33308700	-2.51872000
C	-2.26236700	1.69527400	0.67353500
C	-6.79651100	-0.33460000	0.67770000
H	-7.74442000	-0.28706100	1.22154600
C	-6.78718800	-0.27787200	-0.72540000
H	-7.72690200	-0.18610000	-1.27754200
C	-0.46432900	-2.95886500	0.71809400
H	-1.04890200	-3.69130700	1.28990100
C	-5.59152300	-0.46438800	1.38593800
H	-5.60015500	-0.51459400	2.47990100
C	-2.42948700	4.12833700	0.65590100
H	-2.51646600	5.07260400	1.20115000
C	3.07097400	4.38065300	-0.69040200
H	3.30267800	5.29482800	-1.24461500
C	-4.37110300	-0.53660200	0.69146700
C	0.10261400	-3.28864700	-0.64719500
H	1.10927700	-3.76530700	-0.61644200
H	-0.57734000	-3.97247800	-1.18904100
H	-2.49251200	-2.23024000	-0.20110700
H	0.23265400	0.34000700	0.03093100

$[3(\mu\text{-}H)(H)_2]_b^+$

Ru	1.37898700	-1.06086900	0.04631700
Ru	-1.43193100	-0.99494500	0.02405900
C	2.06684500	0.35810600	-1.44224400
H	1.36590000	0.35922700	-2.29138500
N	-0.00019000	-2.07927800	-1.17370900
C	2.99540600	-0.72373700	-1.40168200
H	2.95190300	-1.45171500	-2.22355600
C	2.30165800	1.70098300	-0.82995000
C	2.04636800	0.54925900	1.36273000
H	1.39808000	0.67229900	2.24325900
N	0.11610000	-2.06248900	1.44018700
C	-3.11723200	-0.60739800	1.35149300
H	-3.14323200	-1.34230800	2.17164100
C	-2.46795300	2.96451800	1.63200600
H	-2.58011000	2.88395800	2.71828300
C	4.31121800	-0.61706200	-0.70450800
C	-4.25397400	-0.34481200	-0.84975700
C	5.53063000	-0.65999500	-1.40468000
H	5.52966000	-0.77546200	-2.49379500

C	-1.91646000	0.67577000	-1.34598300
H	-1.17194200	0.74759200	-2.14941100
C	-2.10932500	3.17858900	-1.14737800
H	-1.94503400	3.26235400	-2.22657300
C	2.42074100	3.05828200	1.19036200
H	2.38697900	3.13807600	2.28236900
C	2.99410800	-0.52213500	1.41194600
H	2.98225400	-1.14492300	2.31804500
C	4.31003500	-0.48732500	0.70232100
C	-2.18568100	0.45995600	1.50792600
H	-1.57467800	0.44537200	2.42114800
C	6.74422600	-0.55638900	-0.70866600
H	7.69074500	-0.59078200	-1.25600300
C	-2.88437600	-0.36379300	-1.44402300
H	-2.75728600	-1.03895200	-2.30675300
C	2.27272400	1.80065200	0.57752700
C	2.60997900	4.20716900	0.40700800
H	2.72558700	5.18232400	0.88937900
C	-2.12760700	1.90821500	-0.54044300
C	2.48211900	2.85678000	-1.61172900
H	2.49575500	2.77788700	-2.70433600
C	-2.30364300	4.33063300	-0.37413700
H	-2.29751700	5.31409900	-0.85252500
C	6.74423200	-0.42087500	0.69041100
H	7.69100100	-0.35138900	1.23404500
C	0.02116700	-2.15648400	-2.63712100
H	0.21998000	-1.16471200	-3.06910600
H	-0.94289700	-2.52603400	-3.03825100
H	0.81579400	-2.84578400	-2.97832800
C	0.07991900	-1.90269500	2.89766800
H	0.97216300	-2.39995500	3.31457500
H	-0.82415800	-2.35415100	3.34113200
H	0.13220200	-0.83764900	3.16143200
C	5.53063600	-0.39245600	1.39416000
H	5.53107800	-0.30688700	2.48611500
C	-5.40815600	-0.27556600	-1.65209700
H	-5.31344400	-0.17972500	-2.73874900
C	-2.30020300	1.79775900	0.86183200
C	-6.79646500	-0.48870600	0.33457100
H	-7.78663600	-0.55007700	0.79523500
C	-6.67707900	-0.33329800	-1.05746800
H	-7.57332700	-0.27291400	-1.68142700
C	-0.63071600	-3.02327300	0.88613800
H	-1.28856000	-3.64151300	1.51545900
C	-5.64815600	-0.57985300	1.13515900
H	-5.74197600	-0.71455200	2.21780100
C	-2.48730800	4.22316400	1.01574000
H	-2.62663600	5.12331900	1.62120900
C	2.64381900	4.10648700	-0.99420600
H	2.78798300	5.00223700	-1.60556200
C	-4.37215800	-0.49621500	0.54840000
C	-0.38116000	-3.36935600	-0.55622700
H	0.41520100	-4.14153600	-0.65860600
H	-1.30059700	-3.79784600	-1.01163800
H	2.36218100	-2.28597700	0.14844000
H	-0.29731600	0.12490500	0.21391000

$[3(\mu\text{-H})(H)_2]_c^+$

Ru	-1.29715400	-0.57413000	0.00000400
Ru	1.29722000	-0.57408200	0.00000400
C	-2.09917100	1.01831200	1.40816800
H	-1.41727900	1.26271500	2.23534800
N	0.00008000	-1.68252300	1.24560400
C	-2.74464000	-0.22893900	1.56132900
H	-2.56368600	-0.76949600	2.49979800
C	-2.64480800	2.20773500	0.70013500
C	-2.09914800	1.01831500	-1.40815400
H	-1.41725100	1.26271700	-2.23533000
N	0.00008100	-1.68252700	-1.24558900
C	2.74473300	-0.22880800	-1.56131300
H	2.56381100	-0.76935400	-2.49979600
C	3.11967400	3.32998500	-1.40521100
H	3.10314200	3.33467100	-2.50025700
C	-3.77922200	-0.86949400	0.72473500
C	3.77933300	-0.86937600	0.72473500
C	-4.70613500	-1.71855400	1.39502400
H	-4.68974700	-1.73516700	2.48951700
C	2.09924700	1.01842000	1.40821600
H	1.41742100	1.26279800	2.23545600
C	3.11970100	3.32998300	1.40520800
H	3.10319000	3.33466700	2.50025500
C	-3.11999900	3.32973500	-1.40521400
H	-3.10348000	3.33441800	-2.50026100
C	-2.74462600	-0.22893200	-1.56132800
H	-2.56366800	-0.76948400	-2.49979900
C	-3.77921900	-0.86948600	-0.72474700
C	2.09922700	1.01841900	-1.40820500
H	1.41740000	1.26280200	-2.23544300
C	-5.64636900	-2.47637300	0.70624500
H	-6.37628800	-3.07617700	1.25736200
C	2.74474600	-0.22881000	1.56131300
H	2.56382100	-0.76936400	2.49979100
C	-2.64479400	2.20773800	-0.70012900
C	-3.60422800	4.44316900	-0.70257600
H	-3.96912100	5.31640600	-1.25110200
C	2.64470100	2.20789100	0.70013500
C	-3.12002900	3.32972800	1.40521600
H	-3.10353300	3.33440600	2.50026300
C	3.60371400	4.44351200	0.70256800
H	3.96844700	5.31681500	1.25109600
C	-5.64636700	-2.47636400	-0.70628100
H	-6.37628500	-3.07616100	-1.25740800
C	0.00007200	-1.62827900	2.70649400
H	-0.00005800	-0.58402100	3.05223300
H	0.89024300	-2.13935100	3.12163700
H	-0.88996100	-2.13959500	3.12162700
C	0.00007200	-1.62828800	-2.70647900
H	-0.88995700	-2.13961400	-3.12160900
H	0.89024600	-2.13935400	-3.12162000
H	-0.00006800	-0.58403200	-3.05222300
C	-4.70613000	-1.71853800	-1.39504900
H	-4.68973800	-1.73513800	-2.48954200
C	4.70624600	-1.71842200	1.39503100
H	4.68986600	-1.73503500	2.48952400
C	2.64468800	2.20789200	-0.70013100
C	5.64648500	-2.47622700	-0.70627600
H	6.37641000	-3.07602000	-1.25739800

C	5.64648600	-2.47623400	0.70624700
H	6.37641200	-3.07603300	1.25736200
C	0.00005800	-3.08970300	-0.77064100
H	0.89084600	-3.61271300	-1.17137900
H	-0.89074700	-3.61268000	-1.17137900
C	4.70624300	-1.71841000	-1.39505100
H	4.68985900	-1.73501400	-2.48954400
C	3.60370000	4.44351400	-0.70257800
H	3.96842200	5.31681800	-1.25111200
C	-3.60424300	4.44316600	0.70257200
H	-3.96914900	5.31640000	1.25109500
C	3.77933000	-0.86937000	-0.72474600
C	0.00005800	-3.08970000	0.77066100
H	-0.89074800	-3.61267600	1.17139900
H	0.89084500	-3.61271000	1.17140100
H	0.00005200	0.58497900	0.00000800

[K][3_2(μ-H)]

Ru	-1.76390	-0.62259	-0.16828
Ru	-4.07168	0.82364	0.31673
C	-6.57879	2.04321	1.48264
N	-2.18898	0.71189	1.44429
N	-2.42871	1.17056	-1.11275
C	-3.37149	-3.17278	0.20106
C	-0.49195	-3.08474	-1.45815
C	-1.02435	-2.36302	0.85391
H	-0.43343	-2.15445	1.76047
C	-1.21230	-1.83585	-1.85260
H	-0.78084	-1.28548	-2.70464
C	-6.45563	-0.94102	0.93324
C	-3.45683	-2.92864	-1.18396
C	-0.43010	-3.37453	-0.07558
C	-6.58190	-0.68907	-0.44918
C	-2.46618	-2.27128	0.97605
H	-2.86364	-1.98448	1.96130
C	-2.65630	-1.77932	-1.70711
H	-3.19770	-1.17813	-2.45225
C	-5.34421	-0.23013	1.63932
H	-4.81993	-0.83783	2.39589
C	-2.33382	2.04240	1.07905
H	-2.36943	2.84106	1.82727
C	-4.30017	-3.71971	-1.98071
H	-4.37608	-3.51678	-3.05631
C	-7.33206	-1.84211	1.56008
H	-7.22037	-2.04702	2.63209
C	0.16903	-4.57170	0.35630
H	0.20024	-4.80025	1.42914
C	-2.45568	2.28907	-0.29851
H	-2.58739	3.29386	-0.71128
C	-7.58360	-1.34100	-1.18722
H	-7.66842	-1.15384	-2.26485
C	-5.58666	0.25629	-1.04544
H	-5.21901	-0.03772	-2.04265
C	0.08391	-3.97925	-2.37936
H	0.03823	-3.75075	-3.45165
C	-4.13344	-4.20124	0.77791

H	-4.07891	-4.37540	1.85979
C	-6.70191	2.29541	0.09738
C	-4.98251	-4.98444	-0.02049
H	-5.59313	-5.77010	0.43825
C	-5.41263	1.20586	1.90836
H	-4.93333	1.54585	2.84251
C	-8.32602	-2.49827	0.81647
H	-8.99288	-3.21587	1.30811
C	-5.65445	1.69443	-0.78664
H	-5.33106	2.34863	-1.61386
C	-7.49912	2.61421	2.37766
H	-7.39274	2.42579	3.45337
C	0.71110	-5.15653	-1.93892
H	1.16249	-5.84176	-2.66544
C	-2.00511	0.48100	2.87629
H	-2.21684	-0.57036	3.11980
H	-2.67016	1.12384	3.48461
H	-0.95565	0.69452	3.15441
C	-7.74294	3.11498	-0.36997
H	-7.82749	3.31873	-1.44475
C	-2.54598	1.43825	-2.54669
H	-1.53729	1.51701	-2.98863
H	-3.08768	2.38207	-2.74076
H	-3.08340	0.61741	-3.04428
C	-5.06462	-4.74478	-1.40038
H	-5.73866	-5.34371	-2.02299
C	0.74498	-5.45922	-0.56737
H	1.22173	-6.38213	-0.21821
C	-8.45197	-2.24738	-0.55799
H	-9.21754	-2.76825	-1.14445
C	-8.53126	3.44202	1.90546
H	-9.23260	3.89950	2.61269
C	-8.65305	3.69267	0.53084
H	-9.44998	4.34698	0.15921
H	-0.00008	-0.00007	-0.19027
Ru	1.76392	0.62262	-0.16850
Ru	4.07166	-0.82376	0.31634
C	6.70200	-2.29534	0.09710
N	2.42873	-1.17051	-1.11314
N	2.18898	-0.71205	1.44394
C	3.45694	2.92869	-1.18394
C	0.43013	3.37459	-0.07606
C	1.21252	1.83584	-1.85292
H	0.78120	1.28545	-2.70503
C	1.02423	2.36307	0.85354
H	0.43314	2.15445	1.75998
C	6.58193	0.68926	-0.44871
C	3.37145	3.17281	0.20107
C	0.49214	3.08475	-1.45861
C	6.45534	0.94092	0.93375
C	2.65651	1.77936	-1.70717
H	3.19806	1.17815	-2.45219
C	2.46601	2.27133	0.97592
H	2.86330	1.98454	1.96124
C	5.58684	-0.25601	-1.04539
H	5.21938	0.03826	-2.04260
C	2.45564	-2.28909	-0.29896
H	2.58730	-3.29388	-0.71175
C	4.13333	4.20125	0.77804

H	4.07868	4.37539	1.85992
C	7.58376	1.34139	-1.18639
H	7.66883	1.15445	-2.26403
C	-0.08357	3.97927	-2.37991
H	-0.03781	3.75071	-3.45218
C	2.33366	-2.04252	1.07861
H	2.36919	-2.84126	1.82674
C	7.33155	1.84196	1.56096
H	7.21962	2.04665	2.63298
C	5.34385	0.22978	1.63944
H	4.81937	0.83722	2.39609
C	-0.16897	4.57181	0.35570
H	-0.20029	4.80039	1.42854
C	4.30035	3.71979	-1.98057
H	4.37639	3.51690	-3.05618
C	6.57867	-2.04344	1.48239
C	5.06473	4.74486	-1.40013
H	5.73883	5.34382	-2.02266
C	5.65465	-1.69422	-0.78696
H	5.33150	-2.34822	-1.61443
C	8.45192	2.24772	-0.55679
H	9.21758	2.76875	-1.14296
C	5.41237	-1.20627	1.90810
H	4.93286	-1.54657	2.84203
C	7.74315	-3.11476	-0.37028
H	7.82787	-3.31827	-1.44509
C	-0.74478	5.45933	-0.56804
H	-1.22153	6.38227	-0.21896
C	2.54612	-1.43817	-2.54708
H	3.08285	-0.61693	-3.04473
H	3.08859	-2.38155	-2.74111
H	1.53749	-1.51776	-2.98899
C	7.49890	-2.61457	2.37743
H	7.39235	-2.42638	3.45316
C	2.00500	-0.48110	2.87591
H	0.95480	-0.69178	3.15333
H	2.66790	-1.12600	3.48441
H	2.21961	0.56959	3.11987
C	4.98247	4.98448	-0.02025
H	5.59305	5.77014	0.43858
C	-0.71076	5.15659	-1.93957
H	-1.16205	5.84182	-2.66617
C	8.32563	2.49834	0.81769
H	8.99233	3.21590	1.30961
C	8.65316	-3.69257	0.53055
H	9.45020	-4.34675	0.15890
C	8.53117	-3.44221	1.90520
H	9.23242	-3.89980	2.61244

9 References

[S1] Franck, G., Brill, M., Helmchen, G. Dibenzo[a,e]cyclooctene: Multi-gram Synthesis of a Bidentate Ligand. *Org. Synth.* **89**, 55-65 (2012).

[S2] TURBOMOLE Version 7.1; TURBOMOLE Gmbh, Karlsruhe, Germany, 2013.

[S3] PQS Version 2.4; Parallel Quantum Solutions, Fayetteville, AR, USA, 2001.

[S4] Baker, J. An Algorithm for the Location of Transition-States. *J. Comput. Chem.* **7**, 385−395 (1986).

[S5] Budzelaar, P. H. M. Geometry optimization using generalized, chemically meaningful constraints. *J. Comput. Chem.* **28**, 2226−2236 (2007).

[S6] Becke, A. D. Density-Functional Exchange-Energy Approximation with Correct Asymptotic-Behavior. *Phys. Rev. A: At., Mol., Opt. Phys.* **38**, 3098−3100 (1988).

[S7] Perdew, J. P. Density-Functional Approximation for the Correlation-Energy of the Inhomogeneous Electron-Gas. *Phys. Rev. B:Condens. Matter Mater. Phys.* **33**, 8822−8824 (1986).

[S8] Weigend, F.; Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **7**, 3297−3305 (2005).

[S9] Weigend, F.; Haser, M.; Patzelt, H.; Ahlrichs, R. RI-MP2: optimized auxiliary basis sets and demonstration of efficiency. *Chem.Phys. Lett.* **294**, 143−152 (1998).

[S10] Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **132**, 154104 (2010).

[S11] Neese, F. The ORCA program system, Wiley Interdiscip. Rev.: Comput. Mol. Sci., **2**, 73-78 (2012).

[S12] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; J. A. Montgomery, J.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian09, Revision A.2; Gaussian, Inc.: Wallingford, CT, 2009.

[S13] J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865–3868 (1996).

[S14] a) Harihara.Pc; Pople, J. A. Theor. Chim. Acta. **28**, 213 (1973); b) Harihara.Pc; Pople, J. A. Mol. Phys. **27**, 209 (1974).

[S15] a) P. Fuentealba, P.; H. Preuss, H.; H. Stoll, H.; Szentpaly, L. V. Chem. Phys. Lett., **89**, 418 (1989). b) Quantum Chemistry: The Challenge of Transition Metals and Coordination Chemistry, Wedig, U.; Dolg, M.; Stoll, H.; Preuss, H. Ed. A. Veillard, Reidel, and Dordrecht, 1986, 79.

[S16] F. Weigend, *Phys. Chem. Chem. Phys.*, **8**, 1057-65 (2006).

[S17] (a) Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Comput. Chem.,* **2011**, *32*, 1456. (b) Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **132**, 154104 (2010).