Supporting Information for:

Reversible Homolytic Activation of Water via Metal-Ligand Cooperativity in a T-shaped Ni(II) Complex

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General Methods

All chemicals were purchased from commercial suppliers and used without further purification. All manipulations were carried out under an atmosphere of N_2 using standard Schlenk and glovebox techniques. Glassware was dried at 180°C for a minimum of two hours and cooled under vacuum prior to use. Solvents were dried on a solvent purification system from Pure Process Technologies and stored over 4 Å molecular sieves under N_2. Tetrahydrofuran (THF) was stirred over NaK alloy and run through an additional alumina column prior to use to ensure dryness. Solvents were tested for H_2O and O_2 using a standard solution of sodium-benzophenone ketyl radical anion. The synthesis of the dihydrazonopyrrole ligand $^{Tol,Ph}DHPyH_3$ (**1**, $^{Tol,Ph}DHPyH_3$ = 2,5-bis((2-phenylhydrazono)(*p*-tolyl)methyl)-pyrrole) was based on the procedure in our previous publication.[1] 2,4,6-tri-*tert*-butylphenoxy radical was prepared by reacting 2,4,6-tri-tert-butylphenol with PbO_2 in THF and then used directly without any further purification. C_6D_6, $CDCl_3$, and CD_2Cl_2 were dried over 4 Å molecular sieves under N_2. ^1H, $^{13}C\{^1H\}$, $^{31}P\{^1H\}$, and NOESY NMR spectra were recorded on Bruker DRX 400 or 500 spectrometers. Chemical shifts are reported in ppm units referenced to residual solvent resonances for ^1H and $^{13}C\{^1H\}$ spectra. UV-Vis Spectra were recorded on a Bruker Evolution 300 spectrometer and analyzed using VisionPro software. Experiments requiring a dip probe utilized Hellma Analytics Excalibur Standard Tauchsonde Granzquarz-Tauchsonde (serial no. 13594). IR spectra were obtained on a Bruker Tensor II spectrometer with the OPUS software suite. All IR samples were prepared as KBr pellets in a homemade press. EPR spectra were recorded on a Elexsys E500 Spectrometer with an Oxford ESR 900 X-band cryostat and a Bruker Cold-Edge Stinger. Electrochemical measurements were performed using a BAS Epsilon potentiostat and analyzed using BAS Epsilon software version 1.40.67NT. Cyclic voltammetry measurements were made using a glassy carbon working electrode, platinum wire counter electrode, and silver wire pseudo-reference electrode, and referenced to internal Fc/Fc^+. GC-MS data were collected using an Agilent 7890B GC equipped with an Agilent HP-5MS column coupled to an Agilent 5977A EI-MS. Isotope patterns were compared to the NIST library to confirm assignments. Combustion analysis was performed by Midwest Microlabs.

Syntheses

$[^{Tol,Ph}DHPyH]Ni(NC_5H_5)(THF)$ (**2-Py**)

Pre-ligand **1** (200 mg, 0.41 mmol) was reacted with 2 equivalents of KH (33.2 mg, 0.83 mmol) in THF at room temperature for three hours resulting in a deep red solution, which is assigned as the doubly-deprotonated ligand. Separately, one equivalent of $(DME)NiCl_2$ (90.8 mg, 0.41 mmol) and THF was charged into a round-bottom flask and 21 equivalents of pyridine (690 mg, 8.72 mmol) were added resulting in a light blue suspension. The solution of doubly-deprotonated ligand was then added into the light blue suspension slowly. The reaction mixture was stirred at room temperature overnight. Subsequently, $KCl_{(s)}$ was removed by filtration and THF solvent and excess pyridine was removed under vacuum resulting in deep red solid. The crude product was purified by a two-layer recrystallization method using toluene (4 mL)/petroleum-ether (15 mL). Yield: 262.1 mg (0.38 mmol, 91.7%). Single crystals of **2-Py** suitable for X-ray crystallography were obtained by a two-layer method using THF/petroleum-ether as a 1:6 solvent combination. ^1H NMR (400 MHz, C_6D_6, RT): δ = 8.32 (dt, 2H, *J* = 8, 2 Hz, *m*-Ph), 8.09 (d, 2H, *J* = 6 Hz), 7.67 (dt, 2H, *J* = 8, 2 Hz, *m*-Ph), 7.58 (d, 1H, *J* = 4 Hz, pyrrole), 7.55 (d, 1H, *J* = 4 Hz, pyrrole), 7.45 (d, 2H, *J* = 7 Hz), 7.29 (d, 2H, *J* = 8 Hz), 6.95 (d, 2H, *J* = 8 Hz), 6.83 (t, 2H, *J* = 8 Hz, *o*-Ph), 6.76 (t, 2H, *J* =

8 Hz, *o*-Ph), 6.70 (tt, 2H, *J* = 7, 1 Hz, *p*-Ph), 6.55 (tt, 2H, *J* = 7, 1 Hz, *p*-Ph), 6.29 (tt, 2H, *J* = 8, 2 Hz, *p*-pyridine), 6.14 (d, 2H, *J* = 8 Hz), 5.88 (bs, 2H), 5.17 (s, 1H, NH), 2.33 (s, 3H, CH_3), 2.12 (s, 3H, CH_3). ^{13}C {^1H} NMR (125 MHz, $CDCl_3$, RT): δ = 162.6, 156.6, 152.6, 148.5, 139.4, 137.7, 136.8, 135.3, 133.9, 130.2, 129.4, 129.0, 129.0, 128.7, 128.6, 128.6, 127.3, 127.0, 125.3, 123.1, 122.9, 122.7, 119.5, 112.8, 110.8, 21.4, 21.2. IR (KBr Pellet, cm^{-1}): 3343 (N-H). UV-vis (THF, nm): 344, 506. Anal. Calc. C, 71.32; H, 5.69; N, 12.17; Found: C, 71.40; H, 5.96; N, 12.08. Note that the combustion analysis was calculated for a THF solvate as observed in the crystal structure.

[^{Tol,Ph}DHPy]Ni(NC_5H_5) (**3-Py**)

A 20 mL vial was charged with complex **2-Py** (300 mg, 0.39 mmol) and THF (10 mL). Freshly prepared 2,4,6-tri-*tert*-butylphenoxy radical (around 700 mg) was titrated into the reaction mixture until the color of the solution turns to deep green. (Note: It is not necessary to purify the phenoxy radical before use in this step; however, the amount of phenoxy radical used in this step depends on the purity of this *in situ* generated reagent). The reaction mixture was then stirred at room temperature for 2 hours after which the THF solvent was removed under vacuum resulting in deep green solid. The solid was washed by petroleum-ether (3 x 7 mL). The crude product of **3-Py** was then purified by a two-layer recrystallization method using toluene (2 mL) + THF (2 mL)/petroleum-ether (15 mL). Yield: 206.5 mg (0.33 mmol, 85%). Single crystals of of **3-Py** suitable for X-ray crystallography were obtained by a two-layer method using toluene/petroleum-ether as a 1:6 solvent combination. ^1H NMR (400 MHz, C_6D_6, RT): δ = 5.83 (bs). Magnetic susceptibility (Evans Method, CD_2Cl_2, 295 K): μ_{eff} = 1.7 μ_B. EPR (toluene, RT): g = 2.01; (toluene, 12 K): g = 2.02. UV-vis (THF, nm): 352, 590, 646. Anal. Calc. C, 71.87; H, 5.05; N, 13.59; Found: C, 71.85; H, 5.09; N, 13.47.

[[^{Tol,Ph}DHPy]Ni][Cp^*_2Co] (**4**)

A 20 mL vial was charged with **3-Py** (220 mg, 0.36 mmol) and THF (5 mL). A solution of Cp^*_2Co (Cp* = pentamethylcyclopentadienyl; 115 mg, 0.35 mmol) in THF (5 mL) was prepared as well. The THF solution of Cp^*_2Co was added into the THF solution of **3-Py** slowly at room temperature resulting in a deep red solution which is assigned as [**3-Py**][Cp^*_2Co]. (Note: In some cases, the formation of green solid, which is [[^{Tol,Ph}DHPy]Ni][Cp^*_2Co] (**4**), can be observed at this step.) After the reaction mixture stood at room temperature for one hour, ether (9 mL) was added into the reaction vial slowly. The reaction mixture was left at room temperature overnight and a green precipitate of **4** formed. The red solution was decanted, and the volatiles were removed under vacuum. The green solid formed **4** was washed with THF (5 mL) and then the THF wash was used to redissolve the red residue from the mother liquor (putatively [**3-Py**][Cp^*_2Co]). Ether (14 mL) was then added slowly to the dissolved [**3-Py**][Cp^*_2Co] to initiate a second recrystallization. After crystallization the solution was removed and the combined green solid was washed with THF (0.4 mL) and petroleum-ether (10 mL). Yield 286 mg (0.33 mmol, 95%). Single crystals of **4** suitable for X-ray crystallography were obtained by a two-layer method using THF/ether as a 1:1 solvent combination. Anal. Calc. C, 71.73; H, 6.71; N, 8.04; Found: C, 71.52; H, 6.37; N, 8.06. Complex **4** is poorly soluble in organic solvents in which is it stable. This has precluded its characterization by solution techniques. Note that **4** can also be observed when [**3-PMe$_3$**][Cp^*_2Co] is crystallized under analogous conditions.

[^{Tol,Ph}DHPy]Ni (**5**)

Complex **4** (266 mg, 0.31 mmol) was suspended with $AgBF_4$ (59 mg, 0.30 mmol) in THF (10 mL). After the mixture was stirred at room temperature overnight the color of the reaction mixture changed from deep green to deep blue. The solid, which is a mixture of $Ag_{(S)}$ and $[Cp^*_2Co][BF_4]$, was removed by filtration. The THF solvent was then removed under vacuum resulting in a deep blue solid, [^{Tol,Ph}DHPy]Ni (**5**). The solid was further purified by recrystallization using toluene (2 mL) and petroleum-ether (17 mL). Yield 120 mg (0.21 mmol, 67 %). ^{1}H NMR (400 MHz, C_6D_6, RT): δ = 11.46 (bs), 10.36 (bs), 7.68 (bs), 5.59 (bs), 2.90 (bs). Effective Magnetic Moment (Evans Method, CD_2Cl_2, 295 K): μ_{eff} = 1.8 μ_B. EPR (toluene, RT): g = 2.14; (toluene, 12 K): g = 2.10; (THF, 12 K) g = 2.01. UV-vis (THF, nm): 352, 634, 872. Anal. Calc. C, 72.84; H, 5.17; N, 11.96; Found: C, 72.69; H, 5.12; N, 11.68. Note that this complex analyzes as a 0.5 toluene solvate, as observed in the crystal structure.

[^{Tol,Ph}DHPy]Ni(μ-OH)[^{Tol,Ph}DHPyH] (**6**)

Complex **5** (24 mg, 0.045 mmol) was dissolved in toluene (4 mL) and H_2O (3.0 µL) was added via micro-syringe. After the mixture was stirred at room temperature for 1 hour the color of the reaction mixture turned from deep blue to deep purple. The majority of toluene was removed under vacuum and the product [^{Tol,Ph}DHPy]Ni(µ-OH)[^{Tol,Ph}DHPyH] (**6**) was purified via recrystallization using toluene (2 mL) and petroleum-ether (17 mL). Yield: 17 mg (0.02 mmol, 67%). ^{1}H NMR (400 MHz, C_6D_6, RT): δ = 8.38 (bs, 2H), 7.85 (d, 2H, J = 8 Hz), 7.77 (d, 2H, J = 8 Hz), 7.72 (d, 4H, J = 8 Hz, overlapped), 7.71 (s, 2H, pyrrole, overlapped), 7.58 (d, 2H, J = 8 Hz), 7.20-7.09 (m, 14H), 7.05 (t, 2H, J = 8 Hz, *p*-Ph), 6.99 (d, 2H, J = 8 Hz), 6.89 (d, 2H, J = 8 Hz), 6.82 (t, 1H, J = 7 Hz, *p*-Ph), 6.78 (t, 2H, J = 8 Hz, *p*-Ph), 6.61 (t, 1H, J = 7 Hz, *p*-Ph), 5.07 (s, 1H, NH), 2.42 (s, 3H, CH_3), 2.33 (s, 6H, CH_3), 2.13 (s, 3H, CH_3),-4.37 (s, 1H, OH). ^{13}C {^{1}H} NMR (125 MHz, C_6D_6, RT): δ = 159.4, 158.1, 149.8, 139.1, 139.0, 134.9, 134.3, 133.4, 131.7, 130.3, 130.3, 129.8, 129.6, 129.3, 129.2, 128.8, 128.7, 128.5, 128.4, 128.2, 128.0, 127.5, 124.4, 120.9, 120.5, 119.4, 115.0, 113.3, 113.1, 110.6 (three resonances are missing due to overlap with solvent peaks). IR (KBr Pellet, cm^{-1}) 3594 (O-H), 3321 (N-H). UV-vis (THF, nm): 352, 520, 592, 652; (toluene, nm): 358, 564, 810. Anal. Calc. C, 66.81; H, 5.26; N, 12.17; Found: C, 66.46; H, 5.33; N, 12.14. This analysis was calculated for a trihydrate of **6**. Attempts to dry samples further to remove excess water molecules results in analysis that does not match the theoretical values for **6**. This is unsurprising as **6** should not be stable in the absence of excess water as indicated by the accessible equilibria discussed in the text.

([^{Tol,Ph}DHPyH]Ni)$_2$ (**8**)

A solution of PPh_3 (2 mg, 0.008 mmol) in toluene (1 mL) was added to a solution of complex **5** (5 mg, 0.009 mmol) and H_2O (4 µL) in toluene (2 mL). After heating the reaction at 85 °C overnight, a mixture of $OPPh_3$, [[^{Tol,Ph}DHPy(O)]Ni] (**7**), [[^{Tol,Ph}DHPyH]Ni]$_2$ (**8**), and other unidentified species formed as products. Complex **8** was also formed as a mixture of products by heating complex **5** (5 mg, 0.009 mmol) in deuterated benzene (0.5 mL) for 3 days at 75 °C under an atmosphere of H_2. As complex **8** could not be generated cleanly in bulk, only ^{1}H NMR and a crystal structure are reported. ^{1}H NMR (400 MHz, C_6D_6, RT): δ = 10.00 (s, 2H, N-H), 8.13 (d, 4H, J = 8 Hz), 7.95 (d, 4H, J = 8 Hz), 7.90 (d, 4H, J = 8 Hz), 7.14 (d, 4H, J = 8 Hz), 7.09 (d, 2H, J = 4 Hz, pyrrole), 7.05-6.99 (m, 6H), 6.90 (d, 4H, J = 8 Hz), 6.80 (d, 4H, J = 8 Hz), 6.70 (q, 4H, J = 8 Hz), 6.61 (t, 4H, J = 8 Hz), 2.20 (s, 6H, CH_3), 1.91 (s, 6H, CH_3).

Reactions of **6** with pyridine and PMe_3

Complex **5** (5 mg) was combined with excess H_2O (0.05 mL) to generate **6** in situ in toluene (2 mL) at room temperature for both reactions. When pyridine (1.3 mg) was added it reacted to form **3-Py** as the major product and trace amounts of **2-Py**. When PMe_3 (0.1 mL) was added, **2-PMe$_3$**, **3-PMe$_3$**, and $OPMe_3$ were generated. Products were identified using ^{1}H NMR.

Thermolysis of **6**

Complex **5** (3 mg, 0.0054 mmol) was dissolved in deuterated benzene (0.5 mL) and H_2O (3.0 µL) was added via micro-syringe. After stirring for half an hour at room temperature the reaction turned from a deep blue to a deep purple indicative of the formation of **6**. Formation of **6** was confirmed by ^{1}H NMR. The solution was then heated at 70 °C overnight in a J-Young NMR tube in the presence of excess water. These conditions were chosen to mimic the conditions used during the phosphine oxidation experiments. A slightly lower temperature was utilized such that the reaction could be conducted in deuterated benzene rather than toluene and monitored by ^{1}H NMR. After heating, **7** and **8** as well as residual **6** were identified by ^{1}H NMR as the major species in the product mixture.

NMR Spectra

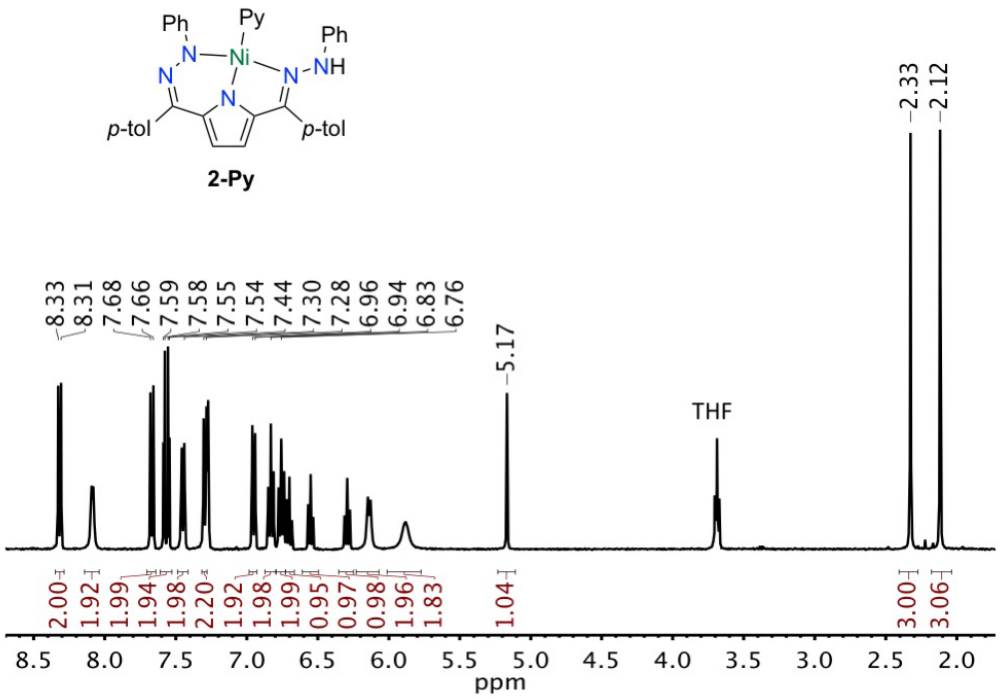

Figure S1. ^{1}H NMR of **2-Py** in C_6D_6.

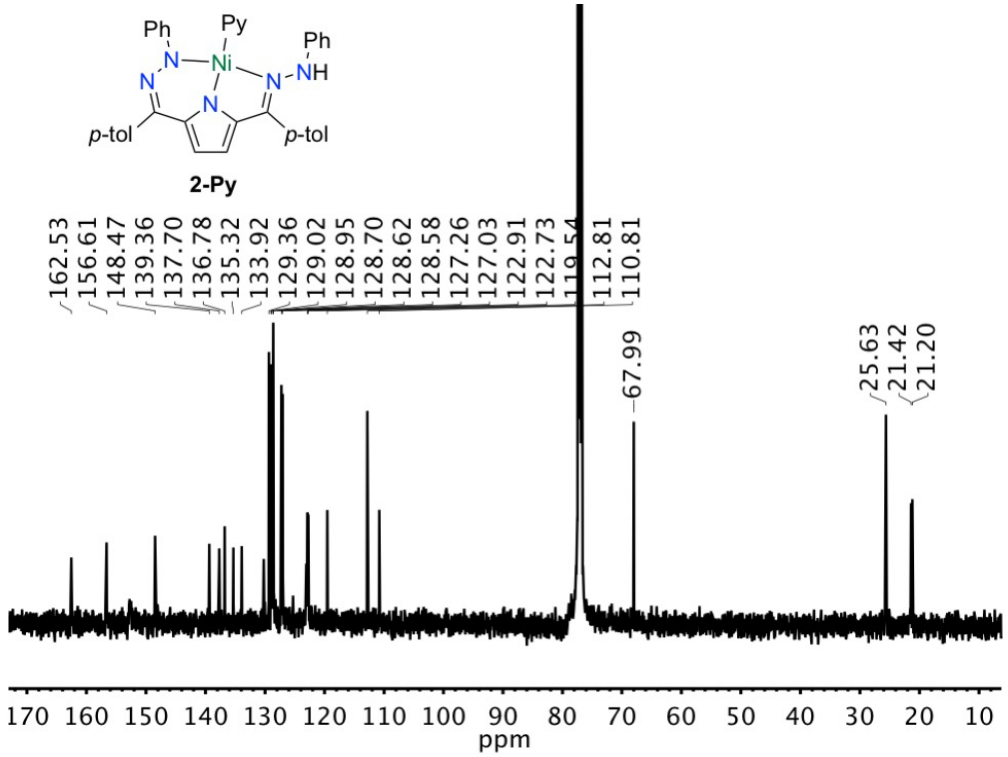

Figure S2. ^{13}C NMR of **2-Py** in C_6D_6.

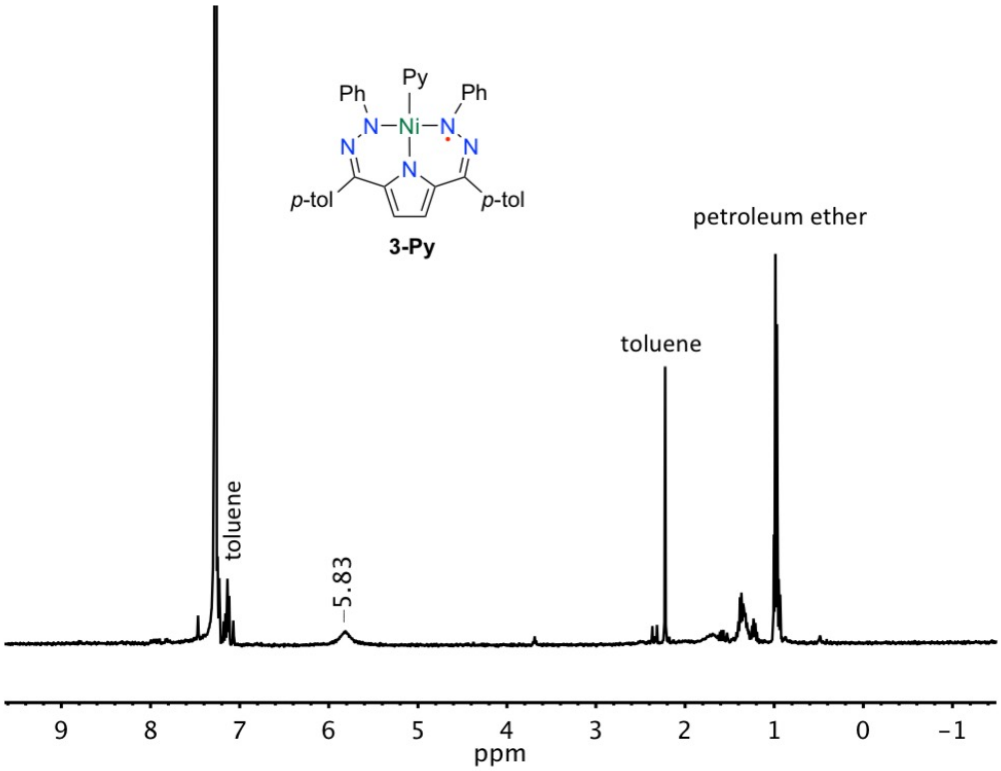

Figure S3. ^{1}H NMR of **3-Py** in C_6D_6. Wider scans reveal that the feature at 5.83 is the only observable signal associated with **3-Py**. We tentatively assign this to the pyridine protons, but this assignment is speculative due to paramagnetic shifting and broadening from the ligand radical.

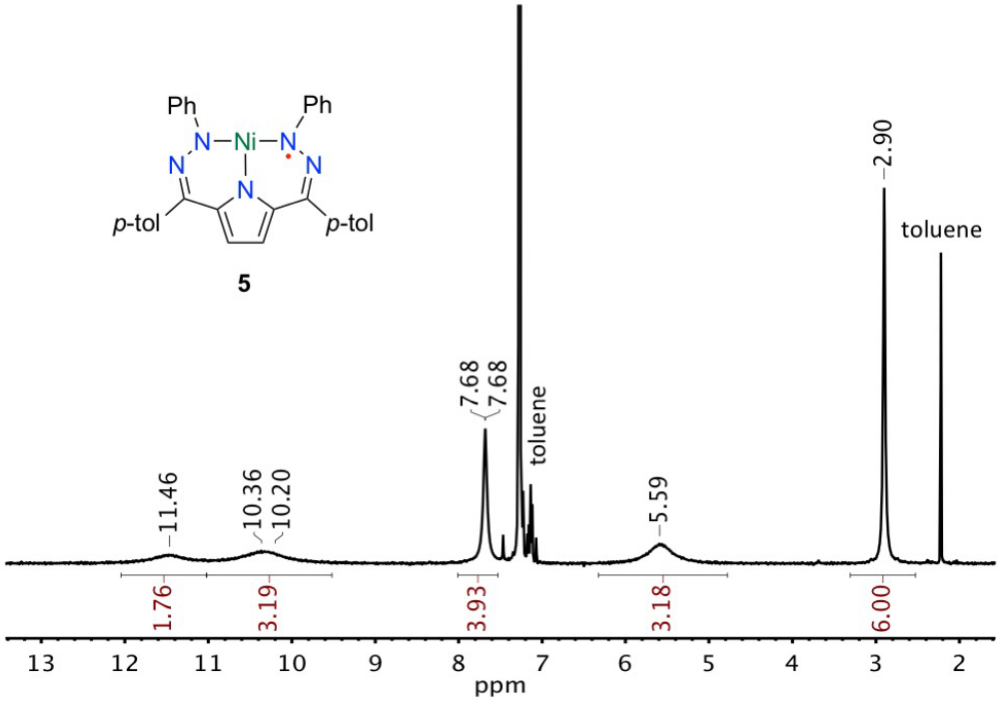

Figure S4. ^{1}H NMR of **5** in C_6D_6.

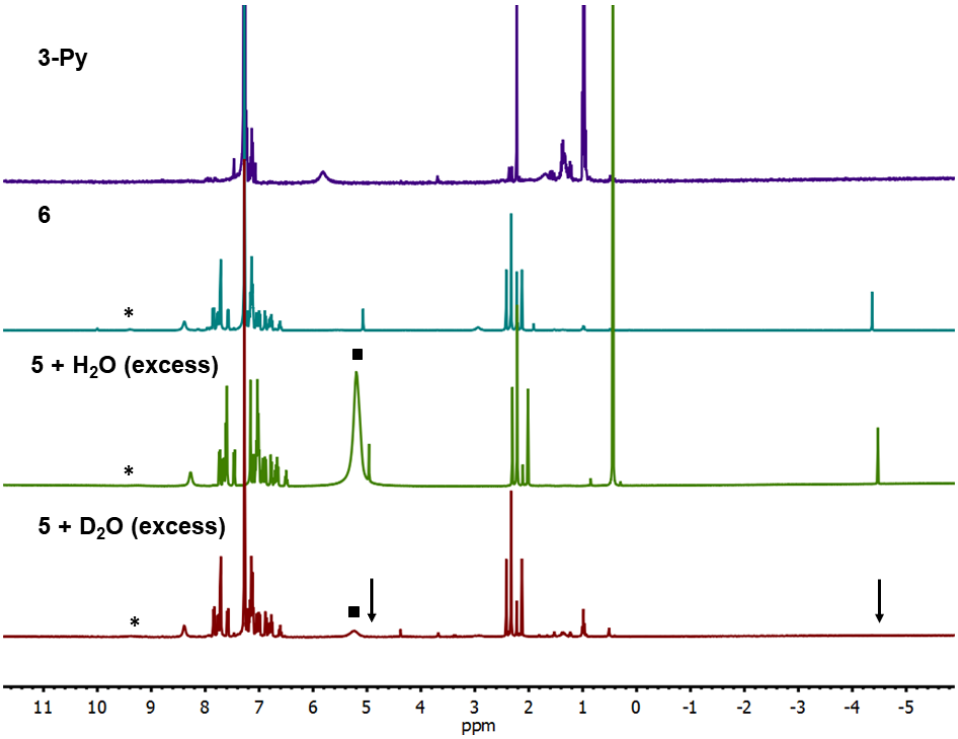

Figure S5. ^{1}H NMR of **3-Py**, **6**, **5** + excess H_2O, and **5** + excess D_2O in C_6D_6. The arrows indicate the decreased signal for the OH and NH peaks when synthesized with D_2O. The asterisk indicates an unidentified paramagnetic intermediate present in solution upon the addition of water. The square indicates the peak tentatively assigned as **3-H$_2$O**.

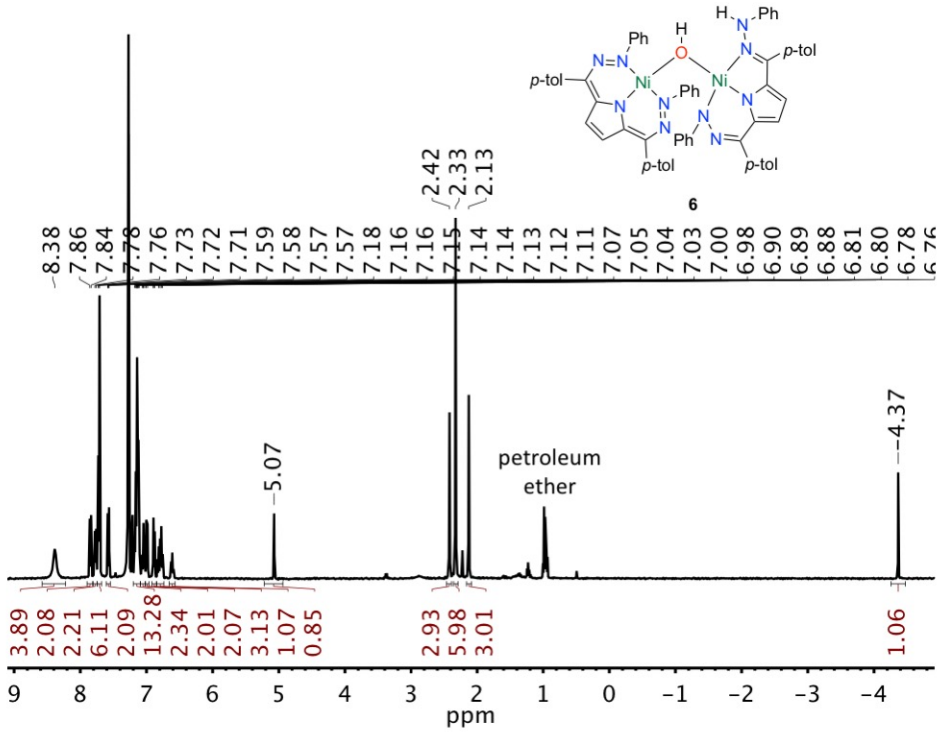

Figure S6. ^{1}H NMR of **6** in C_6D_6.

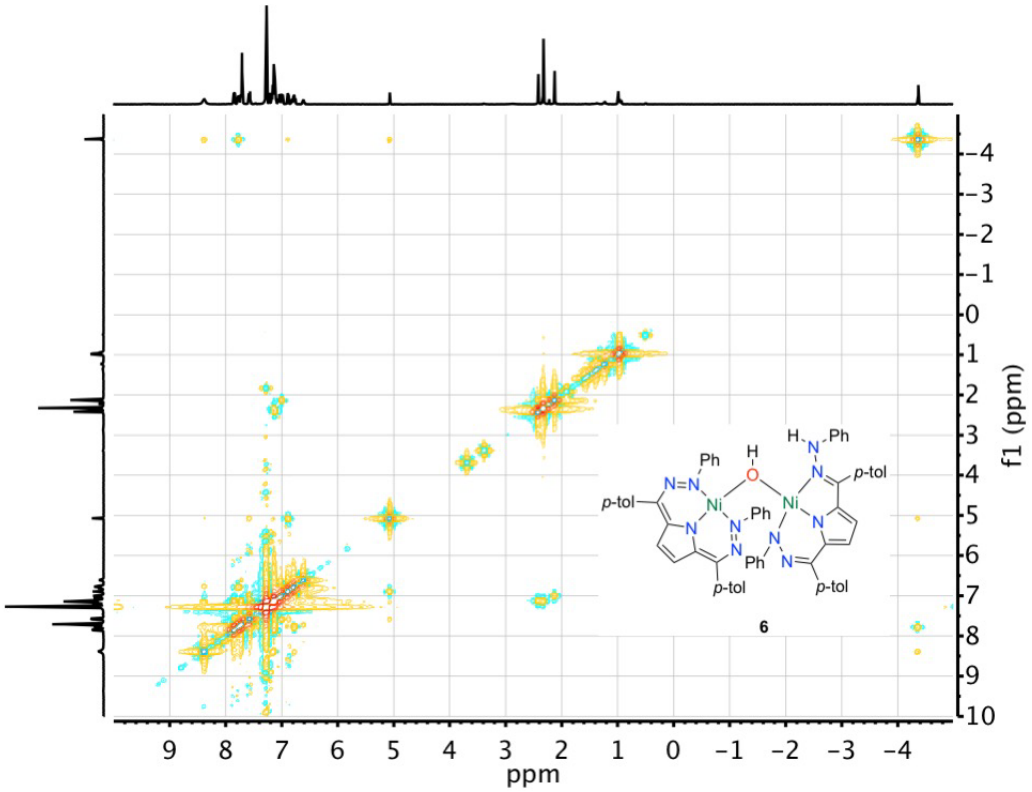

Figure S7. NOESY NMR of **6** in C_6D_6.

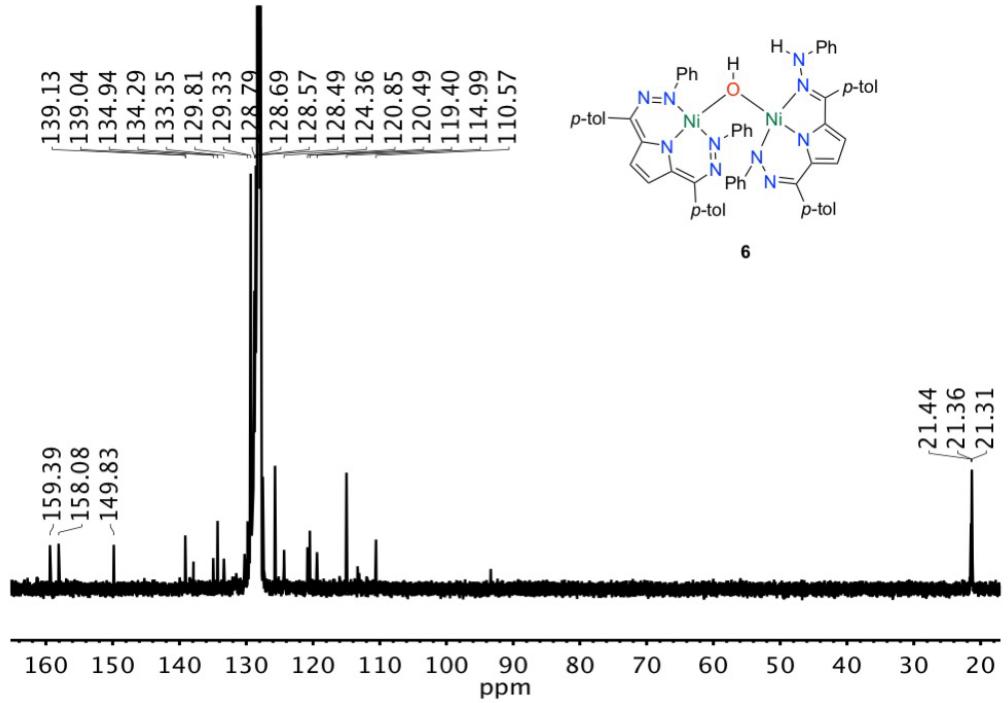

Figure S8. ^{13}C NMR of **6** in C_6D_6.

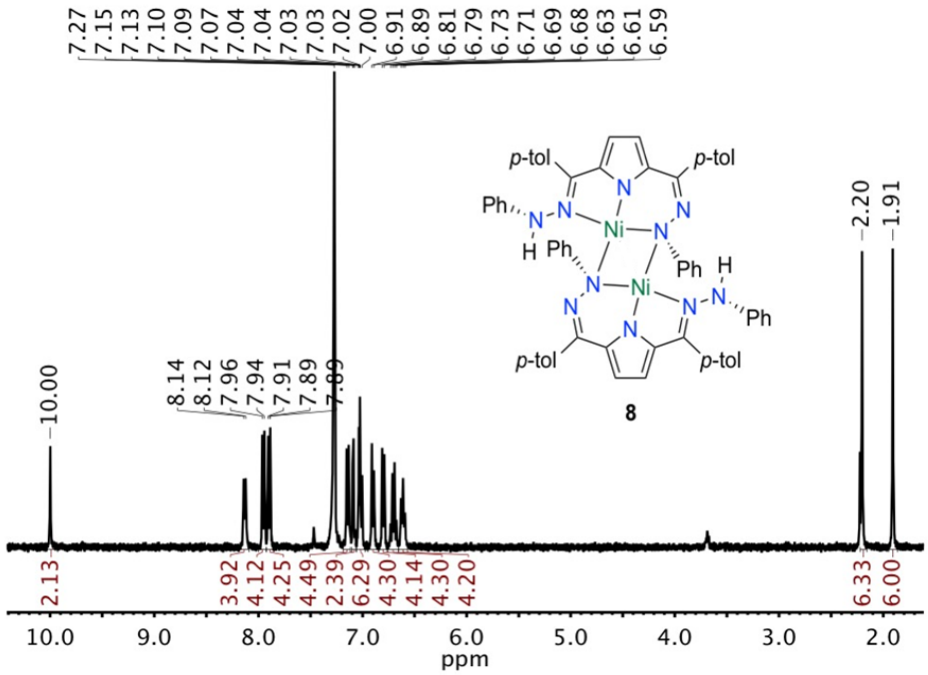

Figure S9. ^{1}H NMR of **8** in C_6D_6.

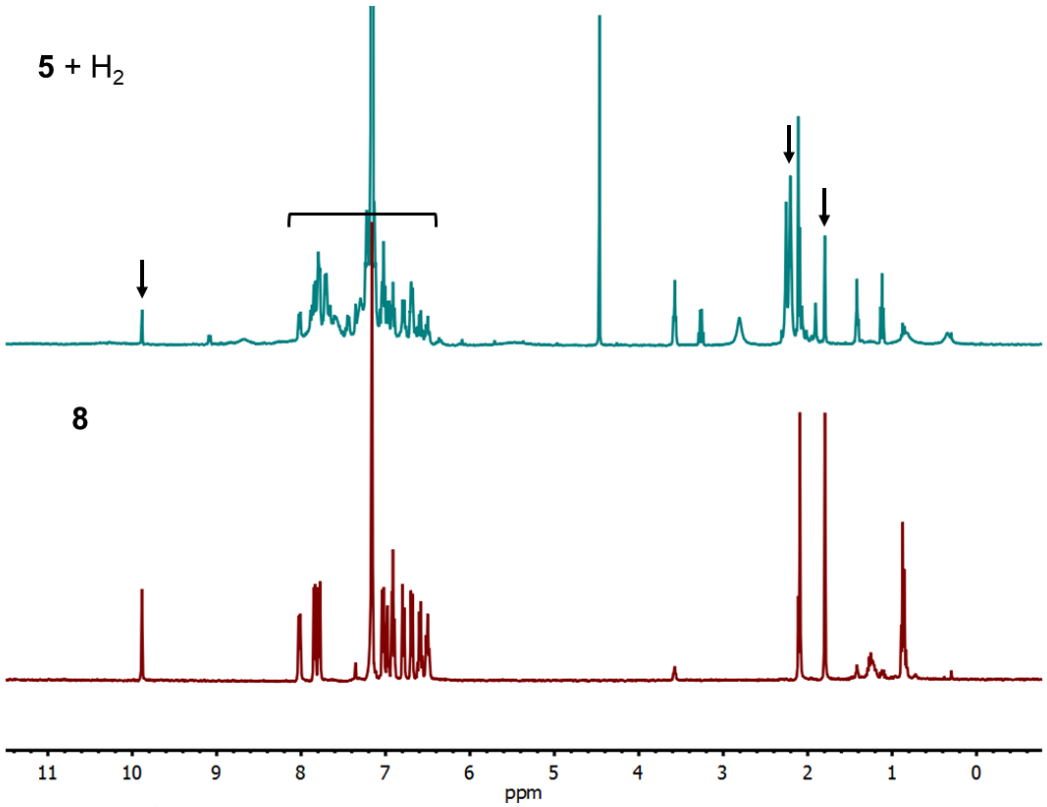

Figure S10. ^{1}H NMR of **8** in C_6D_6 and **5** + 1 atm of H_2 after 24 hours of heating at 85 °C in C_6D_6. Arrows and bracket indicate where **8** can be found in the mixture of products formed.

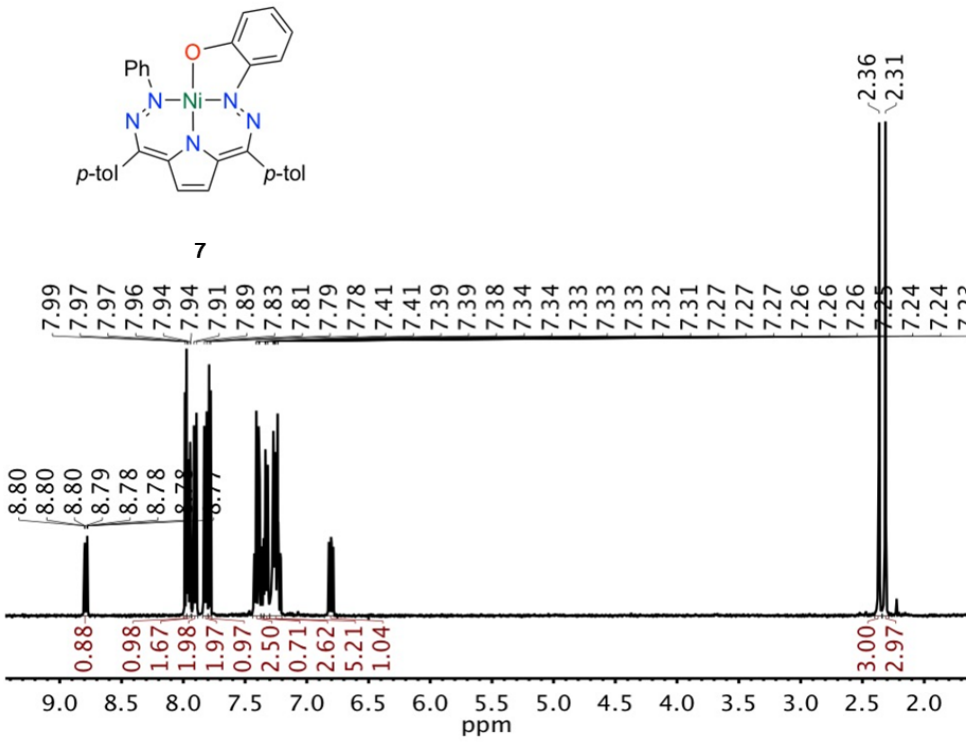

Figure S11. ^{1}H NMR of **7** in C_6D_6.[1]

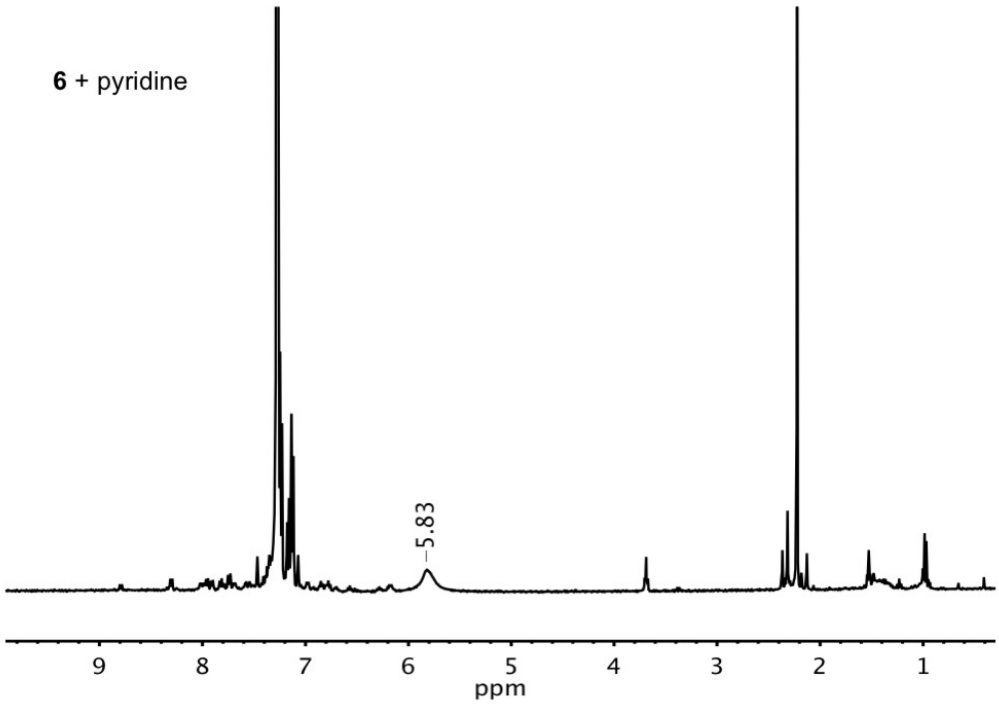

Figure S12. ^{1}H NMR of **6** + pyridine in C_6D_6.

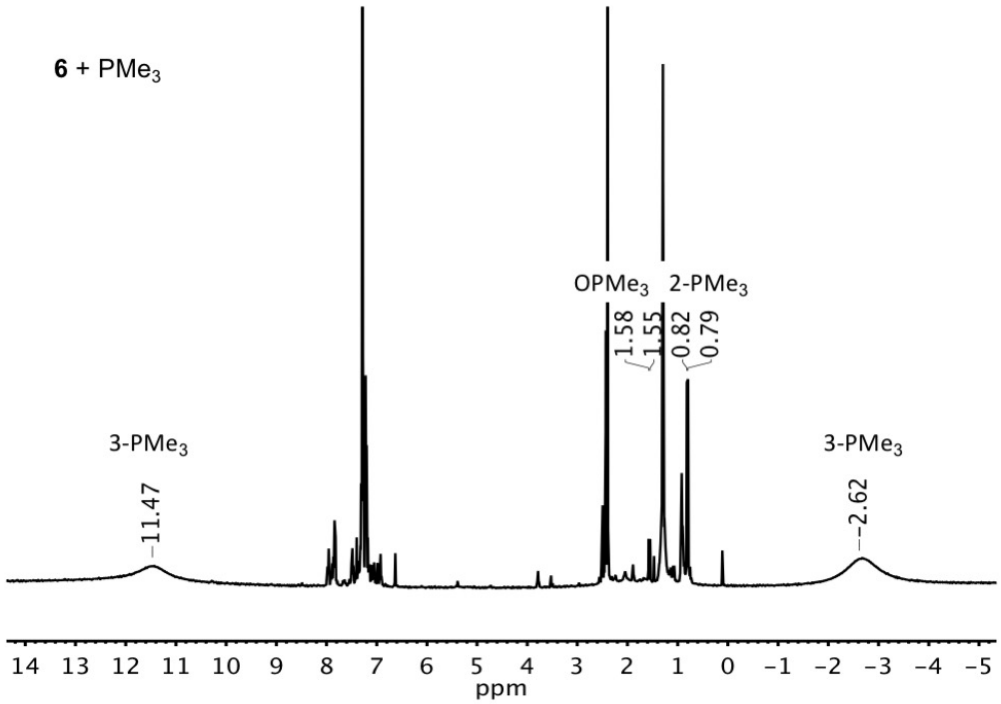

Figure S13. ^{1}H NMR of **6** + PMe_3 in C_6D_6.

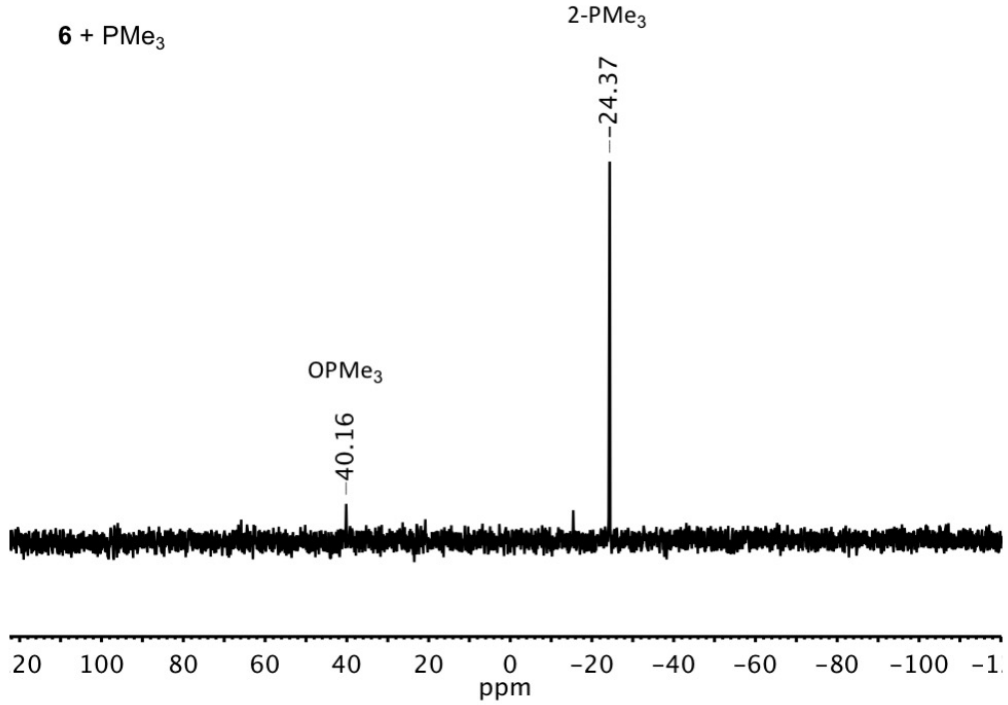

Figure S14. ^{31}P NMR of **6** + PMe_3 in C_6D_6.

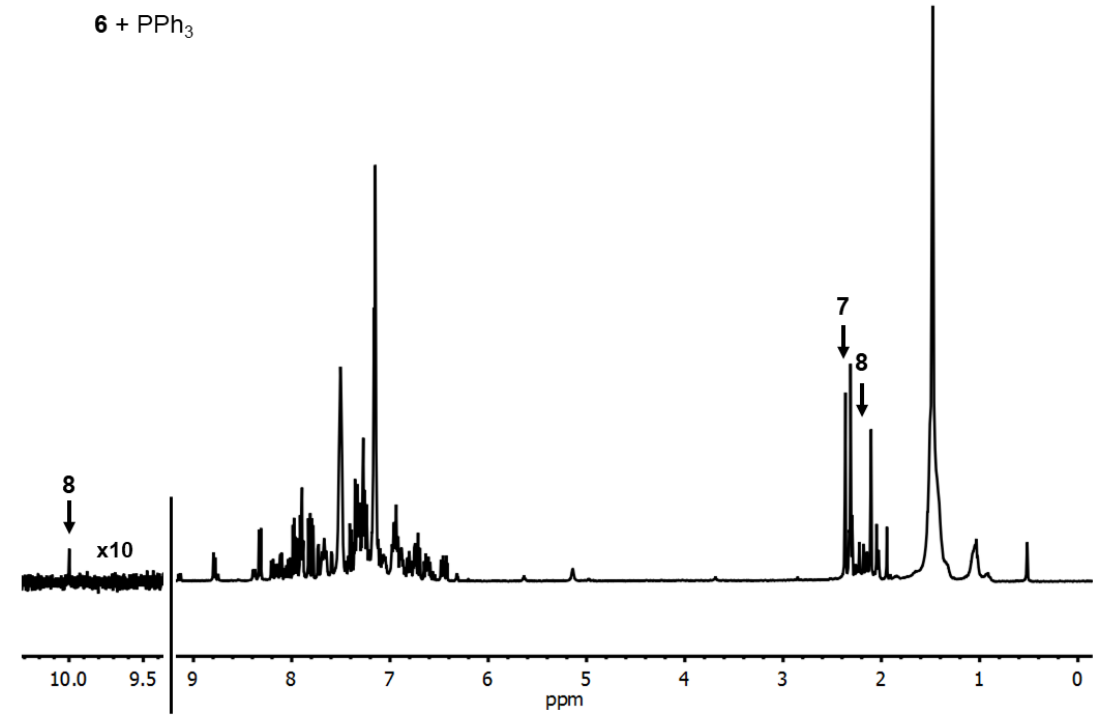

Figure S15. ^{1}H NMR of **6** + PPh_3 in C_6D_6.

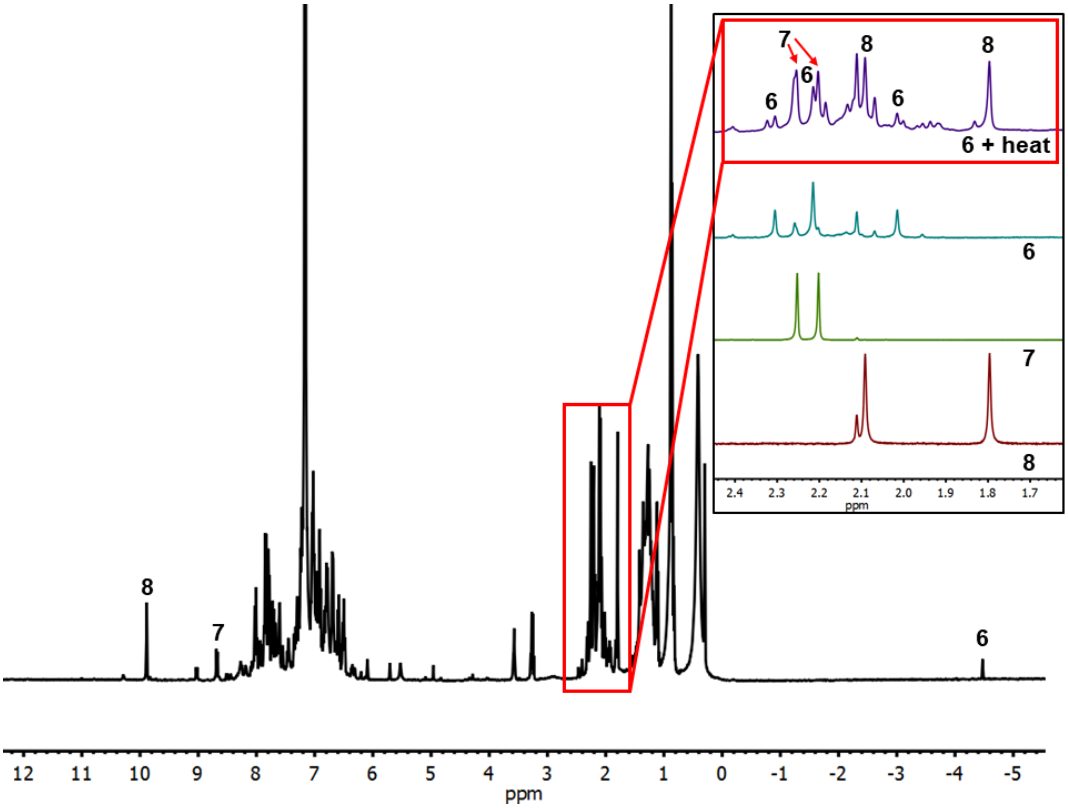

Figure S16. ^{1}H NMR of thermolysis of **6** at 70 °C overnight in C_6D_6.

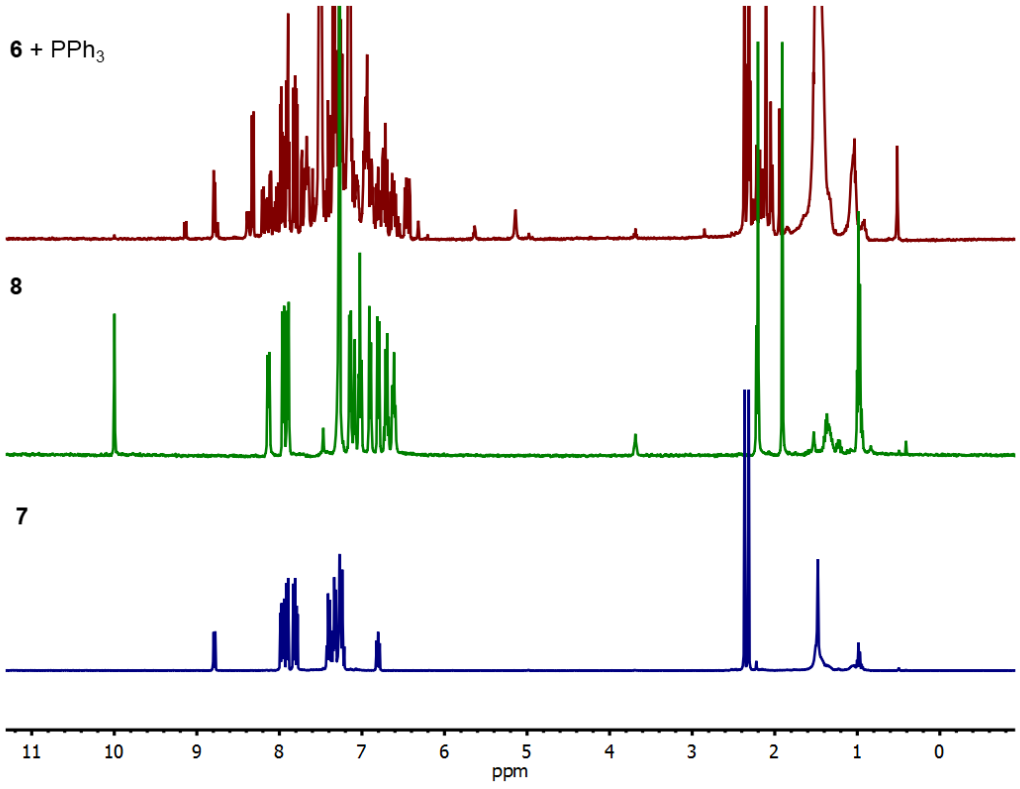

Figure S17. ^{1}H NMR of **6** + PPh_3, **7**, and **8** in C_6D_6.

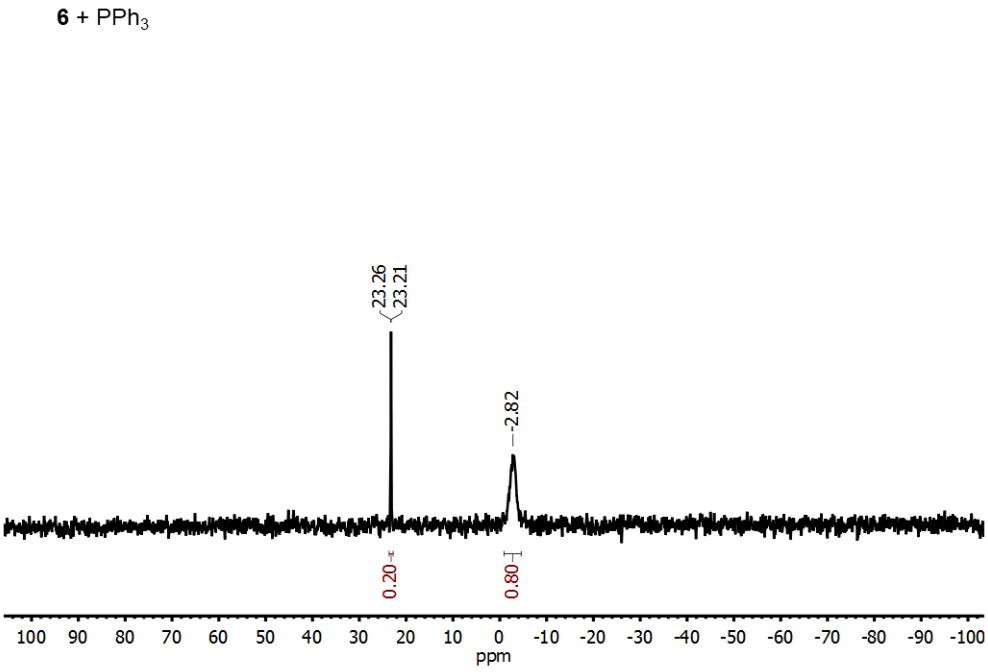

Figure S18. ^{31}P NMR of **6** + PPh_3 in C_6D_6.

IR Spectra

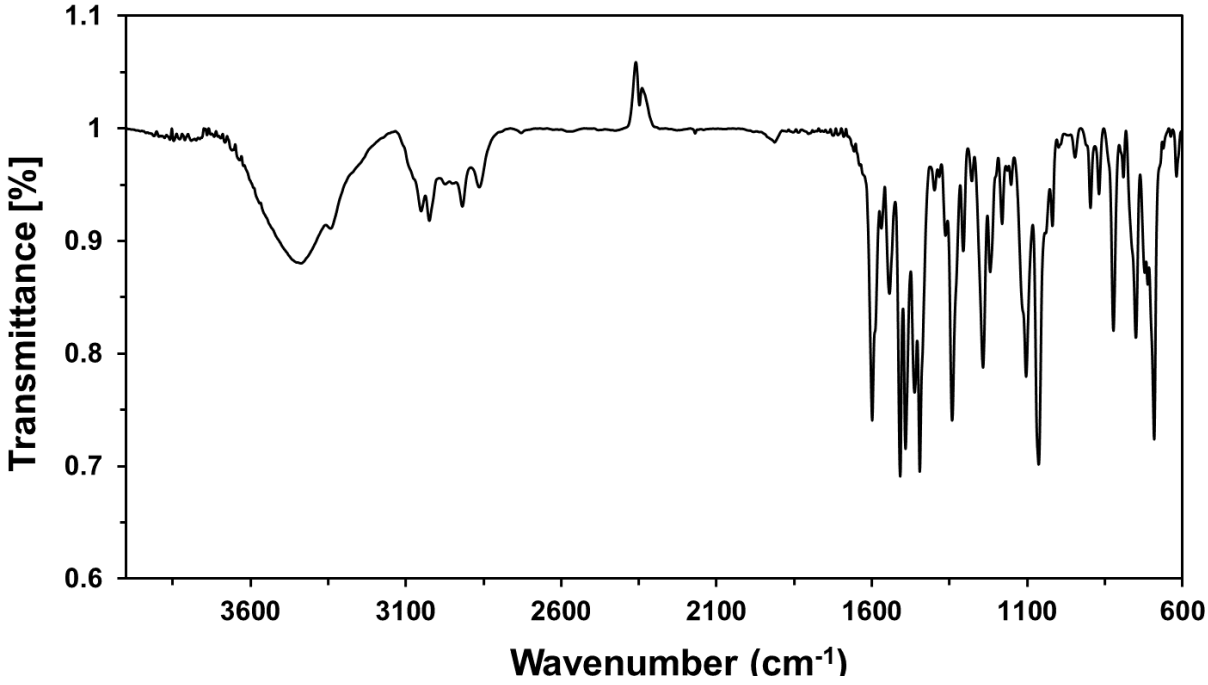

Figure S19. IR (KBr pellet) of **2-Py**.

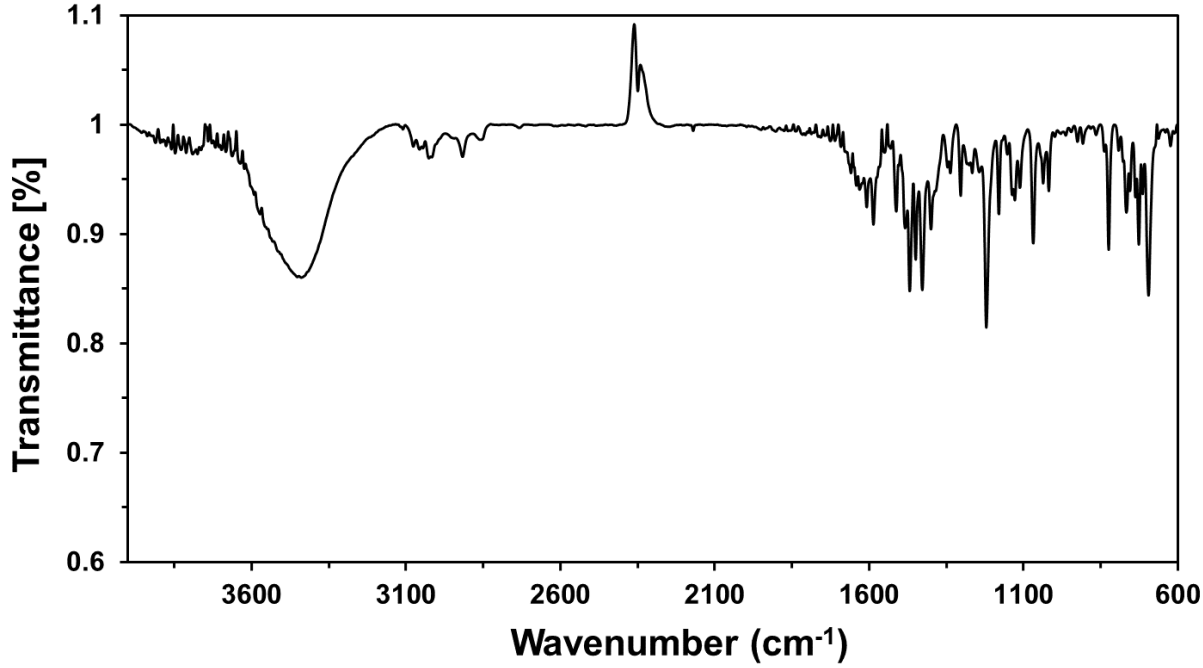

Figure S20. IR (KBr pellet) of **3-Py**.

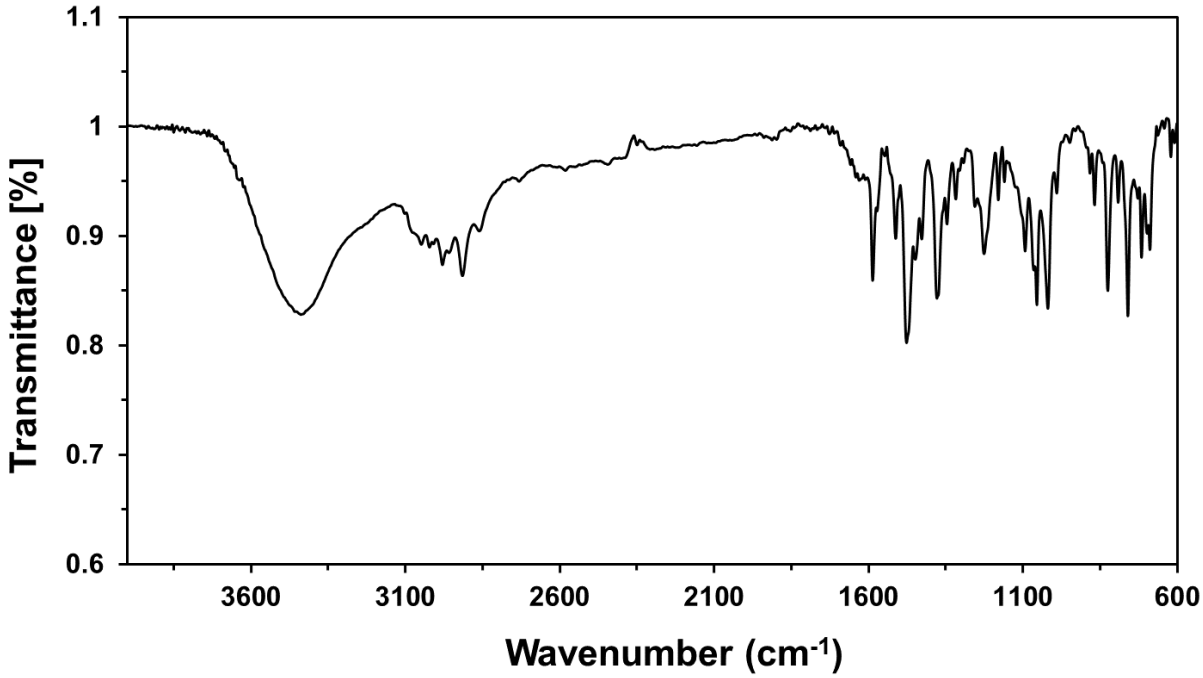

Figure S21. IR (KBr pellet) of **4**.

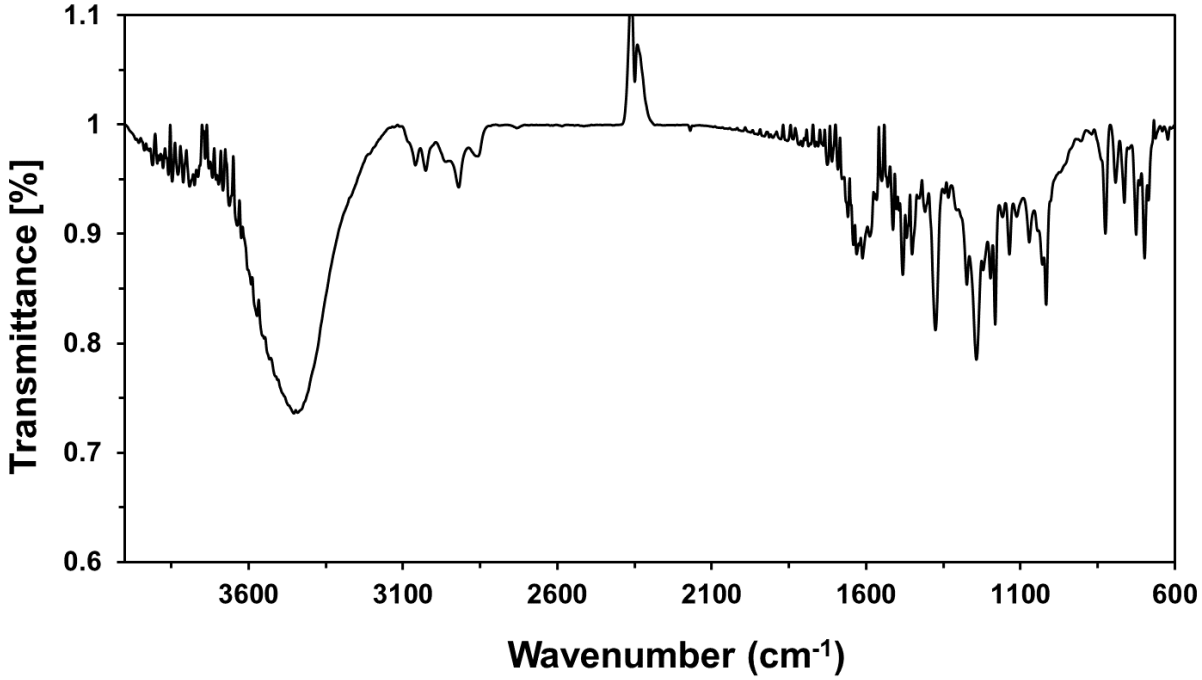

Figure S22. IR (KBr pellet) of **5**.

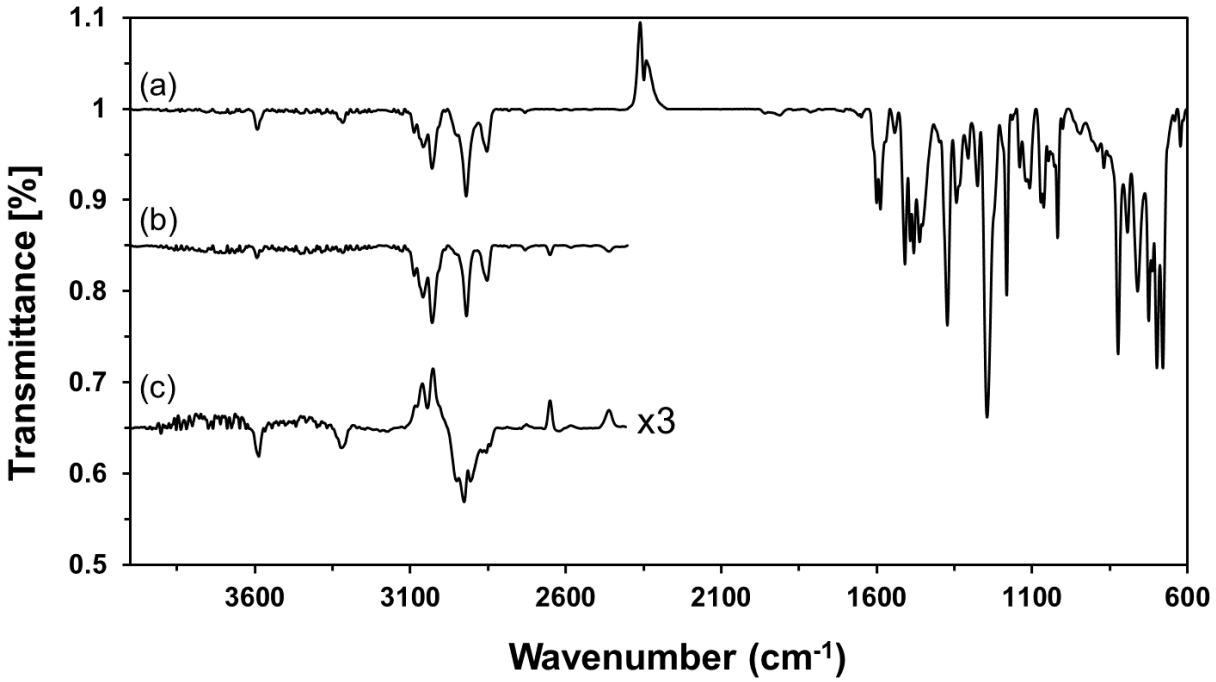

Figure S23. IR (concentrated solution in benzene dried on KBr cell) of (a) **6-H_2O** (b) **6-D_2O** and (c) the difference between **6-H_2O** and **6-D_2O**.

UV-vis Spectra

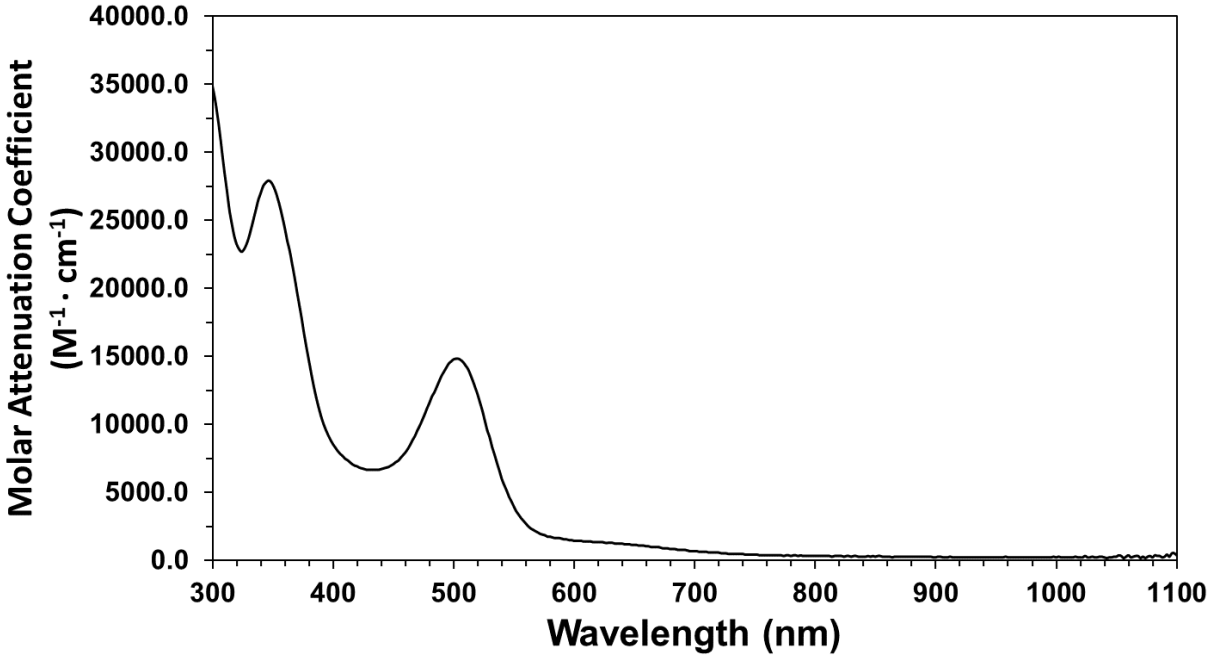

Figure S24. UV-vis trace of **2-Py** in THF.

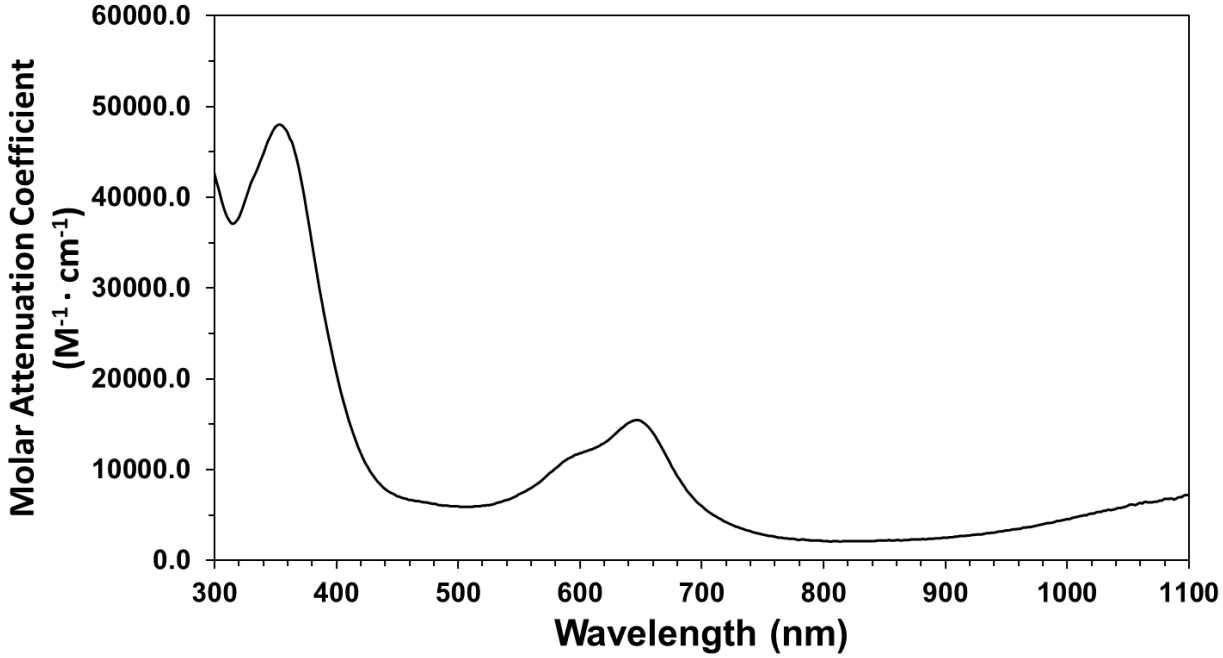

Figure S25. UV-vis trace of **3-Py** in THF.

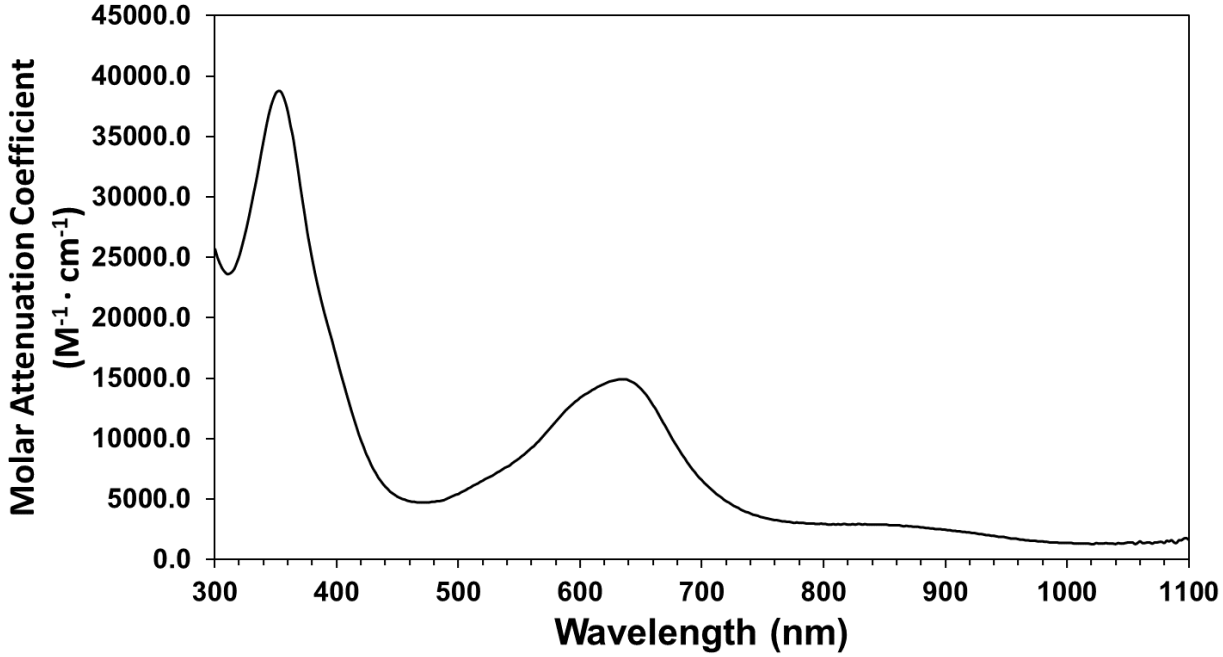

Figure S26. UV-vis trace of **5** in THF.

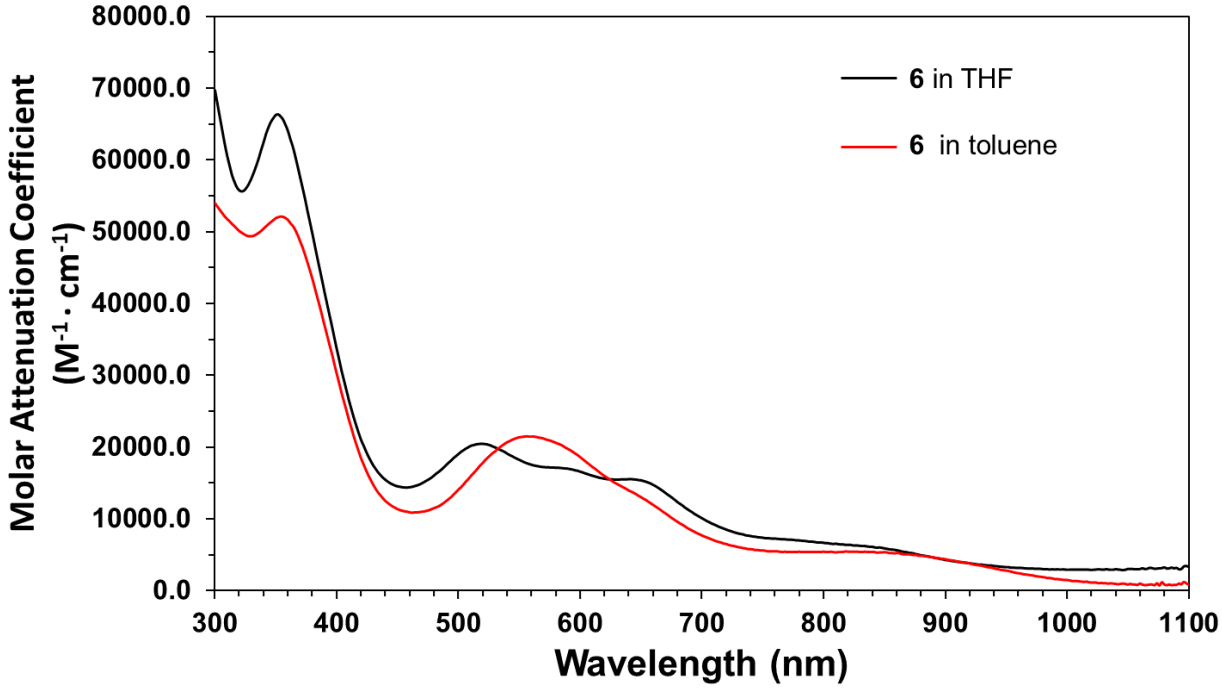

Figure S27. UV-vis of **6** in THF (black) and toluene (red).

EPR Spectra

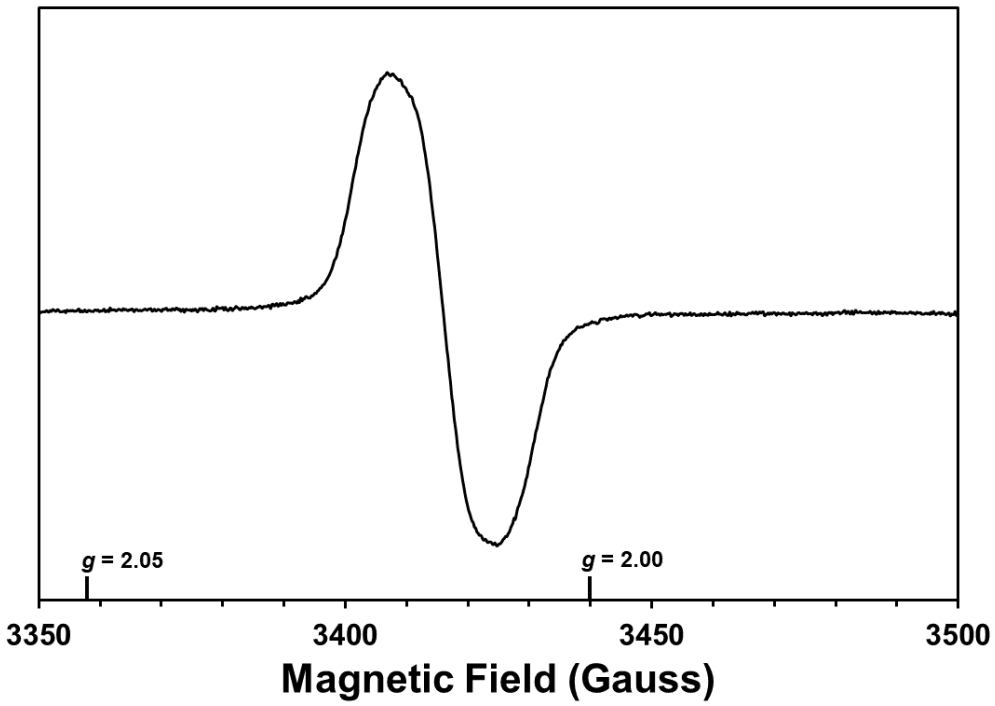

Figure S28. EPR spectrum of **3-Py** in toluene, RT. MW power = 2.01 mW, MW frequency = 9.63 GHz.

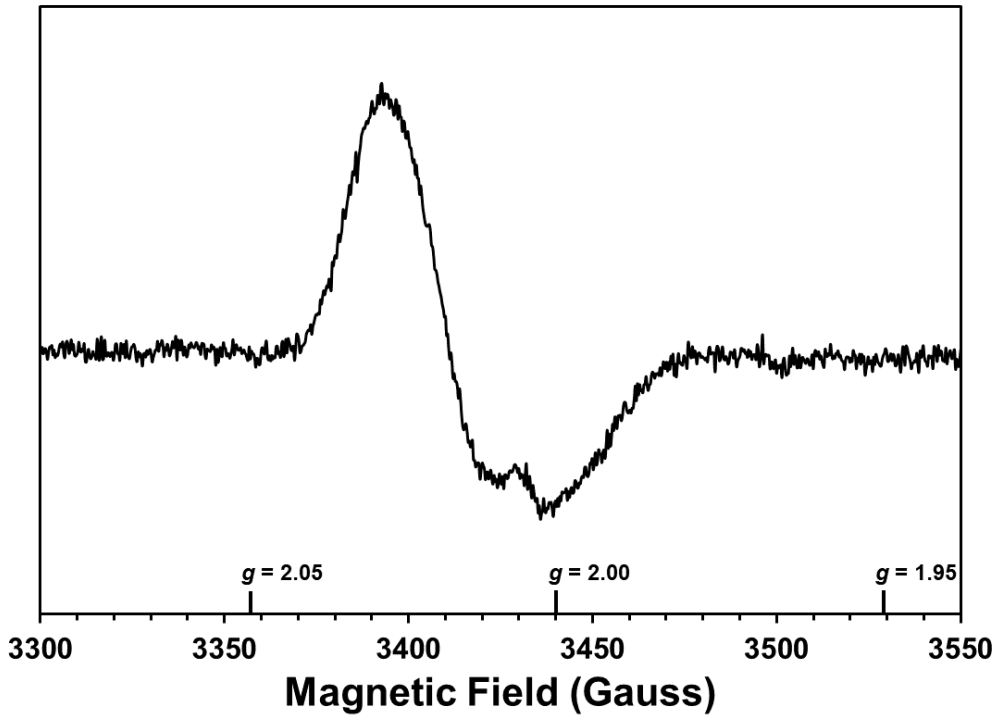

Figure S29. EPR spectrum of **3-Py** in toluene, 12 K. MW power = 6.35 mW, MW frequency = 9.63 GHz.

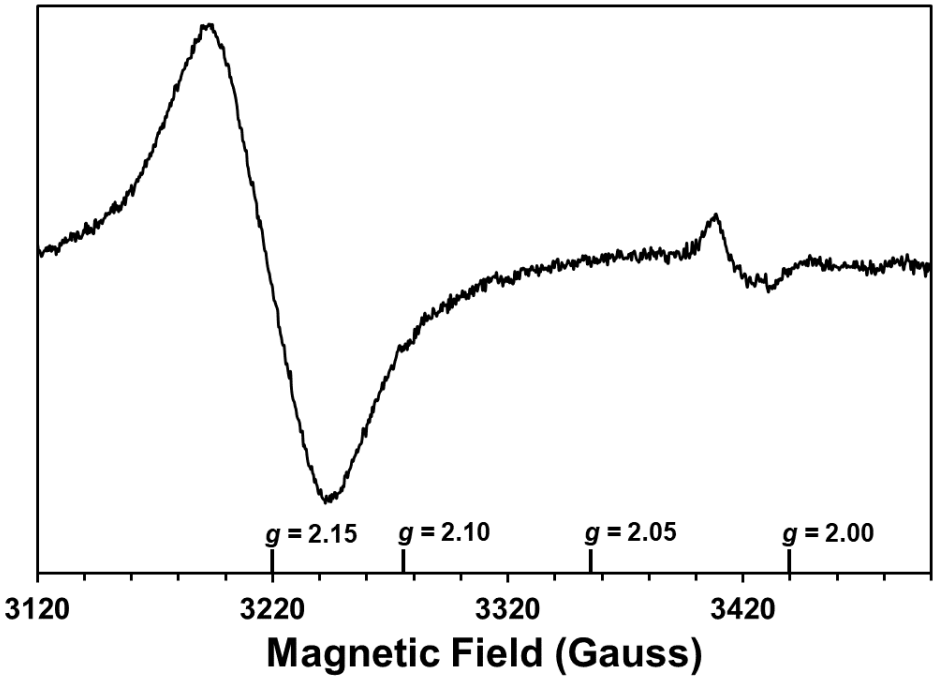

Figure S30. EPR spectrum of **5** in toluene, RT. MW power = 3.17 mW, MW frequency = 9.63 GHz.

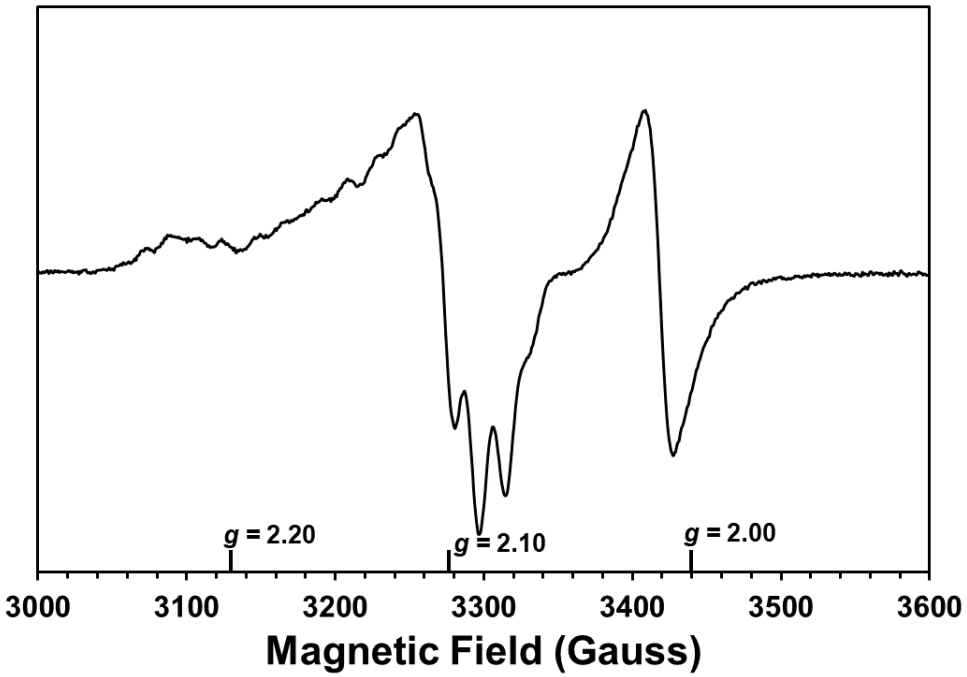

Figure S31. EPR spectrum of **5** in toluene, 12 K. MW power = 3.17 mW, MW frequency = 9.63 GHz. The feature at g = 2.00 likely arises from binding of some small impurity such as THF in the toluene solution.

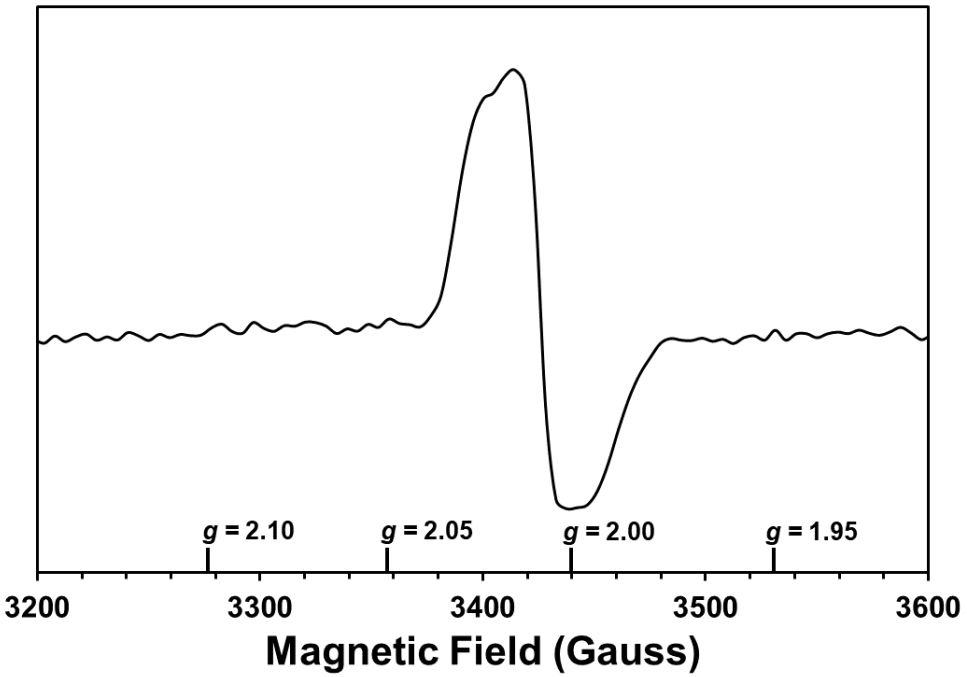

Figure S32. EPR spectrum of **5** in THF, 12 K. MW power = 2.01 mW, MW frequency = 9.63 GHz.

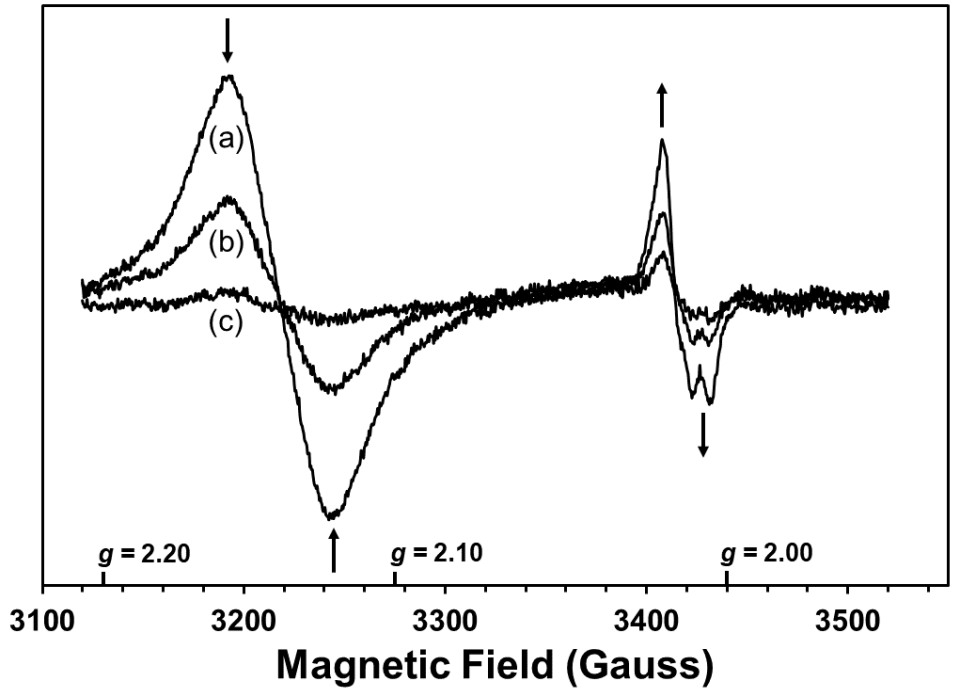

Figure S33. EPR spectrum of the reaction of **5** + 1 μL H_2O in toluene where (a) is prior to mixing, (b) is just after mixing, and (c) is 20 minutes after mixing, RT. MW power = 2.008 mW, MW frequency = 9.631 GHz.

SQUID Data

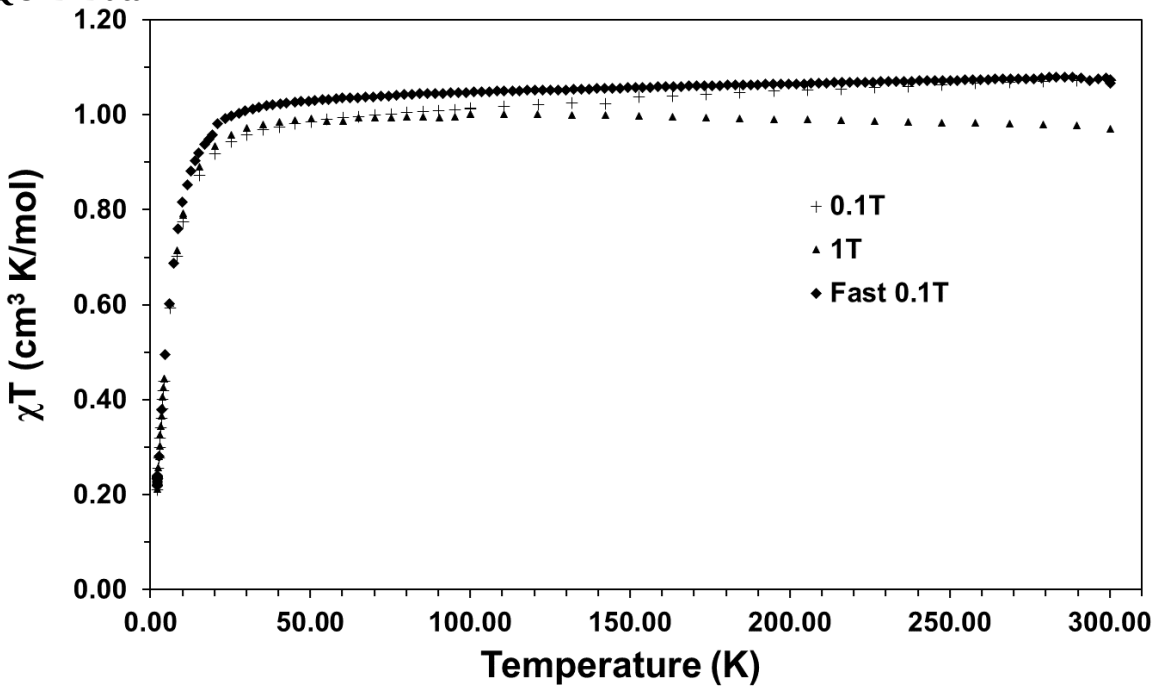

Figure S34. SQUID of **4**.

Electrochemistry

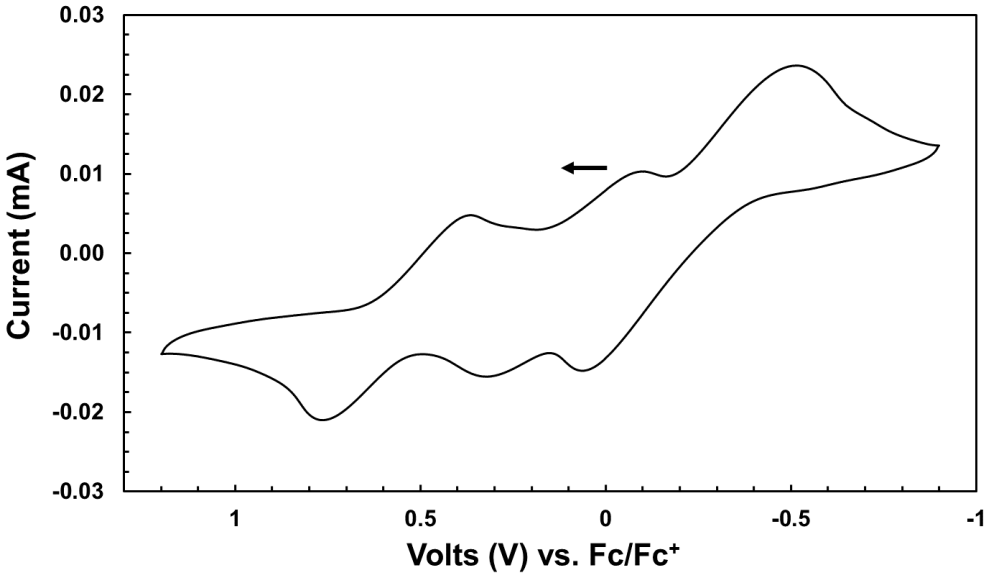

Figure S35. Cyclic voltametry of 1.5 mM **5** in THF. Electrolyte: $[Bu_4N][PF_6]$, Scan rate: 100 mV/s.

Gas Chromatography-Mass Spectrometry

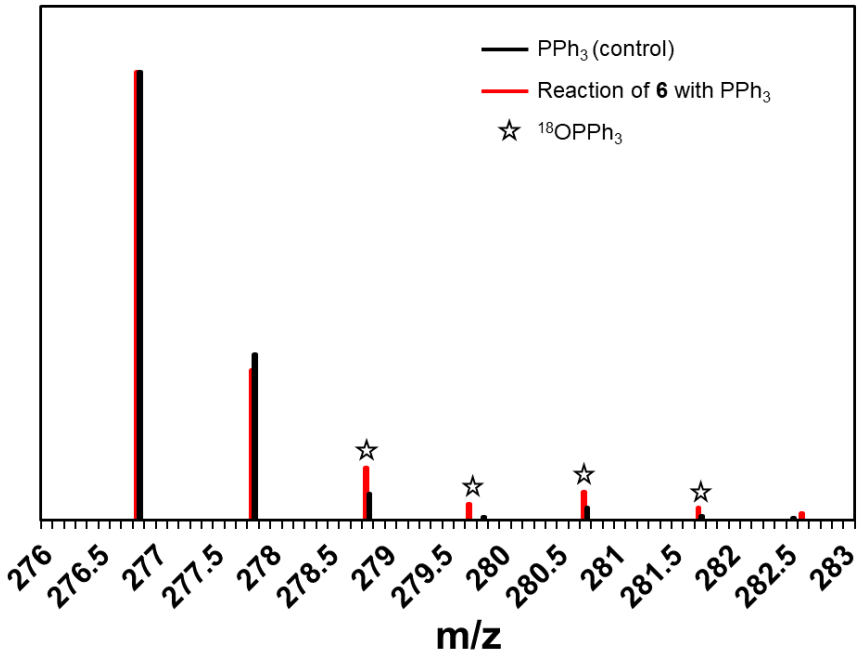

Figure S36. MS data from GC-MS analysis of **5** + $H_2{}^{18}O$ + PPh_3 (red) and a control sample with only the PPh_3 starting material (black) in benzene. Note that the displayed mass spectrum is selected from the GC region for $OPPh_3$. The $^{16}OPPh_3$ in the reaction mixture is due to either an impurity of $^{16}OPPh_3$ in the starting PPh_3 or from some oxidation to $^{16}OPPh_3$ from air during the GC-MS analysis.

X-Ray Crystallography

General Description

Suitable crystals reported in this manuscript were mounted on a cryo-loop and transferred into the cold nitrogen stream of a Bruker D8 Venture diffractometer. Crystal structure of complex **6** and **8** were collected at The Advanced Photon Source at Argonne National Laboratory (beamline 15-ID-B,C,D). The diffraction data were measured at 100 K using synchrotron X-ray radiation with a wavelength of λ = 0.41328 Å. Data were collected using ϕ scans. Data reduction and integration were performed with the Bruker APEX3[2] software package. Data were scaled and corrected for absorption effects using the multi-scan procedure as implemented in SADABS.[4] The structure was solved by SHELXT[4] and refined by a full-matrix least-squares procedure using OLEX2[5] (XL refinement program[6]). The crystallographic data of **2-Py**, **3-Py**, **4** and **5** were collected by using Mo K_α radiation (0.71073 Å). The final unit cell was obtained from the xyz centroids of 4589 (**2-Py**), 9950 (**3-Py**), 9807 (**4**), 9994 (**5**), 9702 (**6**), and 9425 (**8**) reflections after integration. Intensity data were corrected for Lorentz and polarization effects, scale variation for decay and absorption: a multiscan absorption correction was applied, based on the intensities of symmetry-related reflections measured at different angular setting (*SADABS*).[7] The structures were solved by direct methods using the program *SHELXS*[8] integrated in Olex 2.[9] Most of the hydrogen atoms were generated by geometrical considerations and constrained to idealized geometries and allowed to ride on their carrier atoms with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms. Structure refinement was performed with the program package *SHELXL*[7] integrated in Olex 2.[9] Crystallographic data are presented in the table below.

[^{Tol,Ph}DHPyH]Ni(NC_5H_5) (**2-Py**): CCDC 1860790
Hydrogen atom of the NH functional group in **2-Py** was located in the difference density map during refinement. Two refractions were omitted due to the influence from the beam stop.

[^{Tol,Ph}DHPy]Ni(NC_5H_5) (**3-Py**): CCDC 1860792
There was no special treatment for the refinement of complex **3-Py**.

[[^{Tol,Ph}DHPy]Ni][Cp*$_2$Co] (**4**): CCDC 1569427
The structure was solved as by the twin law: [-1 0 0 0 1 0 0 0 -1 2] and BASF = 0.53670.

[^{Tol,Ph}DHPy]Ni(0.5 Toluene) (**5**): CCDC 1860791
There was no special treatment for the refinement of complex **5**.

[^{Tol,Ph}DHPy]Ni-OH-Ni[^{Tol,Ph}DHPyH] (**6**): CCDC 1860789
All elements were refined with anisotropic thermal parameters including those of disordered toluene and benzene rings. Hydrogen atoms were included in idealized positions for structure factor calculations except those of NH- and OH groups. These H-atoms were found in the difference Fourier map and were refined freely with thermal parameters being constrained to be 1.2 times of the U_{eq} value of the N or O atoms. Crystal contained many disordered solvent molecules located in large solvent accessible voids. The diffuse contribution to scattering was accounted by applying a solvent mask algorithm as implemented in OLEX2.[10] The algorithm

located a void centered at (0.5, 0, 0.5) with a volume of 1172.4 Å^3 and the electron count of 184 electrons. Anomalous scattering and absorption coefficients for λ = 0.41328 Å used (SHELX format): DISP C -0.0001 0.0005 5.2; DISP H 0 0 0.6; DISP N 0.0005 0.001 7.2; DISP O 0.0017 0.0018 10.2; DISP Ni 0.2306 0.4106 1001.3.

[[^{Tol,Ph}DHPyH]Ni]$_{20}$ Complex (**8**): CCDC 1860793
All elements were refined with anisotropic thermal parameters including those of disordered toluene and benzene rings. Hydrogen atoms were included in idealized positions for structure factor calculations except the H-atom connected to an N5 atom. This H-atom was found in the difference Fourier map and was refined freely without any additional constraints. No additional electron density is observed near other N-atoms. Crystal contained many disordered solvent molecules located in large solvent accessible voids. The diffuse contribution to scattering was accounted by applying a solvent mask algorithm as implemented in OLEX2.[10] The algorithm located two voids centered at (-0.865, 0, 0.25) and (-0.555, 0, 0.75) with a volume of 805.1 Å^3 and the electron count of 172 for both voids. Anomalous scattering and absorption coefficients for λ = 0.41328 Å used (SHELX format): DISP C -0.0001 0.0005 5.2; DISP H 0 0 0.6; DISP N 0.0005 0.001 7.2; DISP Ni 0.2306 0.4106

Table S1. Crystallographic Data.

	2-Py	**3-Py**	**4**
Chem formula	$C_{45}H_{48}N_6NiO_2$	$C_{37}H_{31}N_6Ni$	$C_{52}H_{56}CoN_5Ni$
M_r	763.60	618.39	868.65
Cryst syst	triclinic	triclinic	monoclinic
Color, habit	Orange, needle	Green, block	Green, block
Size (mm)	0.4 x 0.12 x 0.05	0.33 x 0.25 x 0.20	0.33 x 0.30 x 0.25
Space group	P-1	P-1	Pc
a (Å)	11.8068(14)	10.8266(7)	11.6597(7)
b (Å)	13.0124(15)	12.1078(8)	16.9613(11)
c (Å)	13.3226(15)	12.8979(8)	12.2584(8)
α (º)	71.802(3)	91.267(2)	90
β (º)	84.699(4)	114.454(2)	116.630(2)
ɣ (º)	79.232(4)	93.084(2)	90
V (Å^3)	1908.9(4)	1535.01(17)	2167.1(2)
Z	2	2	2
ρ_{calc}, g·cm^{-3}	1.328	1.338	1.331
μ (mm^{-1})	0.555	0.669	0.859
F(000)	808	646	916
temp (K)	100(2)	100(2)	100(2)
θ range (º)	2.380-24.802	2.361-27.197	2.213-28.370
data collected (h,k,l)	13, -12; 15, -15; 15, -15	13, -13; 15, -15; 16, -16	15, -15; 22, -22; 16, -16
min,max transm	0.639; 0.745	0.6582; 0.7455	0.668; 0.746
rflns collected	28953	32363	53581
indpndt reflns	6541	6827	10753

observed reflns $F_o \geq 2.0\ \sigma(F_o)$	4446	6121	10284
R(F) (%)	0.0513	0.0310	0.0595
wR (F^2) (%)	0.1054	0.0763	0.1575
GooF	1.019	1.044	1.070
Weighting a,b	0.036; 1.1887	0.0327; 0.9315	0.0961; 1.2664
Params refined	493	399	545
Min, max resid dens	-0.322; 0.362	-0.213; 0.404	-0.840; 0.092

Table S1. Crystallographic Data. (Continued)

	5	**6**	**8**
Chem formula	$C_{135}H_{111}N_{20}Ni_4$	$C_{64}H_{54}N_{10}Ni_2O$	$C_{32}H_{27}N_5Ni$
M_r	2248.27	1096.59	540.29
Cryst syst	monoclinic	triclinic	orthorhombic
Color, habit	Blue, plate	Violet, block	Green, block
Size (mm)	0.40 x 0.15 x 0.02	0.02 x 0.02 x 0.02	0.02 x 0.02 x 0.02
Space group	C2	P -1	Pcca
a (Å)	28.6944(17)	12.0657(16)	26.848(3)
b (Å)	7.3064(5)	23.067(3)	14.5340(17)
c (Å)	28.2539(17)	23.079(3)	16.6359(19)
α (º)	90	76.493(3)	90
β (º)	113.099(2)	81.913(3)	90
ɣ(º)	90	81.444(3)	90
V ($Å^3$)	5448.6(6)	6138.6(14)	6491.6(13)
Z	2	4	8
ρ_{calc}, $g \cdot cm^{-3}$	1.370	1.187	1.106
μ (mm^{-1})	0.745	0.160	0.150
F(000)	2346	2288.0	2256.0
temp (K)	100(2)	100(2)	100(2)
θ range (º)	2.250-27.156	1.996-29.522	2.402-30.02
data collected (h,k,l)	36, -36; 9, -9; 36, -36	14, 28, 28	33, 18, 20
min,max transm	0.6647; 0.7455	0.550; 0.744	0.715; 0.744
rflns collected	43574	135413	139459
indpndt reflns	11737	22723	6689
observed reflns $F_o \geq 2.0\ \sigma(F_o)$	10141	17677	5693
R(F) (%)	0.0378	0.0866	0.0286
wR (F^2) (%)	0.0752	0.1680	0.0803
GooF	1.031	1.094	1.053
Weighting a,b	0.0298; 3.2367	0.0453; 20.3719	0.0417; 2.3478
Params refined	728	1576	445
Min, max resid dens	-0.311; 0.415	-1.005, 1.132	-0.3, 0.3

Kinetic Studies

Reaction Order and Kinetic Isotope Effect (KIE = k_H/k_D):

A stock solution was prepared by dissolving 3 mg of **5** in 5 mL of THF. The following conditions were used to determine the reaction order and KIE. Each reaction was followed for at least 12 mins. The kinetic data was fitted by using the first eight data points (8 mins).

Table S2. Conditions and results of reaction order and KIE studies[a].

	[**5**] (mM)	Stock Solution (mL)	THF (mL)	H_2O/D_2O (μL)	$[A]_{int}$[b] (A.U.)	Rate[c] ([A]/min)
1-H_2O	0.186	1.0	0	5	1.996	-0.06420
2-H_2O	0.093	0.5	0.5	5	1.023	-0.01742
3-H_2O	0.047	0.25	0.75	5	0.526	-0.00495
4-D_2O	0.093	0.5	0.5	5	1.037	-0.00738
5-D_2O	0.149	0.8	0.2	5	1.584	-0.01755

a: A cuvette with 0.2 cm path length was used.

b: Initial absorbance was obtained by the intersect of linear fitting

c: Reaction rate was obtained by the slope of linear fitting

Reaction order was calculated by the following equations:

$$\text{reaction order} = \log([Ni]_1/[Ni]_2) / \log(\text{rate}_1/\text{rate}_2)$$

By using this equation, reaction orders are 1.95, 1.89 and 1.92 when using H_2O as substrate, and 2.04 when D_2O was used. Therefore, this reaction is second order to the Ni complex.

The KIE was calculated by the following equations:

$$k_H/k_D = \text{rate}_H*([Ni]_D)^2 / \text{rate}_D*([Ni]_H)^2$$

By using all possible 6 combinations, the following KIEs can be obtained: 2.35, 2.43, 2.61, 2.30, 2.38 and 2.56; the averaged KIE is 2.4 with a standard deviation of 0.1.

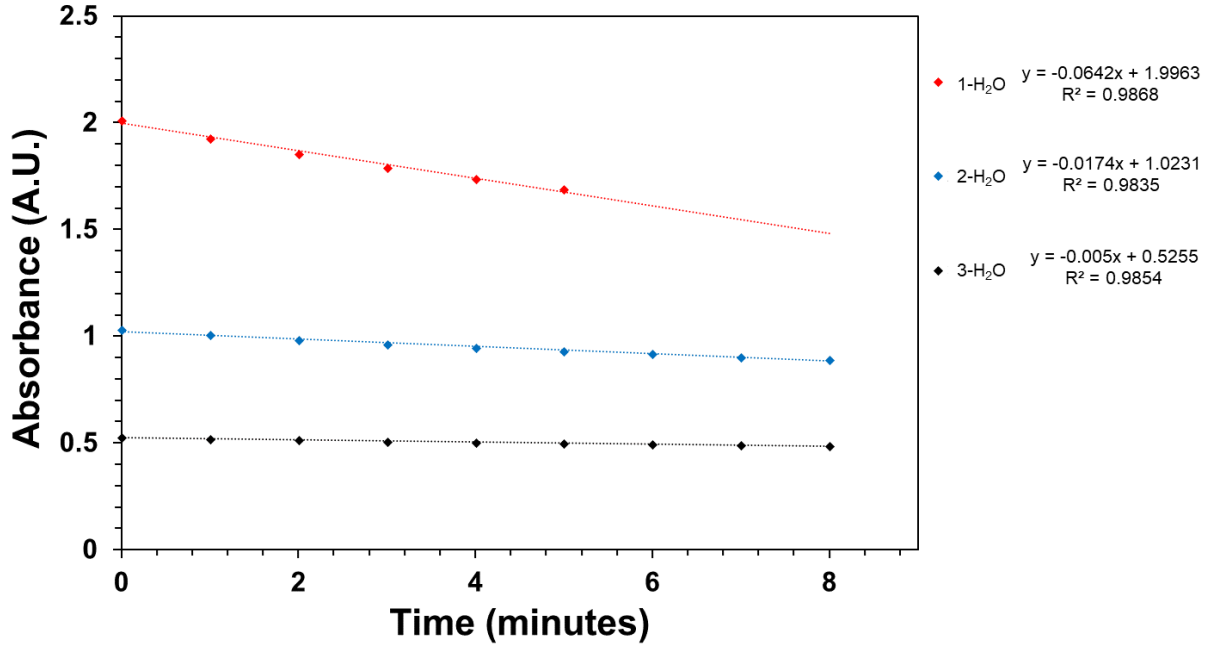

Figure S37. Raw data and lines of best fit for order and KIE studies using H_2O and **5**.

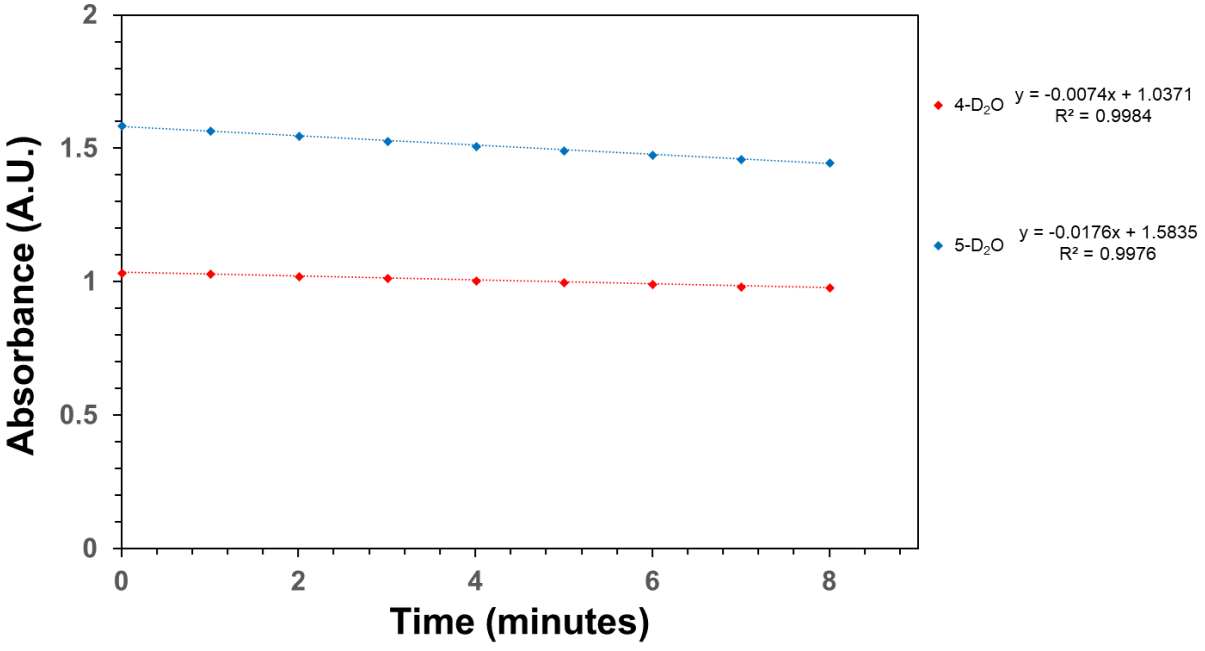

Figure S38. Raw data and lines of best fit for order and KIE studies using D_2O and **5**.

Table S3. Raw data for KIE studies. All values for trials are for Absorbance (A. U.)

Time (min)	1-H_2O	2-H_2O	3-H_2O	4-D_2O	5-D_2O
0	2.014	1.033	0.528	1.036	1.586
1	1.928	1.008	0.521	1.031	1.568

2	1.853	0.985	0.515	1.023	1.548
3	1.791	0.964	0.509	1.015	1.528
4	1.738	0.947	0.504	1.007	1.511
5	1.691	0.931	0.499	1	1.494
6	-	0.917	0.495	0.992	1.477
7	-	0.904	0.492	0.985	1.461
8	-	0.892	0.488	0.979	1.447

$\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$:

The following two stock solutions were prepared:

Solution 1: Dissolving 9.5 mg of **5** in 4.5 mL dry THF.
Solution 2: Adding 0.5 mL H_2O into 100 mL dry THF.

Procedure:
4 mL of *solution 2* and a stir bar were charged into a dip probe setup. The solution was stirred in a water bath, which was at the target temperature of kinetic study, under positive nitrogen pressure. After the solution was stirred for a least 5 mins, a baseline of the experiment was collected. After which, 0.2 mL of *solution 1* was introduced to the bottom of reaction flask by using syringe and then the reaction was followed for 18 mins. The first data point was discarded and the rate of reaction was obtained by using linear fit based one the rest 17 data points.

Table S4. Results of kinetic studies.

No.	Temperature (K)	Rate ([A]/min)	k_{obs} (M^{-2} s^{-1})	ln(k_{obs}/T)	Avg. ln(k_{obs}/T)	STD of ln(k_{obs}/T)
1-1		0.00666	3192.9	2.3804		
1-2		0.00589	2823.6	2.2575		
1-3	RT	0.00505	2424.1	2.1050	2.4147	0.2103
1-4	(295.4)	0.00835	4006.4	2.6074		
1-5		0.00901	3537.5	2.4829		
1-6		0.01074	4201.1	2.6549		
2-1		0.01162	5573.3	2.9006		
2-2	306.5	0.01005	4820.3	2.7554	2.8378	0.0745
2-3		0.01113	5338.3	2.8575		
2-4		0.01149	5511.0	2.8893		
3-1		0.01491	7151.3	3.1178		
3-2	316.5	0.01371	6575.7	3.0339	3.0628	0.0813
3-3		0.01275	6115.3	2.9613		
3-4		0.01522	7300.0	3.1384		
4-1		0.0199	9544.6	3.3703		
4-2	328.2	0.0189	9065.0	3.3187	3.3710	0.0598
4-3		0.02166	10388.8	3.4550		
4-4		0.01931	9261.7	3.3402		

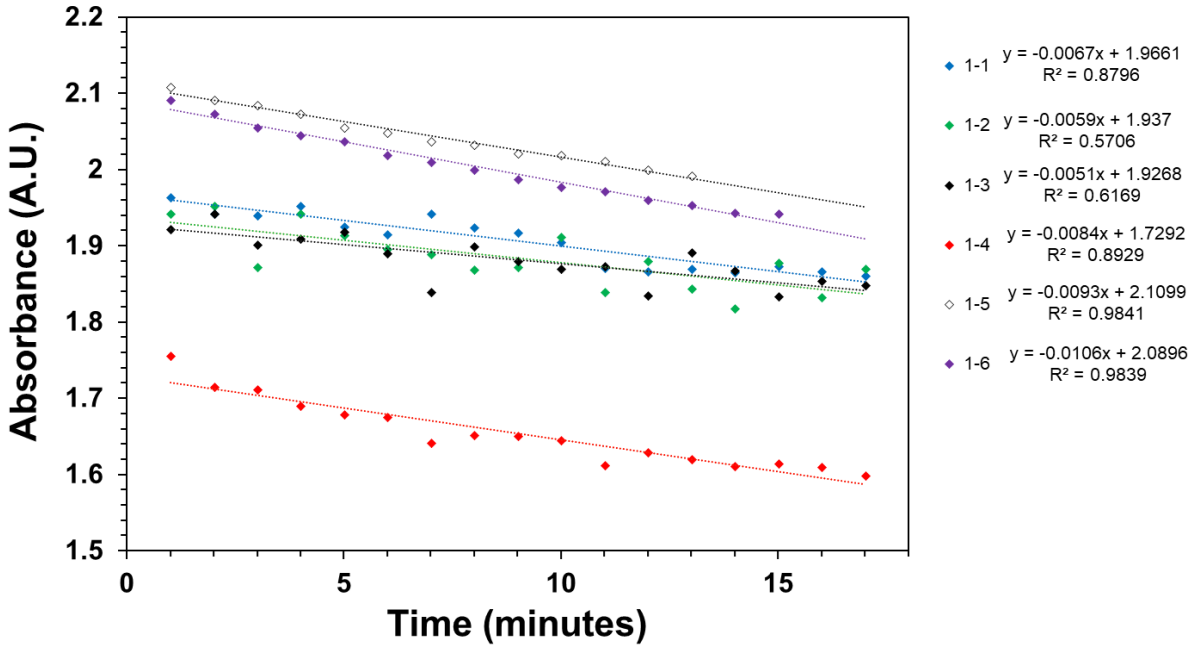

Figure S39. Raw data and lines of best fit at 295.4 K. Absorbance values collected at 644 nm.

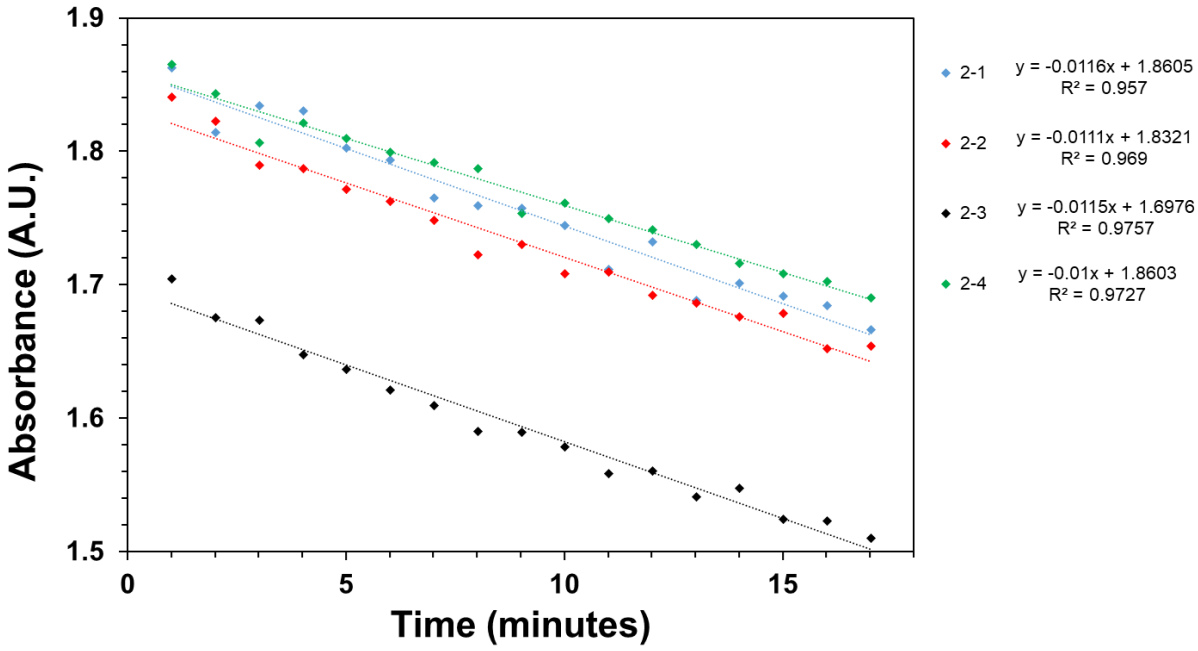

Figure S40. Raw data and lines of best fit at 306.5 K. Absorbance values collected at 600 nm.

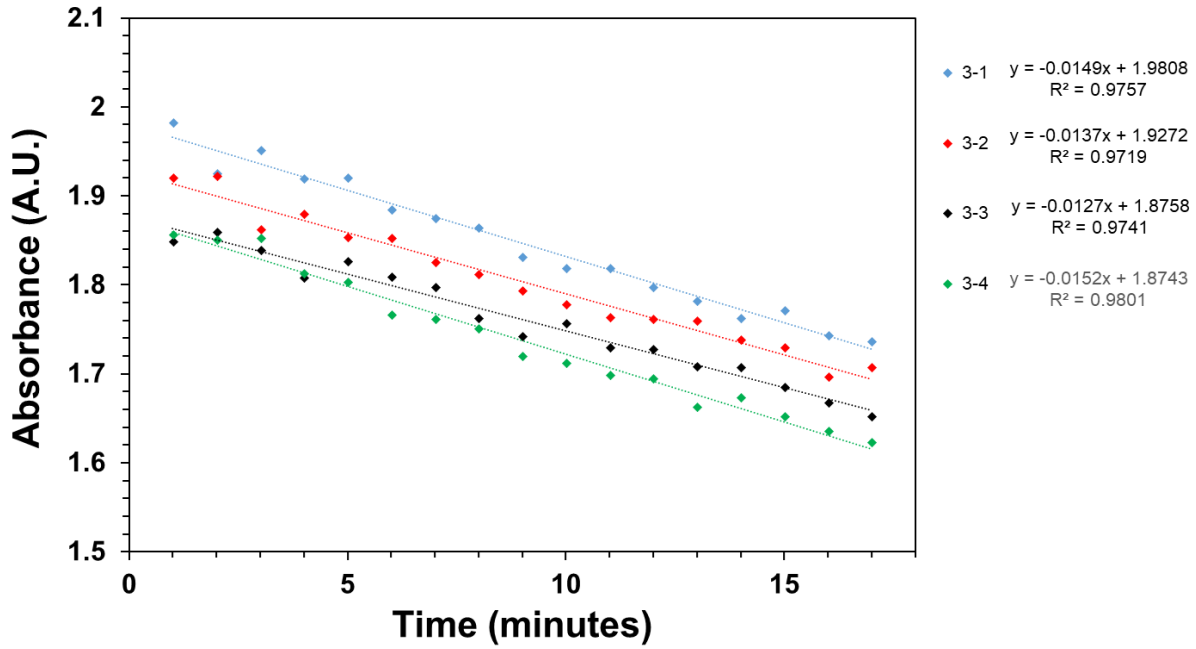

Figure S41. Raw data and lines of best fit at 316.5 K. Absorbance values collected at 600 nm.

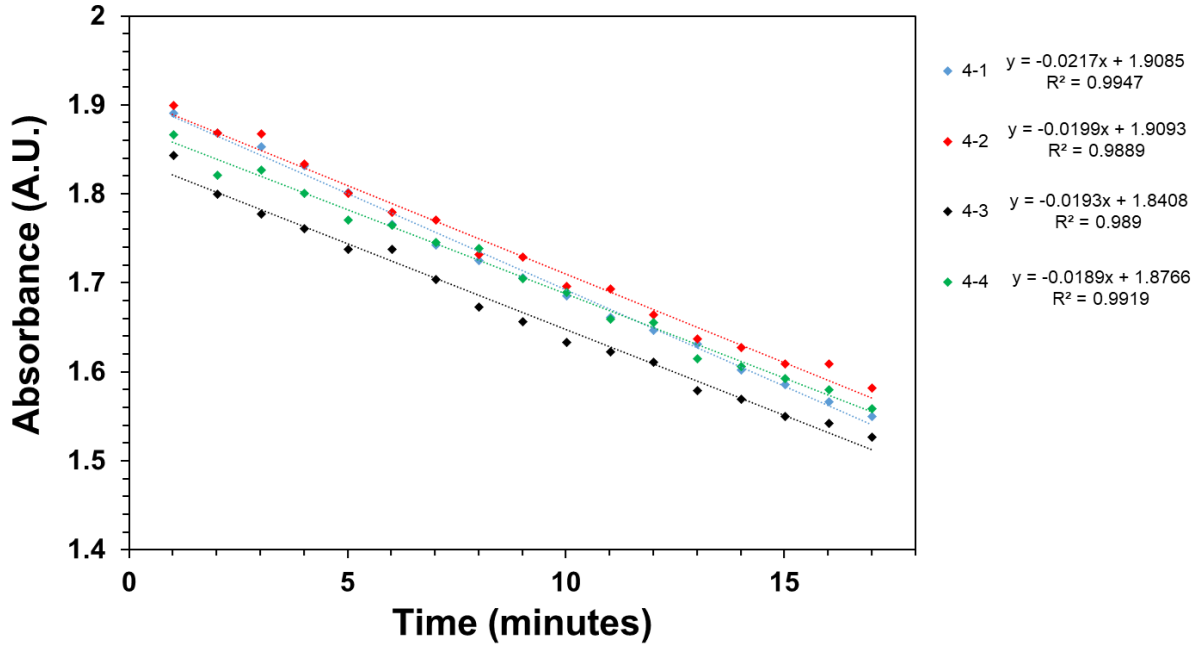

Figure S42. Raw data and lines of best fit at 328.2 K. Absorbance values collected at 600 nm.

Table S5. Raw data for kinetic studies. All values for trials are for Absorbance (A. U.)

Time (min)	1-1	1-2	1-3	1-4	1-5	1-6	2-1	2-2	2-3	2-4
0	2.019	1.798	1.944	1.943	2.129	2.098	1.873	1.857	1.722	1.875
1	1.964	1.756	1.922	1.943	2.108	2.092	1.863	1.841	1.705	1.866
2	1.943	1.715	1.943	1.953	2.092	2.073	1.815	1.823	1.676	1.844
3	1.94	1.712	1.902	1.873	2.085	2.056	1.835	1.79	1.674	1.807
4	1.953	1.691	1.91	1.943	2.074	2.045	1.831	1.788	1.648	1.822
5	1.926	1.679	1.919	1.914	2.056	2.037	1.803	1.772	1.637	1.81
6	1.915	1.676	1.891	1.896	2.049	2.019	1.794	1.763	1.622	1.8
7	1.942	1.642	1.84	1.889	2.037	2.01	1.766	1.749	1.61	1.792
8	1.924	1.652	1.899	1.869	2.033	2	1.76	1.723	1.591	1.788
9	1.918	1.651	1.88	1.873	2.022	1.988	1.758	1.731	1.59	1.754
10	1.905	1.645	1.87	1.912	2.019	1.978	1.745	1.709	1.579	1.762
11	1.871	1.613	1.874	1.84	2.011	1.972	1.712	1.71	1.559	1.75
12	1.867	1.63	1.835	1.88	2	1.961	1.733	1.693	1.561	1.742
13	1.87	1.621	1.892	1.844	1.992	1.954	1.689	1.687	1.542	1.731
14	1.866	1.611	1.868	1.818	-	1.944	1.702	1.677	1.548	1.717
15	1.874	1.615	1.834	1.878	-	1.942	1.692	1.679	1.525	1.709
16	1.867	1.61	1.854	1.833	-	-	1.685	1.653	1.524	1.703
17	1.861	1.599	1.849	1.87	-	-	1.667	1.655	1.511	1.691

Table S5. Raw data for kinetic studies. All values for trials are for Absorbance (A. U.) (Continued.)

Time (min)	3-1	3-2	3-3	3-4	4-1	4-2	4-3	4-4
0	2.041	1.986	1.862	1.882	1.934	1.87	1.89	1.849
1	1.983	1.921	1.849	1.857	1.892	1.9	1.844	1.867
2	1.926	1.923	1.86	1.851	1.869	1.869	1.801	1.822
3	1.952	1.863	1.84	1.853	1.854	1.868	1.778	1.828
4	1.92	1.88	1.809	1.813	1.833	1.834	1.762	1.802
5	1.921	1.854	1.827	1.804	1.803	1.802	1.739	1.772
6	1.885	1.853	1.81	1.767	1.767	1.78	1.739	1.766
7	1.875	1.826	1.798	1.762	1.743	1.772	1.705	1.746
8	1.865	1.812	1.763	1.751	1.726	1.733	1.674	1.74
9	1.832	1.794	1.743	1.72	1.707	1.73	1.657	1.706
10	1.819	1.779	1.757	1.713	1.686	1.697	1.634	1.69
11	1.819	1.764	1.73	1.699	1.662	1.694	1.623	1.66
12	1.798	1.762	1.728	1.695	1.648	1.665	1.612	1.656
13	1.782	1.76	1.709	1.663	1.632	1.638	1.58	1.616
14	1.763	1.739	1.708	1.674	1.603	1.628	1.57	1.607
15	1.772	1.73	1.686	1.653	1.587	1.61	1.551	1.593

16	1.744	1.697	1.668	1.636	1.567	1.61	1.543	1.581
17	1.737	1.708	1.653	1.624	1.551	1.583	1.528	1.559

DFT Calculations

General Description

Geometry optimizations and single point calculations were performed with the Gaussian09[11] program using density functional theory (DFT). In order to increase computational efficiency, the *p*-tol groups in some cases were replaced by Ph. Geometries were fully optimized starting from the X-ray structures or structures generated by Avogadro using the B3LYP exchange-correlation functional with the 6-31G(d) basis set. Geometry optimizations were performed without constraints, and the resulting structures were confirmed to be minima on the potential energy surface by frequency calculations (number of imaginary frequencies = 0).

The reaction coordinate scans were performed with the ORCA software suite.[12] The BP86 functional was used with a 6-31G basis set on C and H and a TZVPP basis set used on Ni, N, and O. Note that no maximum is observed along the reaction coordinate, making reliable assessment of a transition state geometry difficult. Nevertheless, the energy changes along the reaction coordinate are small, consistent with the experimental energy of activation. The negative energies of reaction compared with those calculated for the intermediates is likely a result of the different functionals in these two calculations.

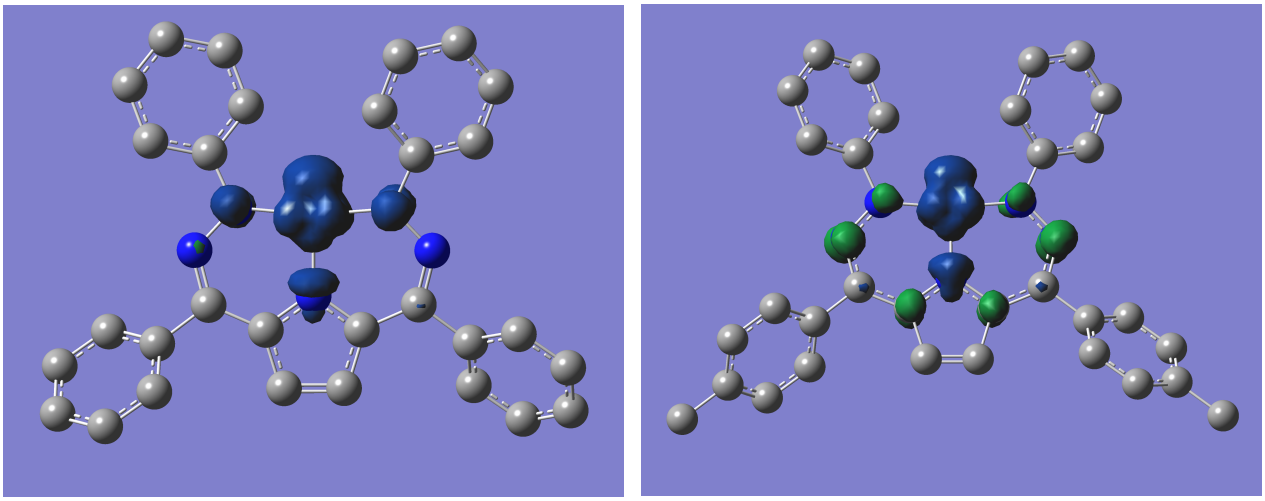

Figure S43. Calculated spin density plot of **4** (left) and **5** (right).

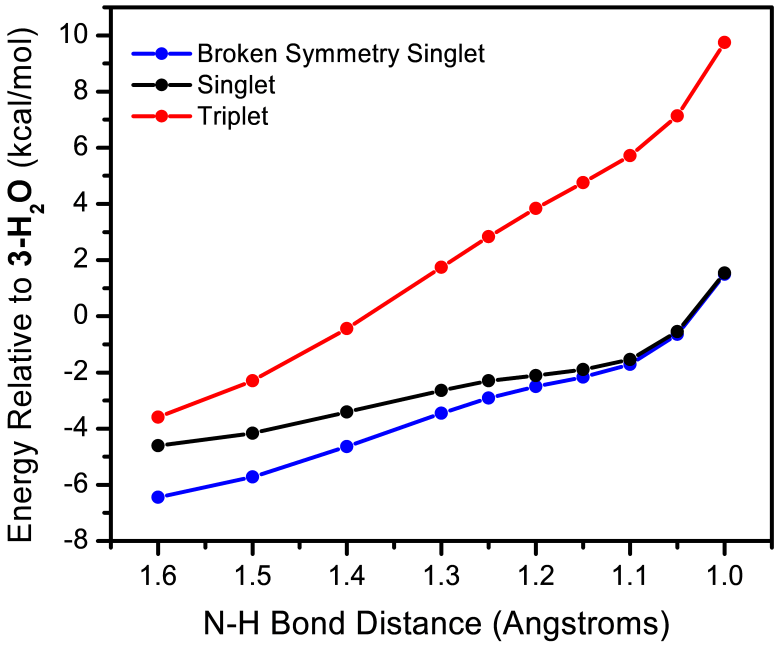

Figure S44. Calculated energies for the reaction coordinate of two molecules of **3-H₂O** converting to **6**.

Table S6. Calculated H and G.

Species	H (kcal/mol)	H (Hartrees)	G (kcal/mol)	G(Hartrees)
H_2O	-47947.3	-76.7156893	-47945.1	-76.712164
2-H₂O	-1941538.8	-3106.462098	-1941241.0	-3105.985587
3-H₂O	-1941155.6	-3105.848966	-1940865.4	-3105.384678
5	-1893192.8	-3029.10855	-1892919.1	-3028.670568
6	-3834369.2	-6134.990723	-3833786.5	-6134.05841
3-H₂O*	-1948856.5	-3093.423008	-1948565.8	-3092.961580
3-H₂O* Transition State	-1948840.1	-3093.396980	-1948552.2	-3092.940056
[^{Tol,Ph}DHPy]Ni(OH)]	-1940772.5	-3105.236013	-1940488.6	-3104.781811
[[^{Tol,Ph}DHPyH•]Ni(H_2O)]$^+$	-1941415.3	-3106.264434	-1941117.7	-3105.788312
[[^{Tol,Ph}DHPy•]Ni(OH)]$^-$	-1940821.2	-3105.313893	-1940539.4	-3104.863117
[^{Tol,Ph}DHPy]Ni(H)	-1893554.3	-3029.68681	-1893272.6	-3029.236112
Note that **3-H₂O*** = [^{Tol,Ph}DHPyH]Ni(OH)				

Optimized Coordinates
2-H₂O
68

Ni	0.02985	0.81268	-0.43050
O	-0.64155	2.35348	-1.37562
N	1.78159	1.35635	-0.15714
N	2.87863	0.60664	-0.05461
N	0.47533	-0.87785	-0.05919
N	-1.73770	0.12599	-0.36214
C	1.65371	-1.47905	0.19186
N	-2.84977	0.86278	-0.81889
C	2.10313	2.72725	-0.33381
C	0.00289	-3.02818	0.46295
H	-0.54482	-3.93827	0.66960
C	5.24394	-0.65110	0.90973
H	5.04567	0.33714	1.31191

C	1.37611	-2.84792	0.52863
H	2.11112	-3.58529	0.81738
C	-3.06412	-2.01387	-0.22478
C	-0.55732	-1.77693	0.08499
C	2.86368	-0.70305	0.11780
C	4.20073	-1.33569	0.26174
C	6.50821	-1.21772	1.03019
H	7.29382	-0.66301	1.54016
C	-5.38194	-3.65010	-0.34694
C	6.78978	-2.49151	0.51397
C	-1.82515	-1.21020	-0.16056
C	1.30752	3.69756	0.30442
H	0.53135	3.36873	0.99237
C	-4.81371	2.18706	-0.28782
H	-5.17501	2.00611	-1.29802
C	4.48662	-2.60231	-0.27144
H	3.71968	-3.13930	-0.82105
C	-4.20294	-4.01694	-1.00976
H	-4.17560	-4.94219	-1.58093
C	-4.24427	-1.64591	0.44567
H	-4.26573	-0.74470	1.04906
C	1.56221	5.05955	0.12499
H	0.94451	5.79279	0.63802
C	3.43692	4.51402	-1.28809
H	4.27311	4.82758	-1.90828
C	-3.13640	1.84897	1.42960
H	-2.20853	1.39232	1.75599
C	3.18422	3.15449	-1.12218
H	3.81241	2.40534	-1.59054
C	2.62458	5.47595	-0.67865
H	2.82759	6.53419	-0.81658
C	5.75614	-3.16693	-0.14312
H	5.94818	-4.14697	-0.57563
C	-3.06433	-3.21806	-0.95272
H	-2.16398	-3.51733	-1.48019
C	-5.37671	-2.45431	0.38379
H	-6.27141	-2.15442	0.92460
C	-3.60370	1.61172	0.13081
C	-5.08040	3.23329	1.88112
H	-5.65174	3.86030	2.55912
C	-6.62315	-4.50578	-0.43391
H	-7.22708	-4.24103	-1.31237
H	-7.25969	-4.37902	0.44789
H	-6.37226	-5.56812	-0.52246
C	-5.54514	2.98679	0.58588
H	-6.48359	3.42063	0.25093
C	-3.87711	2.66077	2.29233
H	-3.50656	2.83667	3.29875
C	8.15652	-3.11418	0.67890
H	8.95459	-2.37556	0.54009
H	8.31762	-3.92324	-0.04154
H	8.28546	-3.54102	1.68305
H	-3.43729	0.32531	-1.45432
H	-1.62115	2.23683	-1.41150
H	-0.40379	3.24934	-1.07629

3-H_2O

67

Ni	0.02811	1.08878	0.17480
N	-1.84510	1.12855	0.36333
N	1.81985	1.20673	-0.40016
N	0.05056	-0.72472	-0.02092
C	-2.37228	-1.08826	-0.11371
N	-2.72679	0.14983	0.19157
N	2.78495	0.31632	-0.22298
C	-3.51374	-2.00141	-0.38939
C	-3.33682	2.25015	1.97282
H	-3.44039	1.30676	2.49817
C	1.43012	3.24831	-1.66235
H	0.42723	2.88927	-1.87740
C	-1.02719	-1.56172	-0.14208
C	-3.46425	-2.96087	-1.41284
H	-2.57390	-3.04343	-2.02857
C	4.88525	-1.59518	-0.39721
H	4.91273	-0.81859	-1.15459
C	3.17445	4.90094	-1.96720
H	3.51283	5.85093	-2.37041
C	2.50527	-0.94477	0.06124
C	-5.74026	-3.68403	-0.93530
C	3.69083	-1.80375	0.31522
C	0.81249	-2.86829	-0.06837
H	1.49818	-3.70296	-0.07468
C	-0.55958	-2.91132	-0.17006
H	-1.18453	-3.78918	-0.23966
C	3.67794	-2.80711	1.29567
H	2.78100	-2.96892	1.88580
C	-4.70846	-1.88556	0.34169
H	-4.77397	-1.13256	1.12008
C	-4.55763	-3.78599	-1.67586
H	-4.49255	-4.51358	-2.48214
C	2.30619	2.42821	-0.92087
C	3.63181	2.86682	-0.72019

H	4.30775	2.23318	-0.15915
C	1.18864	-1.49522	0.02525
C	6.01051	-2.37165	-0.14660
H	6.91790	-2.19636	-0.72137
C	4.05073	4.08691	-1.24010
H	5.07451	4.41084	-1.07065
C	-2.53001	2.29715	0.82507
C	-3.84717	4.60914	1.74218
H	-4.35595	5.49994	2.09900
C	-6.91431	-4.59682	-1.20015
H	-7.86634	-4.05870	-1.12701
H	-6.95344	-5.41962	-0.47333
H	-6.85582	-5.04555	-2.19727
C	-3.05565	4.66339	0.59560
H	-2.95758	5.59339	0.04183
C	-3.98905	3.39524	2.42239
H	-4.60690	3.34311	3.31499
C	-2.40278	3.51482	0.13458
H	-1.83291	3.54139	-0.79078
C	-5.79490	-2.71101	0.07393
H	-6.70495	-2.60088	0.66048
C	4.81167	-3.58255	1.54147
H	4.77437	-4.35028	2.31135
C	5.99721	-3.38289	0.82691
C	1.86380	4.47087	-2.17665
H	1.17586	5.07719	-2.76026
C	7.22997	-4.21289	1.09794
H	7.63836	-4.63856	0.17325
H	7.01333	-5.04070	1.78068
H	8.02727	-3.60961	1.55168
O	0.25793	2.81849	1.05940
H	-0.55187	3.36434	1.12567
H	0.93811	3.36428	0.62057

5

64

Ni	0.00003	1.14177	-0.00184
N	1.84789	1.27742	0.01871
N	-1.84788	1.27745	-0.02000
N	0.00006	-0.73640	-0.00104
C	2.42120	-0.98531	0.02951
N	2.75273	0.31278	-0.01273
N	-2.75258	0.31270	0.01258
C	3.60419	-1.89057	0.08352
C	3.67496	2.83770	-0.62297
H	4.23750	2.01607	-1.04939
C	-1.70692	3.62843	-0.54664
H	-0.76461	3.41349	-1.04582
C	1.10884	-1.52771	0.01974
C	3.69107	-2.93634	1.01459
H	2.88438	-3.09059	1.72523
C	-4.69441	-1.68289	0.77643
H	-4.65181	-0.86880	1.49317
C	-3.43200	5.19297	0.09609
H	-3.82149	6.20665	0.12628
C	-2.42106	-0.98536	-0.03035
C	5.89830	-3.56184	0.19854
C	-3.60406	-1.89066	-0.08356
C	-0.68386	-2.91086	-0.00219
H	-1.33713	-3.77107	0.00605
C	0.68404	-2.91084	0.00064
H	1.33733	-3.77103	-0.00736
C	-3.69155	-2.93633	-1.01468
H	-2.88537	-3.09044	-1.72593
C	4.69517	-1.68263	-0.77563
H	4.65304	-0.86846	-1.49231
C	4.81881	-3.75541	1.06764
H	4.86426	-4.55065	1.80854
C	-2.43253	2.57464	0.02678
C	-3.67420	2.83727	0.62490
H	-4.23594	2.01544	1.05197
C	-1.10869	-1.52775	-0.02150
C	-5.81498	-2.50538	0.72160
H	-6.64248	-2.32523	1.40478
C	-4.16231	4.14102	0.65790
H	-5.12139	4.33900	1.12946
C	2.43243	2.57470	-0.02681
C	3.43149	5.19321	-0.09391
H	3.82082	6.20697	-0.12325
C	7.10702	-4.46700	0.23554
H	8.03474	-3.90469	0.08063
H	7.05765	-5.23044	-0.55263
H	7.18562	-4.99168	1.19335
C	2.20031	4.92947	0.51010
H	1.62857	5.73326	0.96572
C	4.16286	4.14155	-0.65488
H	5.12262	4.33985	-1.12492
C	1.70573	3.62818	0.54578
H	0.76270	3.41288	1.04343
C	5.81574	-2.50506	-0.72009
H	6.64373	-2.32476	-1.40265
C	-4.81928	-3.75545	-1.06702

H	-4.86523	-4.55060	-1.80799	C	-3.58290	-0.68281	3.36559
C	-5.89814	-3.56205	-0.19710	H	-4.56497	-0.21997	3.38737
C	-2.20169	4.92961	-0.50986	C	-2.53320	-0.02876	2.72592
H	-1.63081	5.73363	-0.96615	H	-2.67453	0.93854	2.25804
C	-7.10680	-4.46733	-0.23328	C	-3.12847	-5.65244	-1.14786
H	-7.05594	-5.23193	0.55368	H	-3.05401	-6.65090	-0.72381
H	-7.18700	-4.99065	-1.19172	C	0.73759	3.49277	2.32099
H	-8.03431	-3.90537	-0.07594	C	-7.46367	-1.54224	-0.18361
				H	-7.99407	-2.43764	-0.50077
6				C	1.23782	4.45336	1.42854
131				H	1.75364	4.13602	0.52766
Ni	-1.26398	-0.24058	-0.89885	C	1.81687	-3.69560	0.25731
Ni	1.04586	-0.99202	1.00978	C	5.75422	-1.43140	0.75521
O	-0.39019	-1.68745	0.01376	C	-0.00935	3.93432	3.42729
N	-0.16123	0.02296	2.03882	H	-0.42204	3.20063	4.11214
N	-0.11577	1.26888	2.37914	C	-1.06959	-1.88852	3.25416
N	-3.29729	-2.16870	0.07968	H	-0.07583	-2.32344	3.25541
N	2.39931	0.18247	1.44539	C	2.58029	0.08095	-2.39243
N	0.20154	0.47998	-1.82518	H	2.82778	1.07330	-2.03507
N	-2.18872	1.27503	-1.22208	C	-3.38503	-1.93562	3.95496
N	-2.99718	-0.88991	-0.42110	H	-4.20856	-2.44033	4.45179
N	0.45387	1.76251	-2.10413	C	-2.12420	-2.53238	3.90374
N	2.26264	-2.35328	0.53448	H	-1.95245	-3.49326	4.38101
N	3.56421	-2.32874	0.55857	C	-7.43302	0.57848	0.93728
C	1.24089	-0.34958	-2.31472	H	-7.93288	1.35424	1.51316
C	-1.82042	2.49592	-1.66181	C	0.91643	-1.62561	-2.80969
C	-4.07640	2.51244	-1.36346	H	-0.12316	-1.94178	-2.82047
H	-5.11856	2.80151	-1.33688	C	4.41553	1.26666	1.40010
C	-6.12562	-1.39011	-0.53251	C	-3.32797	-4.19599	-3.05192
H	-5.64040	-2.15648	-1.12499	H	-3.40698	-4.04601	-4.12580
C	-4.00055	-0.00542	-0.52073	C	4.28436	-1.23356	0.84279
C	-5.41447	-0.23836	-0.15436	C	-6.09525	0.74593	0.58269
C	-3.54533	1.24602	-1.01307	H	-5.56494	1.64222	0.88901
C	0.94531	2.04510	2.08643	C	0.70510	-4.22644	0.92283
C	-3.00112	3.29783	-1.76367	H	0.15343	-3.61289	1.62114
H	-3.04447	4.31399	-2.12810	C	-3.32594	-3.07985	-2.21142
C	-1.27426	-0.63977	2.65689	H	-3.40088	-2.08079	-2.62736
C	2.19416	1.51005	1.73331	C	-8.14264	-0.56786	0.56255
C	1.06351	4.21989	-3.35452	C	-3.23094	-5.48637	-2.53281
H	1.46822	3.32517	-3.81564	H	-3.23550	-6.34922	-3.19243
C	0.04862	4.07747	-2.38888	C	1.02397	5.81229	1.65586
C	-0.43938	2.72763	-2.00664	H	1.40164	6.53347	0.93562
C	-3.21981	-3.24785	-0.82103	C	3.46848	2.19210	1.71735
C	3.73262	0.00321	1.22399	C	-0.45069	5.24815	-1.79567
C	-3.12161	-4.55066	-0.29920	H	-1.19988	5.17590	-1.01419
H	-3.05380	-4.68619	0.77796	C	-0.21411	5.29158	3.64670

H	-0.78784	5.61034	4.51441
C	3.55444	-0.74548	-2.94480
H	4.58209	-0.39348	-2.99751
C	1.53887	5.47439	-3.71757
H	2.31852	5.54941	-4.47363
C	6.62206	-0.97894	1.76114
H	6.21598	-0.48414	2.63875
C	0.02840	6.50523	-2.16952
H	-0.38015	7.39285	-1.68993
C	0.30485	6.25786	2.77074
C	7.68233	-2.33746	-0.41629
H	8.08749	-2.87318	-1.27223
C	0.31520	-5.54635	0.69546
H	-0.54285	-5.94531	1.22806
C	6.31033	-2.12576	-0.33222
H	5.65317	-2.48769	-1.11635
C	8.55421	-1.87125	0.57919
C	1.89884	-2.44584	-3.36158
H	1.61818	-3.41953	-3.75470
C	7.99677	-1.19447	1.66996
H	8.64484	-0.84327	2.46983
C	1.02580	6.64641	-3.13956
C	10.04524	-2.08327	0.46596
H	10.28048	-3.08364	0.08542
H	10.54207	-1.96420	1.43420
H	10.49831	-1.36074	-0.22609
C	-9.58759	-0.76162	0.95718
H	-10.18647	-1.12939	0.11597
H	-10.03644	0.17316	1.30810
H	-9.68478	-1.49806	1.76605
C	2.52686	-4.50521	-0.64525
H	3.38096	-4.08808	-1.16162
C	1.01982	-6.34796	-0.20088
H	0.71167	-7.37440	-0.37819
C	3.22544	-2.01465	-3.43387
H	3.98683	-2.64704	-3.88307
C	2.12519	-5.81701	-0.87203
H	2.67829	-6.42888	-1.57963
C	0.09699	7.73099	3.03050
H	0.25744	8.32361	2.12416
H	0.79478	8.10289	3.79292
H	-0.91600	7.93582	3.39495
C	1.52326	8.00719	-3.56790
H	1.20796	8.78789	-2.86746
H	1.13745	8.28167	-4.55904
H	2.61768	8.03505	-3.63294
H	-2.73084	-2.33050	0.90810
H	-0.09860	-2.41503	-0.55588
H	5.47762	1.42087	1.28097
H	3.61169	3.24045	1.93346

[^{Tol,Ph}DHPy]Ni(OH)]

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Ni	-0.02228	1.11810	-0.24992
N	1.83327	1.11049	-0.44756
N	-1.80936	1.24126	0.30599
N	-0.06623	-0.72638	0.00734
C	2.32733	-1.10979	0.08951
N	2.68317	0.14991	-0.22249
N	-2.74010	0.35234	0.24605
C	3.47253	-2.00647	0.38127
C	3.43768	2.22521	-1.93594
H	3.51723	1.29618	-2.49099
C	-1.47361	3.24400	1.65161
H	-0.46822	2.89678	1.85675
C	0.99727	-1.56983	0.10631
C	3.40990	-2.97825	1.39339
H	2.51248	-3.06801	1.99823
C	-4.88737	-1.49593	0.41757
H	-4.88684	-0.70704	1.16217
C	-3.25061	4.85757	1.94399
H	-3.61885	5.78207	2.38036
C	-2.49218	-0.93904	-0.07094
C	5.69844	-3.68058	0.94976
C	-3.70635	-1.75276	-0.30330
C	-0.83551	-2.88938	0.02160
H	-1.52984	-3.71681	0.01882
C	0.52077	-2.93940	0.12009
H	1.14693	-3.81725	0.17982
C	-3.73345	-2.76686	-1.27411
H	-2.85306	-2.95239	-1.88211
C	4.68229	-1.86946	-0.32256
H	4.76036	-1.10449	-1.08778
C	4.50228	-3.80086	1.66583
H	4.42762	-4.53726	2.46293
C	-2.30251	2.48410	0.81870
C	-3.60522	2.91741	0.54134
H	-4.23007	2.32404	-0.11583
C	-1.20422	-1.49077	-0.05272
C	-6.03501	-2.24577	0.19100
H	-6.93093	-2.03561	0.77143
C	-4.07033	4.10546	1.09856

H	-5.07580	4.44730	0.86838
C	2.57096	2.29200	-0.83947
C	4.07785	4.52933	-1.57513
H	4.66127	5.40043	-1.86024
C	6.87453	-4.58622	1.22762
H	7.82111	-4.03461	1.20118
H	6.94739	-5.38611	0.47839
H	6.78906	-5.06439	2.20877
C	3.21534	4.59111	-0.47800
H	3.12917	5.50914	0.09666
C	4.18327	3.34439	-2.30505
H	4.84758	3.28735	-3.16310
C	2.45453	3.48187	-0.11206
H	1.76838	3.53096	0.72355
C	5.76752	-2.69205	-0.04396
H	6.68912	-2.56630	-0.60842
C	-4.88983	-3.51424	-1.49423
H	-4.88484	-4.28983	-2.25668
C	-6.06038	-3.27175	-0.76707
C	-1.95356	4.41891	2.22161
H	-1.31110	4.99688	2.88014
C	-7.31987	-4.06682	-1.01580
H	-7.75617	-4.42931	-0.07747
H	-7.12709	-4.93431	-1.65482
H	-8.08606	-3.45535	-1.51021
O	-0.21019	2.80550	-0.85507
H	0.50638	3.03317	-1.46348

[[^{Tol,Ph}DHPyH•]Ni(H_2O)]$^+$

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Ni	0.01150	0.74909	-0.48867
O	-0.64386	2.20577	-1.53971
N	1.76112	1.33101	-0.17814
N	2.84944	0.62374	-0.02429
N	0.46142	-0.89817	0.03846
N	-1.76869	0.04558	-0.36840
C	1.65255	-1.48131	0.31301
N	-2.85786	0.75756	-0.88982
C	2.02811	2.73050	-0.24509
C	0.01334	-3.02167	0.65885
H	-0.52922	-3.92148	0.91285
C	5.28129	-0.55713	0.69780
H	5.11263	0.45921	1.03544
C	1.38763	-2.82681	0.72600
H	2.12348	-3.53994	1.06709
C	-3.05910	-2.08621	-0.14775
C	-0.54530	-1.79705	0.21099
C	2.84922	-0.71194	0.16081
C	4.18614	-1.31172	0.22317
C	6.55077	-1.11203	0.75488
H	7.37541	-0.51735	1.13961
C	-5.34875	-3.75337	-0.21843
C	6.79221	-2.42929	0.32718
C	-1.84268	-1.25982	-0.10349
C	1.11204	3.61365	0.35312
H	0.27004	3.21735	0.91547
C	-4.64722	2.35255	-0.51517
H	-4.97407	2.17245	-1.53674
C	4.42852	-2.62751	-0.22144
H	3.62218	-3.20869	-0.65559
C	-4.13663	-4.16713	-0.79061
H	-4.07664	-5.14011	-1.27101
C	-4.27316	-1.66468	0.42916
H	-4.33071	-0.71176	0.94556
C	1.33769	4.98910	0.30034
H	0.64273	5.66676	0.78751
C	3.37602	4.60794	-0.94474
H	4.25314	4.99472	-1.45498
C	-3.11082	1.89245	1.30721
H	-2.27123	1.33810	1.71308
C	3.16860	3.23199	-0.88889
H	3.86704	2.53847	-1.34245
C	2.46475	5.49021	-0.35646
H	2.63630	6.56122	-0.40229
C	5.70778	-3.16792	-0.17113
H	5.87405	-4.17698	-0.53895
C	-3.00720	-3.35674	-0.75259
H	-2.08392	-3.69672	-1.21124
C	-5.38993	-2.49274	0.39729
H	-6.31028	-2.15857	0.86890
C	-3.54275	1.65801	-0.00222
C	-4.88924	3.51875	1.59423
H	-5.41348	4.23897	2.21447
C	-6.57515	-4.62842	-0.27737
H	-7.16330	-4.41275	-1.17914
H	-7.22828	-4.46159	0.58461
H	-6.31005	-5.68960	-0.30820
C	-5.31955	3.27062	0.28703
H	-6.18014	3.79817	-0.11362
C	-3.78644	2.82966	2.09556
H	-3.45050	3.00544	3.11348
C	8.17119	-3.03021	0.41437

H	8.94533	-2.29377	0.17460
H	8.28374	-3.88131	-0.26375
H	8.37374	-3.39132	1.43158
H	-3.49759	0.14849	-1.40037
H	-1.61952	2.07975	-1.63409
H	-0.43359	3.13356	-1.32964

[[^{Tol,Ph}DHPy•]Ni(OH)]$^{-}$

66

Ni	-0.02719	1.10769	-0.29631
N	1.85401	1.10179	-0.48518
N	-1.80482	1.25446	0.33242
N	-0.08175	-0.73648	-0.02076
C	2.32916	-1.12339	0.05951
N	2.70535	0.10748	-0.24304
N	-2.78003	0.37483	0.19939
C	3.46213	-2.03506	0.37273
C	3.64180	2.16109	-1.79932
H	3.82243	1.19947	-2.26752
C	-1.40095	3.28977	1.59359
H	-0.37918	2.95462	1.72641
C	0.97600	-1.59361	0.08086
C	3.37053	-3.04058	1.35067
H	2.44554	-3.15913	1.90545
C	-4.94440	-1.42255	0.38547
H	-4.93732	-0.60642	1.10027
C	-3.16215	4.90328	1.99710
H	-3.50357	5.83544	2.44166
C	-2.53334	-0.89640	-0.08341
C	5.68264	-3.72037	0.98917
C	-3.75299	-1.71387	-0.30756
C	-0.88464	-2.86798	-0.00144
H	-1.58212	-3.69374	0.00813
C	0.49139	-2.93578	0.09581
H	1.09920	-3.82810	0.14409
C	-3.79059	-2.76338	-1.24017
H	-2.90114	-2.99091	-1.81892
C	4.70405	-1.88034	-0.27264
H	4.80704	-1.09004	-1.00849
C	4.45689	-3.86491	1.64666
H	4.35033	-4.62741	2.41700
C	-2.27733	2.48683	0.84528
C	-3.60623	2.91515	0.67990
H	-4.28202	2.29647	0.10174
C	-1.23165	-1.48705	-0.07502
C	-6.10354	-2.15741	0.16636
H	-7.00424	-1.91089	0.72736
C	-4.03665	4.11224	1.24772
H	-5.06661	4.43163	1.09899
C	2.61294	2.26003	-0.84697
C	4.17994	4.50580	-1.52602
H	4.78204	5.37313	-1.78715
C	6.85036	-4.63216	1.28820
H	7.79760	-4.07953	1.31740
H	6.96170	-5.41618	0.52533
H	6.72701	-5.13573	2.25377
C	3.15789	4.61220	-0.57987
H	2.96273	5.56568	-0.09392
C	4.41490	3.27101	-2.13486
H	5.20225	3.17008	-2.87932
C	2.37886	3.50603	-0.24196
H	1.57204	3.59863	0.47253
C	5.78394	-2.70263	0.02848
H	6.72792	-2.55456	-0.49471
C	-4.95761	-3.49914	-1.45336
H	-4.95188	-4.30346	-2.18743
C	-6.13559	-3.21531	-0.75606
C	-1.84062	4.47866	2.16581
H	-1.14556	5.07865	2.74958
C	-7.40353	-4.00341	-0.99225
H	-7.82365	-4.38612	-0.05288
H	-7.22342	-4.86157	-1.64917
H	-8.18363	-3.38804	-1.46152
O	-0.23341	2.76857	-0.99882
H	0.51607	2.96892	-1.57563

[^{Tol,Ph}DHPy]Ni(H)

65

Ni	-0.00005	1.17663	-0.00516
N	1.82458	1.28062	-0.07883
N	-1.82440	1.28076	0.07308
N	-0.00010	-0.69772	-0.00112
C	2.40799	-0.97952	0.03854
N	2.71926	0.32532	-0.06533
N	-2.71917	0.32559	0.06348
C	3.59734	-1.86504	0.15452
C	3.49028	2.71406	-1.19284
H	3.72801	1.88501	-1.85006
C	-2.19634	3.60787	-0.64741
H	-1.44448	3.46689	-1.41533
C	1.10192	-1.50048	0.03179
C	3.65000	-2.91149	1.08833

H	2.81231	-3.07509	1.75972
C	-4.73327	-1.63372	0.64004
H	-4.72302	-0.81012	1.34636
C	-3.83567	4.99510	0.47123
H	-4.34968	5.94687	0.57377
C	-2.40825	-0.97945	-0.03971
C	5.90456	-3.50593	0.38776
C	-3.59781	-1.86474	-0.15451
C	-0.68074	-2.88793	-0.00917
H	-1.33932	-3.74383	-0.00526
C	0.68034	-2.88794	0.01252
H	1.33887	-3.74389	0.01103
C	-3.64991	-2.91371	-1.08553
H	-2.81163	-3.07942	-1.75565
C	4.73197	-1.63672	-0.64194
H	4.72121	-0.81522	-1.35072
C	4.78343	-3.71651	1.19818
H	4.80074	-4.51234	1.93950
C	-2.50056	2.54978	0.21484
C	-3.48133	2.71432	1.19932
H	-3.71292	1.88564	1.85924
C	-1.10223	-1.50049	-0.03205
C	-5.85927	-2.44185	0.52810
H	-6.72181	-2.24412	1.16107
C	-4.13497	3.93826	1.33311
H	-4.88008	4.06472	2.11406
C	2.50138	2.54965	-0.21646
C	3.83700	4.99568	-0.46359
H	4.35127	5.94769	-0.56259
C	7.12168	-4.39478	0.48573
H	8.04862	-3.81803	0.39124
H	7.12887	-5.14906	-0.31267
H	7.15178	-4.92968	1.44055
C	2.86362	4.82170	0.52309
H	2.62484	5.63384	1.20429
C	4.14417	3.93833	-1.32209
H	4.89571	4.06468	-2.09688
C	2.18928	3.60829	0.64235
H	1.43102	3.46732	1.40393
C	5.85780	-2.44496	-0.52900
H	6.71971	-2.24936	-1.16349
C	-4.78352	-3.71860	-1.19437
H	-4.80033	-4.51645	-1.93355
C	-5.90544	-3.50538	-0.38573
C	-2.87046	4.82094	-0.52341
H	-2.63793	5.63270	-1.20724
C	-7.12275	-4.39407	-0.48252
H	-7.13044	-5.14686	0.31730
H	-7.15262	-4.93078	-1.43633
H	-8.04957	-3.81691	-0.38945
H	-0.00025	2.61430	-0.01201

([^{Tol,Ph}DHPyH]Ni(OH)

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Ni	0.00070	0.78310	-0.54230
O	-0.46650	2.15750	-1.53680
N	1.74390	1.34730	-0.17130
N	2.83300	0.60060	-0.07630
N	0.44860	-0.90060	-0.05140
N	-1.79790	0.08290	-0.35220
C	1.63670	-1.50380	0.18650
N	-2.92280	0.74310	-0.84390
C	2.06410	2.73370	-0.25170
C	-0.00470	-3.04220	0.51600
H	-0.55030	-3.94610	0.75200
C	5.22350	-0.62970	0.81850
H	5.02610	0.36080	1.21490
C	1.37030	-2.86320	0.55610
H	2.10930	-3.59330	0.85240
C	-3.08390	-2.05520	-0.13580
C	-0.56830	-1.79790	0.12030
C	2.82850	-0.71930	0.08480
C	4.17330	-1.33390	0.20310
C	6.49310	-1.18670	0.91880
H	7.28540	-0.62170	1.40570
C	-5.39520	-3.69720	-0.11050
C	6.77270	-2.46290	0.40660
C	-1.84950	-1.23970	-0.12540
C	1.13790	3.67160	0.22830
H	0.19350	3.32890	0.63160
C	-4.78350	2.24230	-0.48280
H	-5.17860	1.93920	-1.44990
C	4.45420	-2.60440	-0.32400
H	3.67880	-3.15210	-0.85030
C	-4.24270	-4.08480	-0.80550
H	-4.23520	-5.02900	-1.34490
C	-4.23900	-1.66170	0.56500
H	-4.24080	-0.73230	1.12610
C	1.43870	5.03090	0.19710
H	0.71530	5.74590	0.57950
C	3.57880	4.54030	-0.80480
H	4.52670	4.87550	-1.21800

C	-3.07190	2.07750	1.22600
H	-2.15410	1.63480	1.59580
C	3.29230	3.17970	-0.76890
H	4.00210	2.44910	-1.13730
C	2.65670	5.47350	-0.32070
H	2.88680	6.53530	-0.34860
C	5.73130	-3.15470	-0.22190
H	5.92340	-4.13570	-0.65110
C	-3.10370	-3.28270	-0.81890
H	-2.22330	-3.60010	-1.36910
C	-5.36800	-2.47470	0.57710
H	-6.24340	-2.15750	1.13900
C	-3.58610	1.67670	-0.01450
C	-4.93800	3.60470	1.51470
H	-5.45940	4.35170	2.10570
C	-6.63670	-4.55630	-0.11470
H	-7.35080	-4.21540	-0.87620
H	-7.15240	-4.51880	0.85090
H	-6.39990	-5.60220	-0.33410
C	-5.45220	3.19340	0.28150
H	-6.37900	3.62000	-0.09300
C	-3.74790	3.04250	1.97560
H	-3.33760	3.34710	2.93480
C	8.14820	-3.07120	0.54480
H	8.93500	-2.32460	0.38830
H	8.30260	-3.88130	-0.17550
H	8.29920	-3.49220	1.54810
H	-3.54690	0.13580	-1.36850
H	-1.42790	2.11020	-1.68780

([^{Tol,Ph}DHPyH]Ni(OH) Trans. State 67

C	2.45620	-2.29720	-1.32210
C	3.76780	-2.66430	-0.98430
C	1.76010	-3.03010	-2.29610
N	1.80750	-1.18500	-0.72430
C	4.35910	-3.76290	-1.60220
H	4.29800	-2.08640	-0.23620
C	3.66450	-4.49530	-2.56950
H	5.36930	-4.05190	-1.32480
C	2.36560	-4.11880	-2.91960
H	4.13350	-5.34940	-3.04940
H	1.82580	-4.66770	-3.68650
H	0.76750	-2.70230	-2.59330
N	-0.16230	0.45980	-0.10090
C	-1.37730	1.04120	-0.29900
C	0.80910	1.41020	-0.20830
Ni	0.08650	-1.32670	-0.01750
C	-1.17660	2.42530	-0.56110
C	-2.61580	0.26350	-0.24780
C	0.18610	2.66330	-0.48040
H	-1.94510	3.14620	-0.79600
H	0.69800	3.60010	-0.64930
C	2.19130	1.04270	-0.20970
C	-3.87620	0.86390	-0.78300
N	-2.76080	-0.93590	0.23510
C	-4.63750	0.15480	-1.72230
C	-4.36490	2.09510	-0.32410
C	3.24800	2.04530	0.02920
N	2.63680	-0.17990	-0.52060
C	4.51480	1.91170	-0.57090
C	3.03670	3.13690	0.88980
N	-1.62030	-1.56920	0.78430
C	-1.66150	-1.60860	2.22260
O	-0.15160	-3.21730	0.04900
C	-5.83530	0.67430	-2.20610
H	-4.28360	-0.81240	-2.06550
C	-6.32120	1.91200	-1.76310
H	-6.40590	0.10650	-2.93790
C	-5.56940	2.60550	-0.80700
C	-7.60610	2.48560	-2.31270
H	-5.93520	3.55610	-0.42540
H	-3.82050	2.64250	0.43950
H	-8.07260	3.17690	-1.60310
H	-7.42740	3.04370	-3.24170
H	-8.33050	1.69710	-2.54410
C	5.51570	2.84490	-0.33280
H	4.69430	1.06920	-1.22970
C	4.04780	4.06580	1.12420
H	2.08540	3.23860	1.40190
C	5.30240	3.94420	0.51420
H	3.86200	4.89390	1.80430
C	6.38680	4.96930	0.74280
H	6.48310	2.72340	-0.81540
H	6.22500	5.52430	1.67250
H	6.41740	5.70250	-0.07460
H	7.37670	4.50230	0.79320
C	-0.67390	-2.33760	2.91180
C	-2.65710	-0.95010	2.95810
C	-0.68990	-2.39650	4.30190
H	0.08780	-2.87410	2.35640
C	-1.68280	-1.74100	5.03520

H	0.08200	-2.96420	4.81540	H	-3.42850	-0.39580	2.43890
C	-2.66360	-1.02450	4.35240	H	-0.11360	-3.68440	-0.79960
H	-1.69020	-1.79120	6.12050	H	-1.24020	-2.74980	0.34800
H	-3.44750	-0.51140	4.90420				

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