

Supplementary Information

for

**Synthesis and Characterization of Homometallic Cobalt Complexes  
with Metal-Metal Interactions**

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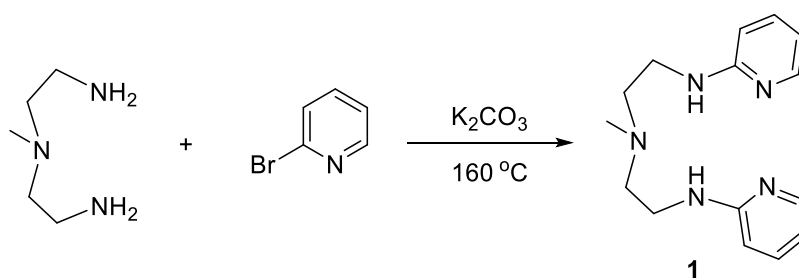
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## 1. Experimental Procedure

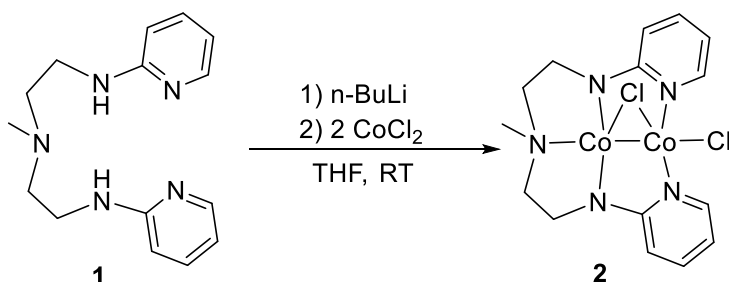
**General Procedure:** All manipulations were performed under an atmosphere of nitrogen using standard Schlenk techniques or in a glovebox. Commercially available chemicals were used as received without further purification. The solvents were obtained by passing through a Solve Purer G5 (MIKROUNA) solvent purification system and further dried over 4 Å molecular sieves. C<sub>6</sub>D<sub>6</sub> and THF-d<sub>8</sub> were dried over Na/K and stored under N<sub>2</sub> atmosphere prior to use. Nuclear magnetic resonance spectroscopy was performed using a Bruker AVIII-400 (<sup>1</sup>H 400 MHz) or a Bruker AVIII-500 (<sup>1</sup>H 500 MHz; <sup>13</sup>C{<sup>1</sup>H} 125 MHz) spectrometer at room temperature (RT). The <sup>1</sup>H and <sup>13</sup>C{<sup>1</sup>H} NMR chemical shifts (δ) are relative to tetramethylsilane. Absolute values of the coupling constants are provided in Hertz (Hz). Multiplicities are abbreviated as singlet (s), doublet (d), triplet (t) and multiplet (m). Absorption spectra were measured on a Lambda 750 spectrometer at room temperature. Fourier transform infrared spectra (FT-IR) were measured on a Nicolet FT-IR 170X spectrophotometer in the range of 4000-400 cm<sup>-1</sup> at 25 °C using KBr plates. Magnetic susceptibility measurements on crystalline samples were performed using a Quantum Design SQUID VSM magnetometer from 300 to 2 K under an external magnetic field of 1000 Oe. Elemental analyses (C, H, N) were performed on a Vario MICRO elemental analyzer at the Center of Modern Analysis, Nanjing University.

### Synthesis of compound 1.



Two equivalents of  $K_2CO_3$  (2.76 g, 20.0 mmol) was added to a solution of  $CH_3N(CH_2CH_2NH_2)_2$  (1.17 g, 10.0 mmol, 1 equiv.) and 2-bromopyridine (3.16 g, 20.0 mmol, 2 equiv.). The reaction mixture was sealed in a Schlenk flask and stirred at 160 °C for 2 days, and subsequently purified by column chromatography (petroleum ether: ethyl acetate:  $CH_3OH = 1 : 10 : 0.1$ ) to give compound **1** as a pale yellow oil (The reaction was performed without solvent.). Yield: 1.68 g (62%).  $^1H$  NMR ( $CDCl_3$ , 500 MHz, 298K)  $\delta$  8.06-8.07 (m, 2H,  $C_5H_4N$ ), 7.35-7.39 (m, 2H,  $C_5H_4N$ ), 6.53-6.55 (m, 2H,  $C_5H_4N$ ), 6.37 (d,  $^3J_{HH} = 8.5$  Hz, 2H,  $C_5H_4NCH_2$ ), 5.06 (s, 2H, NH), 3.35 (dd,  $^3J_{HH} = 11.0$  Hz, 6.0 Hz, 4H,  $NCH_2CH_2$ ), 2.66 (t,  $^3J_{HH} = 6.0$  Hz, 4H,  $NCH_2CH_2$ ), 2.29 (s, 3H,  $NCH_3$ ).  $^{13}C\{^1H\}$  NMR ( $CDCl_3$ , 125 MHz, 298K)  $\delta$  158.8 ( $C_5H_4N$ ), 148.0 ( $C_5H_4N$ ), 137.3 ( $C_5H_4N$ ), 112.7 ( $C_5H_4N$ ), 107.3 ( $C_5H_4N$ ), 56.2 ( $NCH_2CH_2$ ), 41.6 ( $NCH_2CH_2$ ), 39.4 ( $(CH_3)N$ ). HRMS (ESI-TOF) calcd for  $C_{15}H_{21}N_5$   $[M+H]^+$  272.1870, found 272.1864.

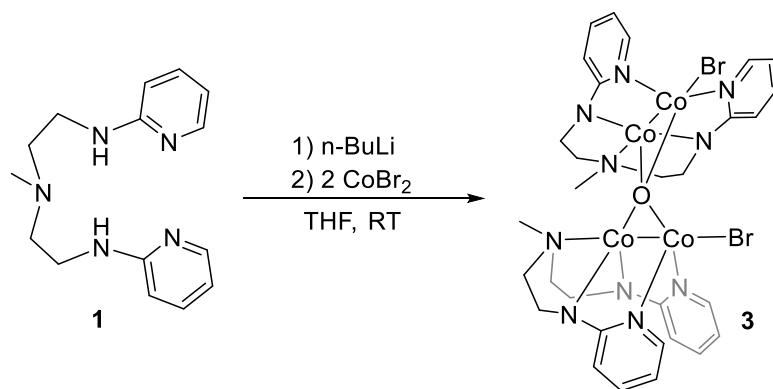
### Synthesis of complex **2**.



A 2.4 M solution of  $n\text{-BuLi}$  in hexanes (0.25 mL, 0.6 mmol) was added dropwise to a solution of compound **1** (81 mg, 0.3 mmol) in THF (20 mL) at room temperature. The mixture was stirred for 2 h, and was then added to the suspension of  $CoCl_2$  (78 mg, 0.6 mmol) in THF (10 mL). After stirring overnight at RT, the mixture was filtered through a sintered glass funnel and the filtrate was concentrated to 1 mL. After the concentrated solution was placed at -30 °C for 24 h, a green solid was afforded (96 mg, 70%). Green crystals of **2** suitable for X-ray diffraction were obtained by placing the concentrated toluene solution at -30 °C for 24 h.  $^1H$  NMR ( $C_6D_6$ , 400 MHz, 298K)  $\delta$  22.86, 11.87, 5.65, 2.10, 1.35, 1.23, 0.29 (The complex **2** exhibits poor solubility in common deuterated solvents, the characteristic peaks shown in the  $^1H$  NMR spectrum were extracted based

on the *in-situ* reaction between lithiated **1** and CoCl<sub>2</sub> in THF-d<sub>8</sub>). FTIR  $\nu/\text{cm}^{-1}$  (KBr): 3025 (w, C-H<sub>Ar</sub>), 2963 (w), 2853 (m), 2812 (m), 1608 (s, C=N), 1539 (m, C=C), 1494 (s), 1438 (s), 1373 (m), 1343 (m), 1296 (m), 1246 (w), 1161 (m), 1125 (w), 1072 (w), 1003 (m), 918 (w), 822 (w), 765 (m), 729 (m), 644 (m), 515 (w, Co-N). Anal. Calcd. For C<sub>15</sub>H<sub>19</sub>Cl<sub>2</sub>Co<sub>2</sub>N<sub>5</sub>: C 39.33; H 4.18; N 15.29. Found: C 39.43; H 4.56; N 15.49.

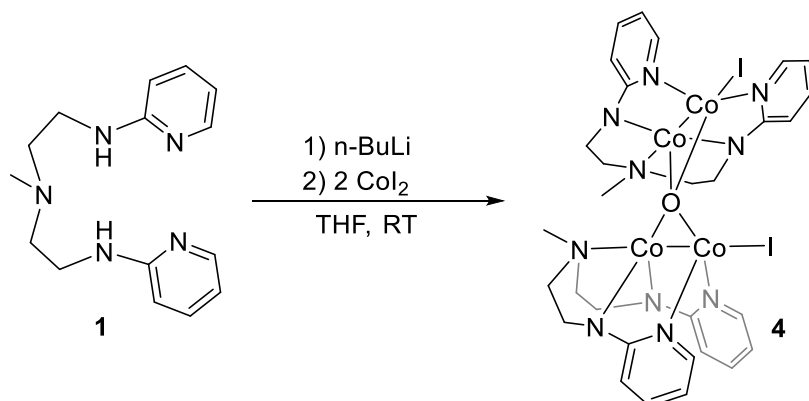
### Synthesis of complex **3**.



A 2.4 M solution of *n*-BuLi in hexanes (0.25 mL, 0.6 mmol) was added dropwise to a solution of compound **1** (81 mg, 0.3 mmol) in THF (20 mL) at room temperature. The mixture was stirred for 2 h, and was then added to the suspension of CoBr<sub>2</sub> (131 mg, 0.6 mmol) in THF (10 mL). After stirring overnight at RT, the mixture was filtered through a sintered glass funnel and the filtrate was concentrated to 1 mL. After the concentrated solution was placed at -30 °C for 24 h, green-brown crystals of **3** suitable for X-ray diffraction were obtained (88 mg, 61%). <sup>1</sup>H NMR (THF-d<sub>8</sub>, 400 MHz, 298K)  $\delta$  72.48, 70.05, 60.40, 59.60, 58.86, 56.46, 55.31, 43.98, 22.77, 21.61, 19.83, 19.25, 13.01, 11.89, 8.39, 7.20, -1.13 (The complex **3** exhibits poor solubility in common deuterated solvents, the characteristic peaks shown in the <sup>1</sup>H NMR spectrum were extracted based on the *in-situ* reaction between lithiated **1** and CoBr<sub>2</sub> in THF-d<sub>8</sub>). FTIR  $\nu/\text{cm}^{-1}$  (KBr): 3025 (w, C-H<sub>Ar</sub>), 2962 (w), 2906 (w), 2856 (m), 1607 (s, C=N), 1537 (m, C=C), 1491 (s), 1437 (s), 1344 (m), 1296 (m), 1249 (m), 1160 (m), 1125 (w), 1001 (m), 918 (w), 856 (w), 818 (w), 764 (m), 730 (m), 637 (m), 515 (w, Co-N). Anal. Calcd. For C<sub>30</sub>H<sub>38</sub>Br<sub>2</sub>Co<sub>4</sub>N<sub>10</sub>O·THF: C 39.94; H 4.54; N 13.70. Found: C

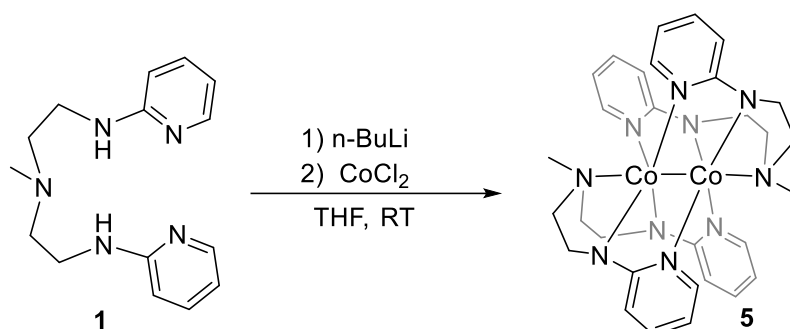
41.03; H 4.53; N 13.61.

#### Synthesis of complex **4**.



A 2.4 M solution of *n*-BuLi in hexanes (0.25 mL, 0.6 mmol) was added dropwise to a solution of compound **1** (81 mg, 0.3 mmol) in THF (20 mL) at room temperature. The mixture was stirred for 2 h, and was then added to the suspension of CoI<sub>2</sub> (188 mg, 0.6 mmol) in THF (10 mL). After stirring overnight at RT, the mixture was filtered through a sintered glass funnel and the filtrate was concentrated to 1 mL. After the concentrated solution was placed at -30 °C for 24 h, red-brown crystals were collected (83 mg, 53%). Red-brown crystals of **4** suitable for X-ray diffraction were obtained by placing the concentrated toluene solution at -30 °C for 24 h. <sup>1</sup>H NMR (THF-d<sub>8</sub>, 400 MHz, 298K) δ 78.13, 61.93, 61.56, 58.25, 57.55, 24.96, 24.58, 22.76, 20.63, 13.88, 12.46, 10.51, 7.78, 6.75, 5.76, 5.64, -2.31 (The complex **4** exhibits poor solubility in common deuterated solvents, the characteristic peaks shown in the <sup>1</sup>H NMR spectrum were extracted based on the *in-situ* reaction between lithiated **1** and CoI<sub>2</sub> in THF-d<sub>8</sub>). FTIR ν/cm<sup>-1</sup> (KBr): 3023 (w, C-H<sub>Ar</sub>), 2902 (w), 2855 (m), 1607 (s, C=N), 1536 (m, C=C), 1491 (s), 1436 (s), 1344 (m), 1294 (m), 1247 (m), 1161 (m), 1126 (m), 1075 (w), 1000 (m), 919 (w), 855 (w), 820 (w), 763 (m), 729 (m), 631 (m), 515 (w, Co-N). Anal. Calcd. For C<sub>30</sub>H<sub>38</sub>Co<sub>4</sub>I<sub>2</sub>N<sub>10</sub>O·Toluene: C 39.11; H 4.08; N 12.33. Found: C 39.31; H 4.13; N 12.10.

### Synthesis of complex 5.



A 2.4 M solution of *n*-BuLi in hexanes (0.25 mL, 0.6 mmol) was added dropwise to a solution of compound **1** (81 mg, 0.3 mmol) in THF (20 mL) at room temperature. The mixture was stirred for 2 h, and was then added to the suspension of CoCl<sub>2</sub> (39 mg, 0.3 mmol) in THF (10 mL). After stirring overnight at RT, the mixture was filtered through a sintered glass funnel and the filtrate was concentrated to 1 mL. After the concentrated solution was placed at -30 °C for 24 h, a yellow-green solid was afforded (57 mg, 58%). Green crystals of **5** suitable for X-ray diffraction were obtained by placing the concentrated toluene solution at -30 °C for 24 h. <sup>1</sup>H NMR (THF-*d*<sub>8</sub>, 400 MHz, 298K) δ 7.76-7.78 (m, 2H, C<sub>5</sub>H<sub>4</sub>N), 6.73 (t, <sup>3</sup>J<sub>HH</sub>= 8.0 Hz, 2H, C<sub>5</sub>H<sub>4</sub>N), 5.76 (t, <sup>3</sup>J<sub>HH</sub>= 6.0 Hz, 2H, C<sub>5</sub>H<sub>4</sub>N), 5.63 (d, <sup>3</sup>J<sub>HH</sub>= 8.8 Hz, 2H, C<sub>5</sub>H<sub>4</sub>N), 2.97 (s, 3H, NCH<sub>3</sub>), 2.82-2.88 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>), 2.73-2.80 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>), 2.61-2.67 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>), 2.34-2.40 (m, 2H, NCH<sub>2</sub>CH<sub>2</sub>) (The complex **5** exhibits poor solubility in common deuterated solvents, the characteristic peaks shown in the <sup>1</sup>H NMR spectrum were extracted based on the *in-situ* reaction between lithiated **1** and CoCl<sub>2</sub> in THF-*d*<sub>8</sub>, tentative assignments based on relative integration.). FTIR  $\nu/\text{cm}^{-1}$  (KBr): 3078 (w, C-H<sub>Ar</sub>), 3020 (w, C-H<sub>Ar</sub>), 2971 (w), 2895 (w), 2848 (m), 2793 (m), 1912 (w), 1862 (w), 1761 (w), 1607 (s, C=N), 1528 (s, C=C), 1446 (s), 1354 (m), 1291 (s), 1249 (m), 1158 (m), 1123 (m), 1090 (w), 1047 (w), 1011 (m), 939 (w), 906 (w), 856 (w), 803 (m), 744 (m), 718 (m), 647 (m), 521 (m, Co-N), 438 (w). Anal. Calcd. For C<sub>30</sub>H<sub>38</sub>Co<sub>2</sub>N<sub>10</sub>: C 54.88; H 5.83; N 21.33. Found: C 54.90; H 5.76; N 21.35.

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**General procedures for the hydrosilylation of terminal alkynes catalyzed by complexes 2-5.**

In a N<sub>2</sub>-filled glovebox, the phenylacetylene (51 mg, 0.5 mmol), phenylsilane (54 mg, 0.5 mmol), Co complex (5 mol%), THF (1.0 mL) and a magnetic stirring bar were added to a 5-mL vial. The vial was sealed with a rubber septum and removed from the glovebox. The reaction mixture was stirred for 24 h at room temperature and then the solvent was removed under reduced pressure. The crude product was purified by column chromatography with petroleum ether as eluent.

## 2. Supplementary Figures

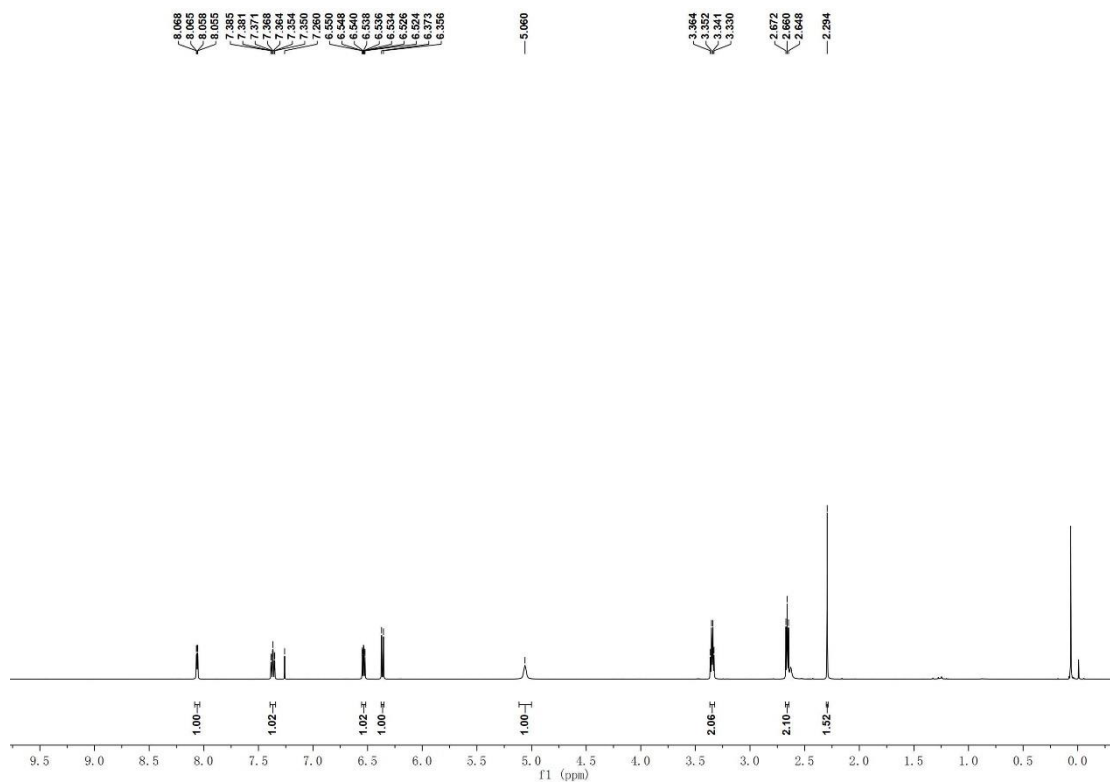


Figure S1. The  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**.

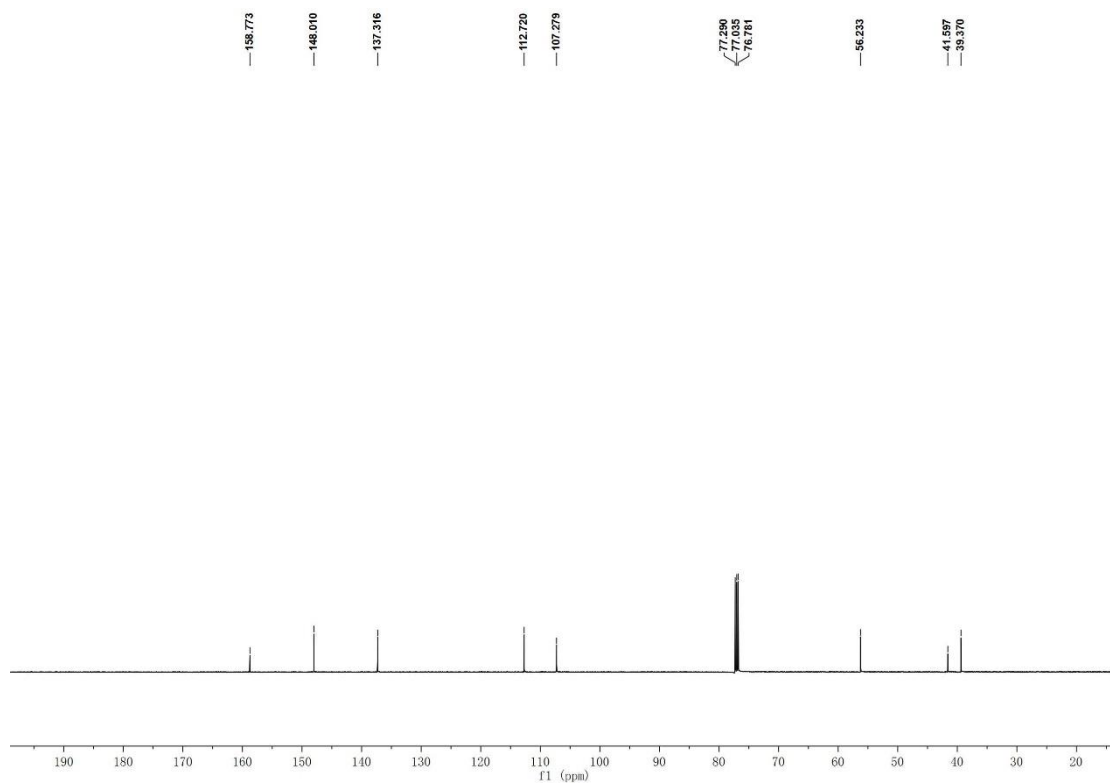
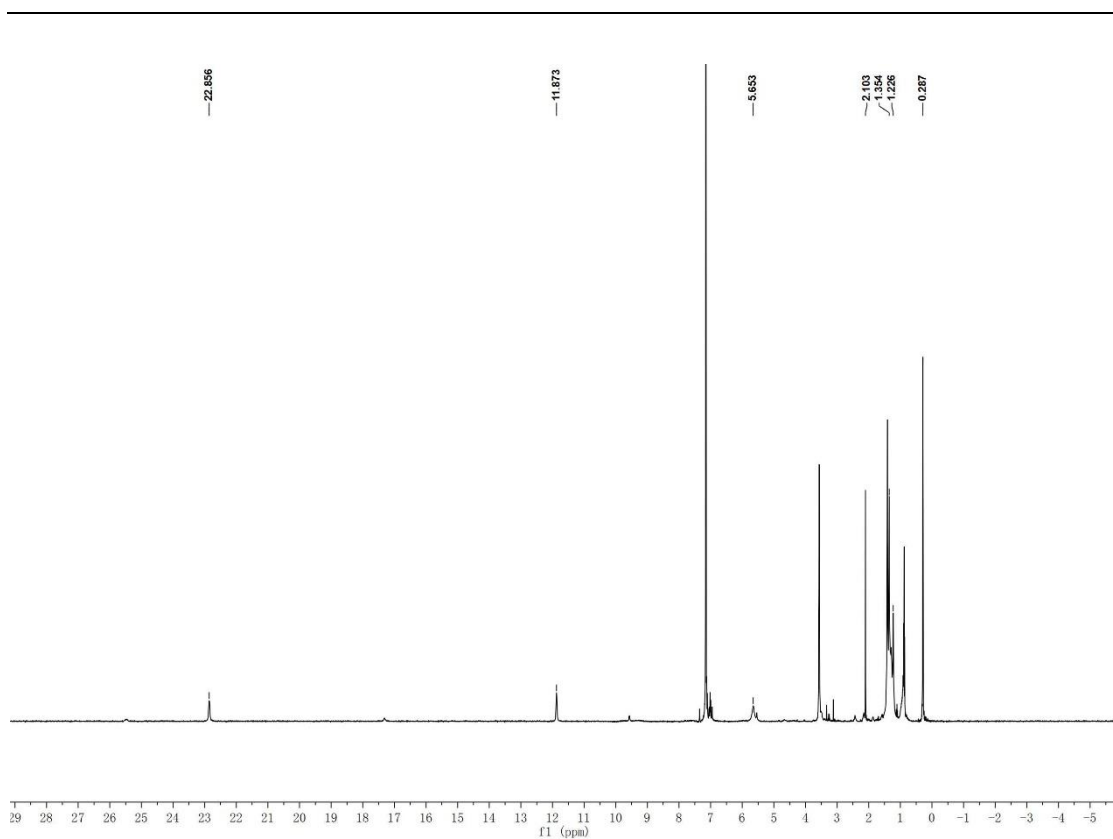
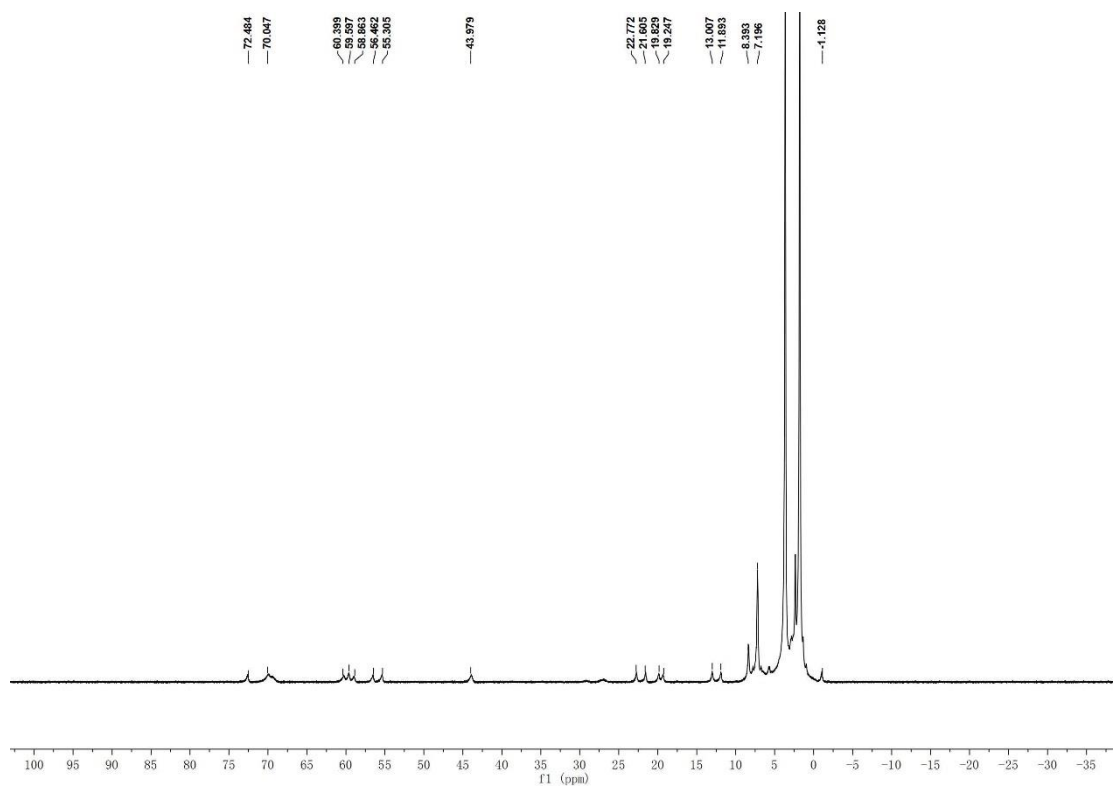


Figure S2. The  $^{13}\text{C}\{^1\text{H}\}$  NMR (125 MHz,  $\text{CDCl}_3$ ) spectrum of compound **1**.

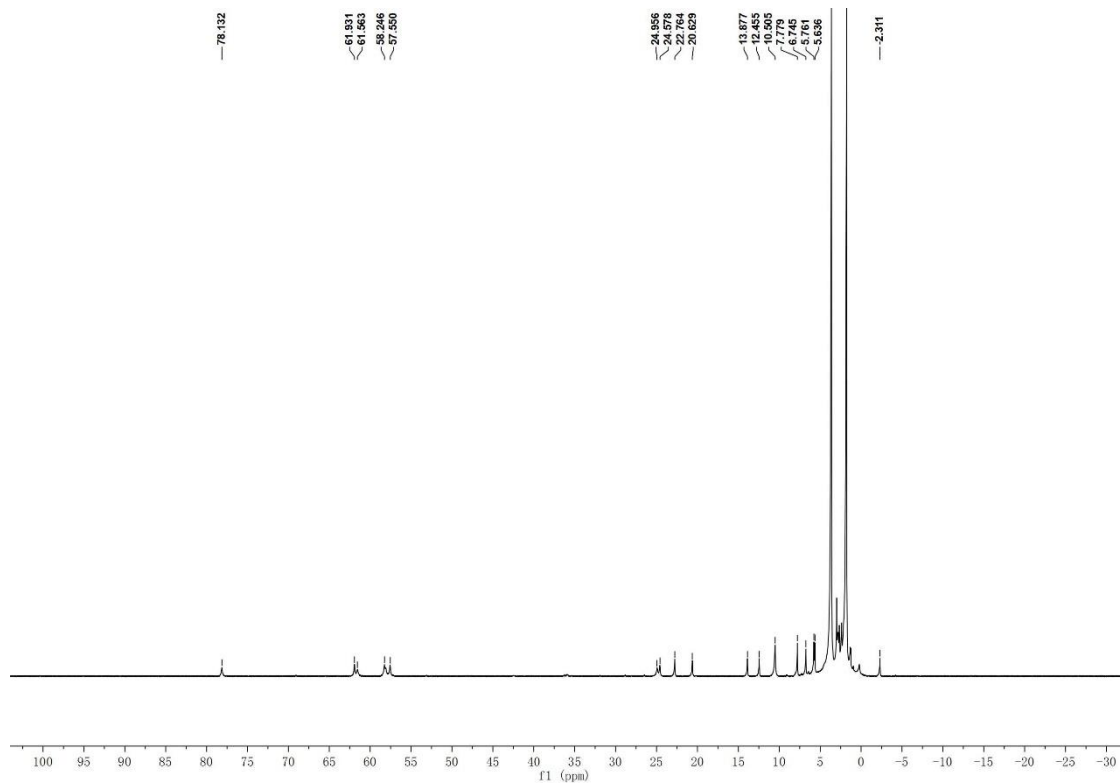




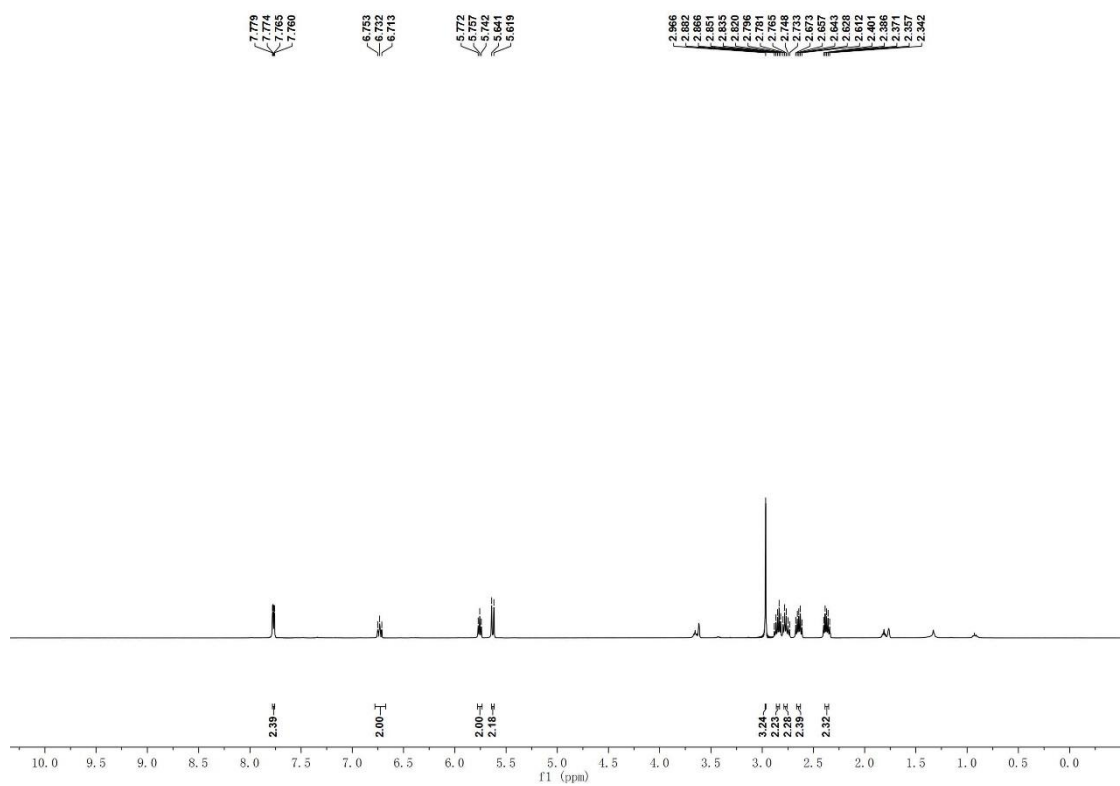
**Figure S3.** The  $^1\text{H}$  NMR (400 MHz,  $\text{C}_6\text{D}_6$ ) spectrum of complex **2**.



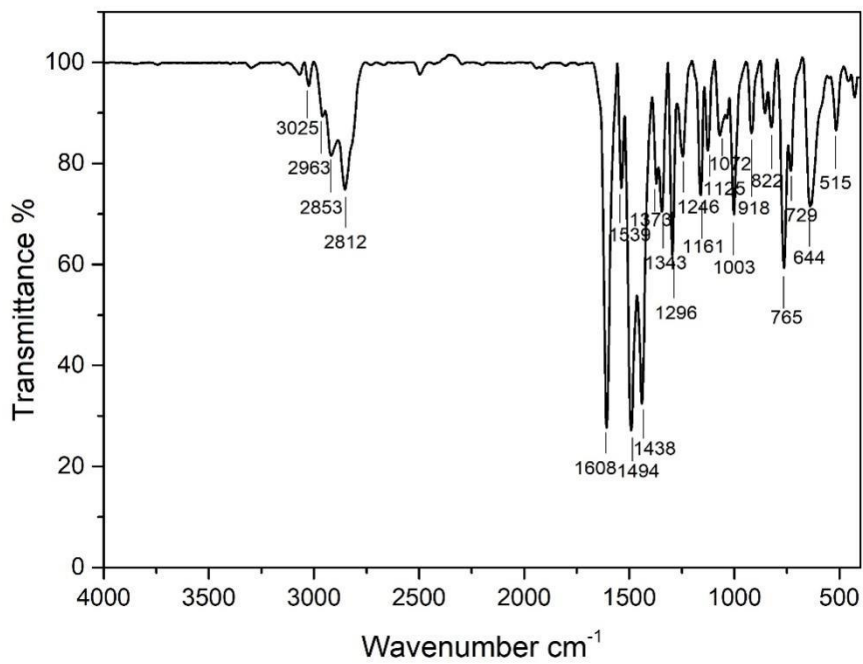
**Figure S4.** The  $^1\text{H}$  NMR (400 MHz,  $\text{THF-d}_8$ ) spectrum of complex **3**.



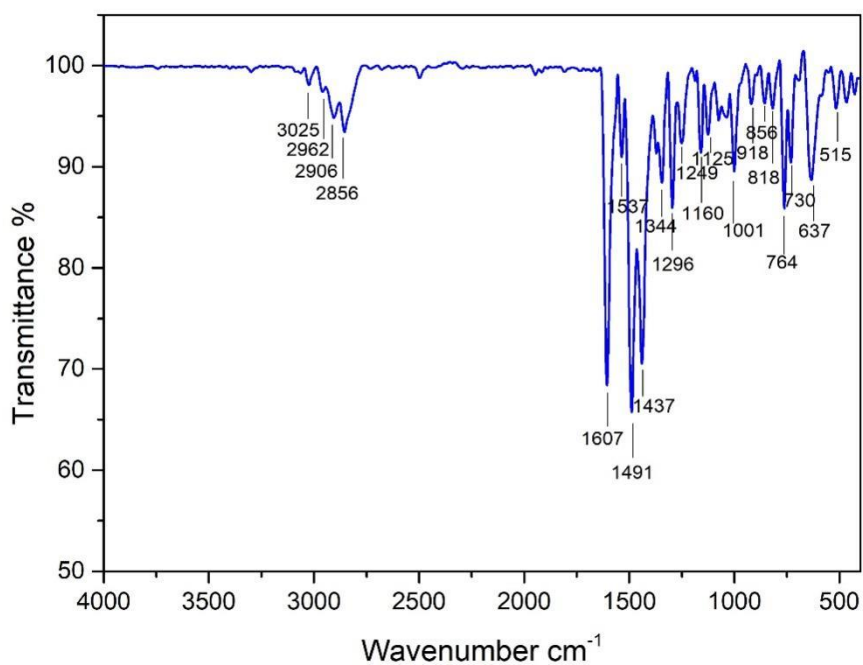
**Figure S5.** The  $^1\text{H}$  NMR (400 MHz, THF- $d_8$ ) spectrum of complex **4**.



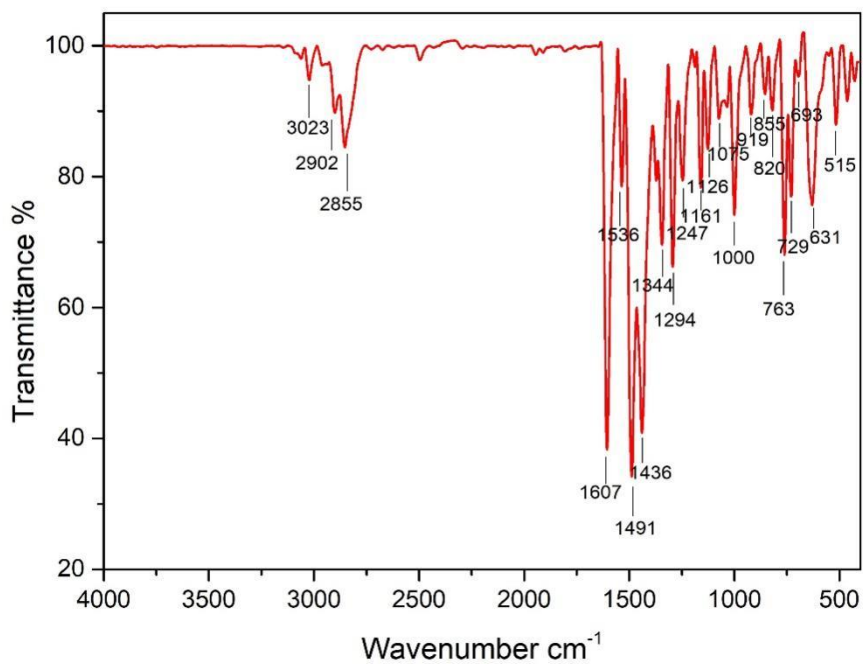
**Figure S6.** The  $^1\text{H}$  NMR (400 MHz, THF- $d_8$ ) spectrum of complex **5**.



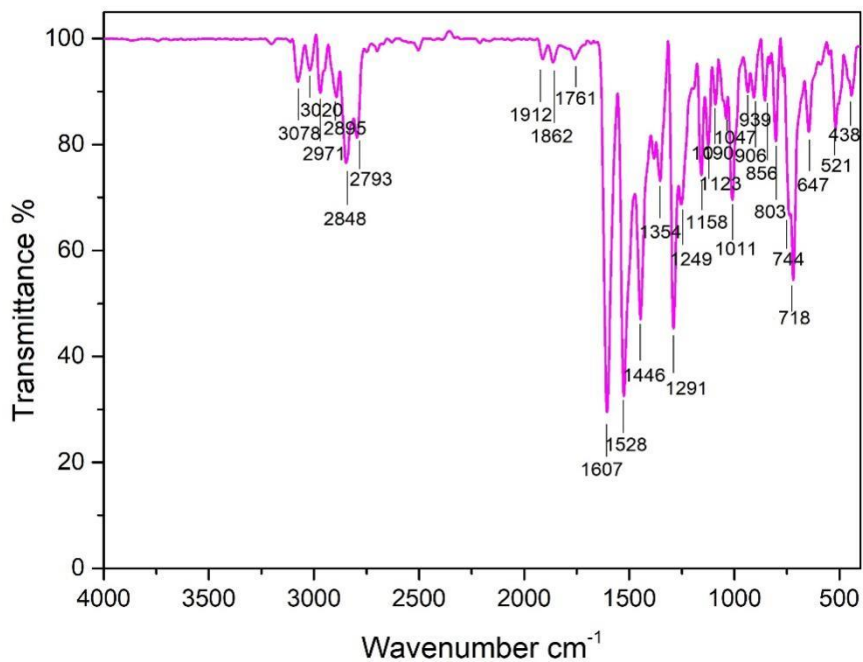
**Figure S7.** FT-IR spectrum of complex 2.



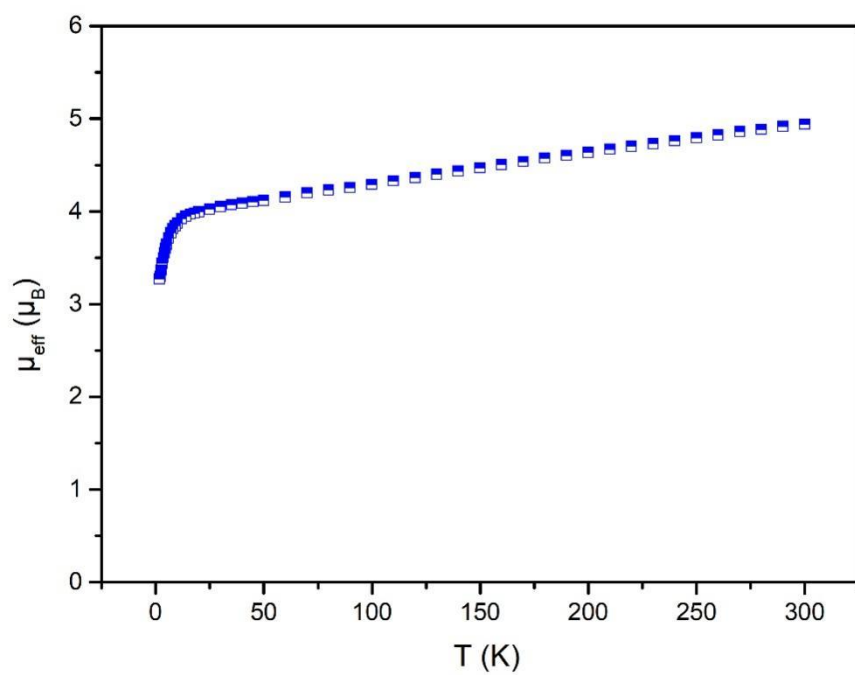
**Figure S8.** FT-IR spectrum of complex 3.



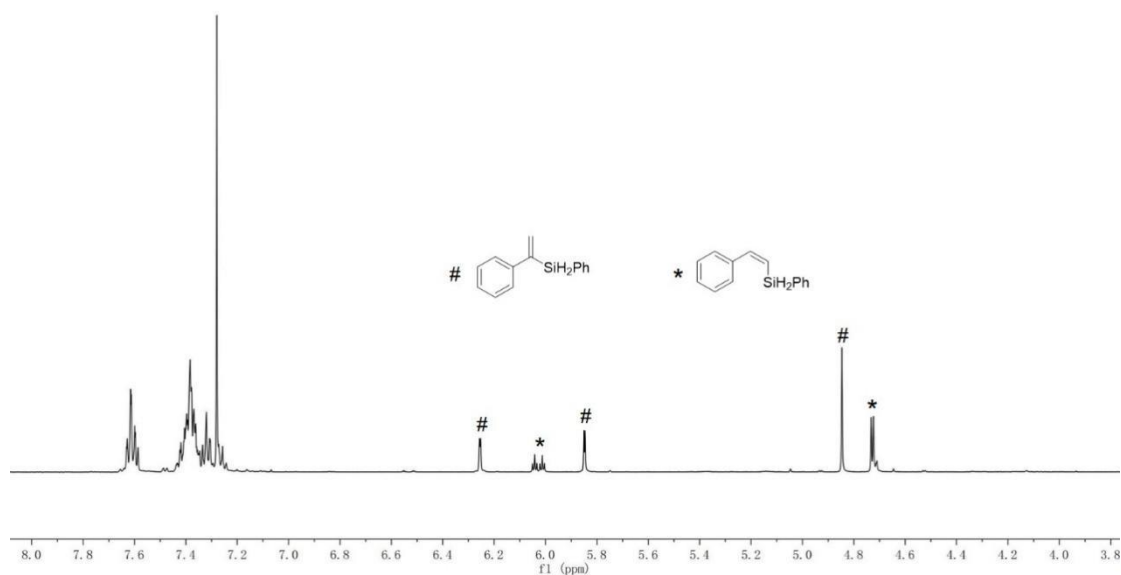
**Figure S9.** FT-IR spectrum of complex 4.



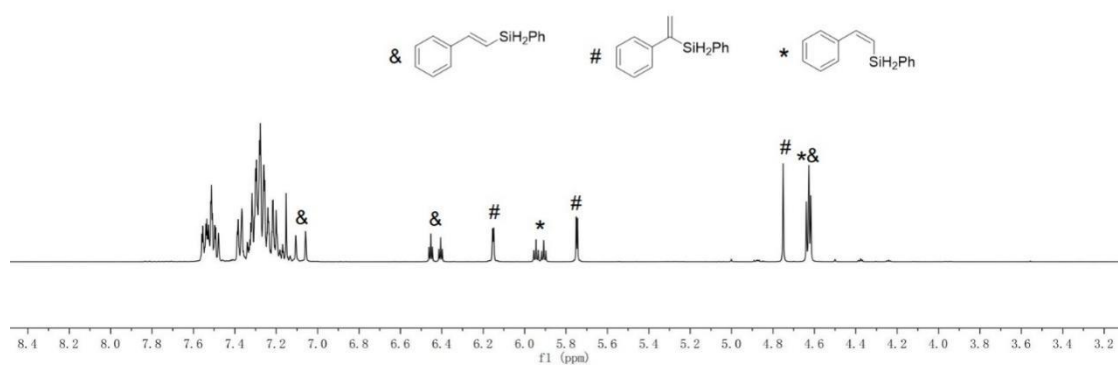
**Figure S10.** FT-IR spectrum of complex 5.



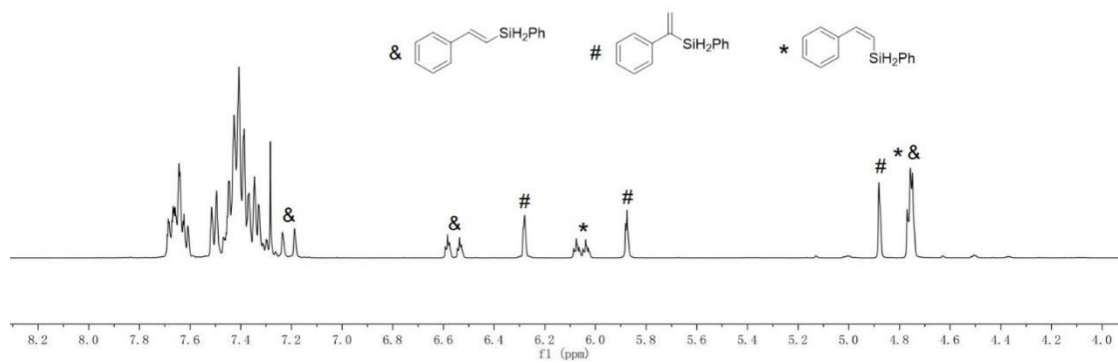
**Figure S11.** Variable-temperature effective magnetic moment data of complex **2** as  $\mu_{\text{eff}}$  vs T.



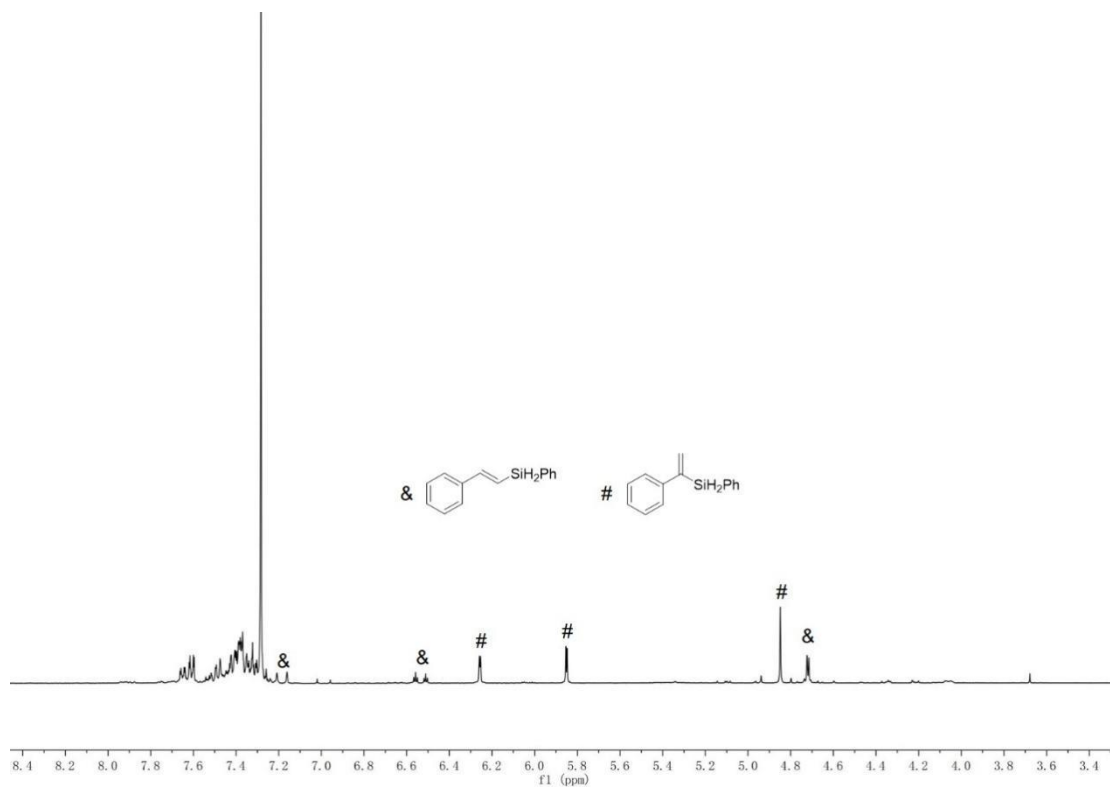
**Figure S12.** The  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) spectrum of hydrosilylated products from the reaction of phenylacetylene with  $\text{PhSiH}_3$  catalyzed by **2**.



**Figure S13.** The  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of hydrosilylated products from the reaction of phenylacetylene with  $\text{PhSiH}_3$  catalyzed by **3**.



**Figure S14.** The  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of hydrosilylated products from the reaction of phenylacetylene with  $\text{PhSiH}_3$  catalyzed by **4**.



**Figure S15.** The  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of hydrosilylated products from the reaction of phenylacetylene with  $\text{PhSiH}_3$  catalyzed by **5**.

### 3. X-ray crystallographic analysis

The crystallographic data were collected using a Bruker APEX-II CCD area detector with a radiation source of Mo(K $\alpha$ ) (0.71073 Å). Multi-scan or empirical absorption corrections (SADABS) were applied. The structures were solved using Patterson methods, expanded using difference Fourier syntheses, and refined using full-matrix least squares fitting on  $F^2$  using the Bruker SHELXTL-2014 program package.<sup>1,2</sup> All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were introduced at their geometric positions and refined as riding atoms. Evaluation of the CIF using the CheckCIF routine at [www.checkcif.iucr.org](http://www.checkcif.iucr.org) gave no A or B alert for these complexes. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre ([www.ccdc.cam.ac.uk/data-request/cif](http://www.ccdc.cam.ac.uk/data-request/cif)). Details regarding the data collection and refinement for these complexes are given in Table S1.

**Table S1.** Crystal data and structural refinement for **2**, **3**, **4** and **5**.

	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>
empirical formula	C <sub>15</sub> H <sub>19</sub> Cl <sub>2</sub> Co <sub>2</sub> N <sub>5</sub>	C <sub>30</sub> H <sub>38</sub> Br <sub>2</sub> Co <sub>4</sub> N <sub>10</sub> O	C <sub>30</sub> H <sub>38</sub> Co <sub>4</sub> I <sub>2</sub> N <sub>10</sub> O	C <sub>30</sub> H <sub>38</sub> Co <sub>2</sub> N <sub>10</sub>
formula weight	458.11	948.23	1044.22	656.56
temperature, K	193(2)	193(2)	193(2)	193(2)
wavelength, Å	0.71073	0.71073	0.71073	0.71073
crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	P2 <sub>1</sub> /n	C2/c	C2/c	P2 <sub>1</sub> /c
<i>a</i> , Å	11.9019(6)	22.7129(11)	22.4229(13)	12.9492(4)
<i>b</i> , Å	11.1915(6)	9.7358(4)	9.8952(6)	12.5051(4)
<i>c</i> , Å	13.7561(7)	18.7476(9)	19.0944(10)	18.2150(6)
$\alpha$ , °	90	90	90	90
$\beta$ , °	92.162(2)	102.994(3)	103.532(3)	106.8170(10)
$\gamma$ , °	90	90	90	90
<i>V</i> , Å <sup>3</sup>	1831.01(16)	4039.5(3)	4119.0(4)	2823.43(16)
<i>Z</i>	4	4	4	4
<i>d</i> <sub>calcd</sub> , g cm <sup>-3</sup>	1.662	1.559	1.684	1.545



$\mu$ , mm <sup>-1</sup>	2.110	3.628	3.117	1.216
$F(000)$	928.0	1888.0	2040.0	1368.0
crystal size, mm	0.10 × 0.10 × 0.10	0.10 × 0.10 × 0.10	0.10 × 0.10 × 0.10	0.10 × 0.10 × 0.10
$\theta_{\max}$ , °	27.475	24.998	27.482	27.512
reflns collected	16803	14900	18798	24771
	4177	3537	4701	6473
indep reflns	[ $R_{\text{int}}=0.0593$ , $R_{\text{sigma}}=0.0519$ ]	[ $R_{\text{int}}=0.0410$ , $R_{\text{sigma}}=0.0352$ ]	[ $R_{\text{int}}=0.0348$ , $R_{\text{sigma}}=0.0311$ ]	[ $R_{\text{int}}=0.0744$ , $R_{\text{sigma}}=0.0685$ ]
data/restraints/par ams	4177/0/218	3537/30/214	4701/0/214	6473/0/381
goodness-of-fit on $F^2$	1.026	1.037	1.051	1.021
final $R$ ( $I > 2\sigma(I)$ )	$R_1 = 0.0308$ , $wR_2 = 0.0775$	$R_1 = 0.0416$ , $wR_2 = 0.1119$	$R_1 = 0.0255$ , $wR_2 = 0.0573$	$R_1 = 0.0454$ , $wR_2 = 0.1077$
$R$ indices (all data)	$R_1 = 0.0398$ , $wR_2 = 0.0828$	$R_1 = 0.0452$ , $wR_2 = 0.1143$	$R_1 = 0.0342$ , $wR_2 = 0.0606$	$R_1 = 0.0724$ , $wR_2 = 0.1233$
Residual electron density (e. Å <sup>-3</sup> )	0.42/-0.35	2.18/-0.69	0.77/-0.49	0.78/-0.73
max/min				
CCDC	2346803	2346804	2346805	2346806

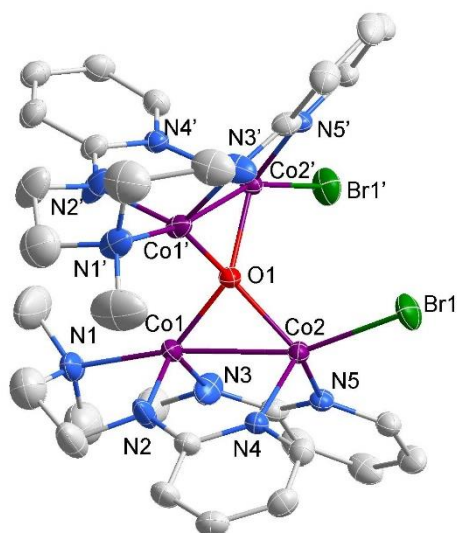


**Figure S16.** X-ray molecular structure of complex **2** drawn with 50% probability. Hydrogen atoms are omitted for clarity.

**Table S2.** Bond distances (Å) and angles (deg) for **2**.

Co2-Co1	2.6184(4)	Co2-Cl1	2.3360(6)
Co2-Cl2	2.2480(6)	Co2-N4	2.0298(18)
Co2-N5	2.0238(17)	Co1-Cl1	2.2680(6)
Co1-N1	2.0619(19)	Co1-N2	1.9057(19)
Co1-N3	1.9086(18)	N4-C6	1.368(3)
N4-C10	1.360(3)	N5-C15	1.357(3)
N5-C11	1.375(3)	N1-C2	1.485(3)
N1-C4	1.491(3)	N1-C1	1.471(3)
N2-C6	1.341(3)	N2-C3	1.461(3)
N3-C11	1.334(3)	N3-C5	1.473(3)
C6-C7	1.425(3)	C15-C14	1.369(3)
C11-C12	1.423(3)	C3-C2	1.518(3)
C10-C9	1.365(3)	C12-C13	1.356(4)
C14-C13	1.402(3)	C7-C8	1.366(3)
C4-C5	1.518(3)	C9-C8	1.390(4)
Cl1-Co2-Co1	54.124(16)	C4-N1-Co1	101.17(14)

C12-Co2-Co1	158.68(2)	C1-N1-Co1	118.15(16)
C12-Co2-C11	104.67(2)	C1-N1-C2	110.7(2)
N4-Co2-Co1	82.75(5)	C1-N1-C4	110.5(2)
N4-Co2-C11	114.14(5)	C6-N2-Co1	125.25(15)
N4-Co2-C12	107.45(5)	C6-N2-C3	117.96(19)
N5-Co2-Co1	84.56(5)	C3-N2-Co1	113.50(14)
N5-Co2-C11	108.44(6)	C11-N3-Co1	128.36(15)
N5-Co2-C12	106.90(5)	C11-N3-C5	119.41(19)
N5-Co2-N4	114.52(7)	C5-N3-Co1	112.16(16)
C11-Co1-Co2	56.573(17)	N4-C6-C7	119.0(2)
N1-Co1-Co2	169.26(5)	N2-C6-N4	116.97(19)
N1-Co1-C11	134.14(6)	N2-C6-C7	124.0(2)
N2-Co1-Co2	88.07(6)	N5-C15-C14	123.8(2)
N2-Co1-C11	114.28(6)	N5-C11-C12	118.8(2)
N2-Co1-N1	86.91(8)	N3-C11-N5	116.40(19)
N2-Co1-N3	116.82(8)	N3-C11-C12	124.8(2)
N3-Co1-Co2	86.02(6)	N2-C3-C2	109.88(19)
N3-Co1-C11	113.71(6)	N4-C10-C9	124.0(2)
N3-Co1-N1	87.78(8)	C13-C12-C11	120.3(2)
Co1-C11-Co2	69.303(18)	N1-C2-C3	111.64(19)
C6-N4-Co2	125.19(15)	C15-C14-C13	117.4(2)
C10-N4-Co2	115.73(15)	C8-C7-C6	120.2(2)
C10-N4-C6	118.7(2)	N1-C4-C5	111.27(19)
C15-N5-Co2	117.26(14)	C10-C9-C8	117.8(2)
C15-N5-C11	119.03(18)	C12-C13-C14	120.5(2)
C11-N5-Co2	123.68(15)	C7-C8-C9	120.2(2)
C2-N1-Co1	103.39(14)	N3-C5-C4	107.69(19)
C2-N1-C4	112.50(18)		



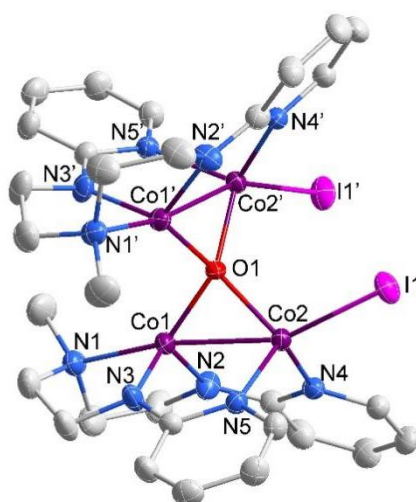
**Figure S17.** X-ray molecular structure of complex **3** drawn with 50% probability. Hydrogen atoms are omitted for clarity.

**Table S3.** Bond distances (Å) and angles (deg) for **3**.

Br1-Co2	2.3999(7)	C11-C12	1.435(6)
Co2-Co1	2.5831(7)	C15-C14	1.379(6)
Co2-O1	1.9424(18)	N2-C6	1.339(6)
Co2-N5	2.046(3)	N2-C3	1.472(6)
Co2-N4	2.058(3)	C10-C9	1.369(6)
Co1-O1	1.921(2)	N1-C1	1.429(8)
Co1-N3	1.917(4)	N1-C2	1.551(8)
Co1-N2	1.931(4)	N1-C4	1.394(8)
Co1-N1	2.071(4)	C8-C7	1.367(7)
N5-C11	1.369(5)	C8-C9	1.395(7)
N5-C15	1.348(5)	C7-C6	1.417(6)
N4-C10	1.348(5)	C12-C13	1.372(7)
N4-C6	1.375(5)	C14-C13	1.384(7)
N3-C11	1.331(6)	C5-C4	1.660(10)
N3-C5	1.465(6)	C3-C2	1.534(8)
Br1-Co2-Co1	160.32(3)	C6-N4-Co2	124.5(3)

O1-Co2-Br1	112.71(7)	C11-N3-Co1	125.9(3)
O1-Co2-Co1	47.69(7)	C11-N3-C5	120.3(4)
O1-Co2-N5	112.47(10)	C5-N3-Co1	112.9(3)
O1-Co2-N4	106.26(13)	N5-C11-C12	118.7(4)
N5-Co2-Br1	106.93(10)	N3-C11-N5	117.3(4)
N5-Co2-Co1	83.30(9)	N3-C11-C12	123.9(4)
N5-Co2-N4	111.44(13)	N5-C15-C14	123.3(4)
N4-Co2-Br1	106.96(10)	C6-N2-Co1	126.6(3)
N4-Co2-Co1	83.83(9)	C6-N2-C3	118.4(4)
O1-Co1-Co2	48.39(6)	C3-N2-Co1	113.8(3)
O1-Co1-N2	107.98(14)	N4-C10-C9	124.5(4)
O1-Co1-N1	141.02(13)	C1-N1-Co1	119.0(4)
N3-Co1-Co2	88.62(11)	C1-N1-C2	100.5(5)
N3-Co1-O1	114.10(15)	C2-N1-Co1	103.3(3)
N3-Co1-N2	119.3(2)	C4-N1-Co1	102.1(4)
N3-Co1-N1	87.08(17)	C4-N1-C1	119.3(6)
N2-Co1-Co2	88.28(11)	C4-N1-C2	111.8(5)
N2-Co1-N1	86.41(16)	C7-C8-C9	119.4(4)
N1-Co1-Co2	170.48(11)	C8-C7-C6	120.7(4)
Co2'-O1-Co2	124.30(19)	C13-C12-C11	119.7(4)
Co1'-O1-Co2	129.54(3)	N4-C6-C7	119.2(4)
Co1'-O1-Co2'	83.92(2)	N2-C6-N4	116.6(4)
Co1-O1-Co2	83.92(2)	N2-C6-C7	124.2(4)
Co1-O1-Co2'	129.55(3)	C10-C9-C8	117.8(4)
Co1'-O1-Co1	110.78(18)	C15-C14-C13	118.2(4)
C11-N5-Co2	124.5(3)	C12-C13-C14	120.4(4)
C15-N5-Co2	115.8(3)	N3-C5-C4	103.6(5)
C15-N5-C11	119.7(4)	N2-C3-C2	109.4(5)
C10-N4-Co2	117.3(3)	C3-C2-N1	108.4(5)

C10-N4-C6	118.2(4)	N1-C4-C5	108.8(5)
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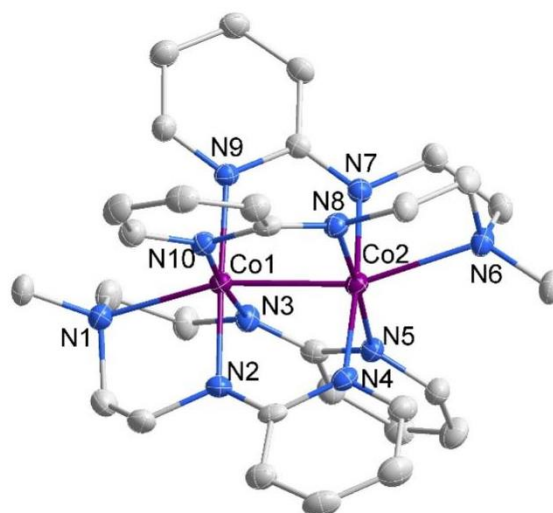
**Figure S18.** X-ray molecular structure of complex **4** drawn with 50% probability. Hydrogen atoms are omitted for clarity.

**Table S4.** Bond distances (Å) and angles (deg) for **4**.

I1-Co2	2.6041(4)	N3-C11	1.337(3)
Co2-Co1	2.5735(5)	N3-C5	1.463(3)
Co2-O1	1.9411(11)	N1-C4	1.497(4)
Co2-N4	2.048(2)	N1-C1	1.459(3)
Co2-N5	2.059(2)	N1-C2	1.467(4)
Co1-O1	1.9245(14)	C6-C7	1.427(4)
Co1-N2	1.919(2)	C10-C9	1.370(4)
Co1-N3	1.933(2)	C11-C12	1.419(4)
Co1-N1	2.074(2)	C15-C14	1.368(4)
N4-C6	1.373(3)	C12-C13	1.363(4)
N4-C10	1.339(3)	C9-C8	1.389(4)
N5-C11	1.376(3)	C13-C14	1.392(4)
N5-C15	1.352(3)	C7-C8	1.362(4)
N2-C6	1.335(3)	C5-C4	1.524(4)

N2-C3	1.465(3)	C3-C2	1.538(5)
Co1'-Co2-I1	158.117(16)	C15-N5-C11	118.3(2)
O1-Co2-I1	110.20(5)	C6-N2-Co1	126.98(18)
O1-Co2-Co1'	47.99(4)	C6-N2-C3	120.7(2)
O1-Co2-N4'	113.00(6)	C3-N2-Co1	111.94(18)
O1-Co2-N5'	105.74(8)	C11-N3-Co1	125.71(19)
N4'-Co2-I1	106.87(6)	C11-N3-C5	118.6(2)
N4'-Co2-Co1'	84.48(6)	C5-N3-Co1	113.80(17)
N4'-Co2-N5'	113.29(8)	C4-N1-Co1	103.85(16)
N5'-Co2-I1	107.64(6)	C1-N1-Co1	118.67(19)
N5'-Co2-Co1'	83.72(6)	C1-N1-C4	108.6(2)
O1-Co1-Co2'	48.54(4)	C1-N1-C2	112.5(2)
O1-Co1-N3	107.33(8)	C2-N1-Co1	100.94(17)
O1-Co1-N1	140.95(7)	C2-N1-C4	111.9(2)
N2-Co1-Co2'	87.93(7)	N4-C6-C7	118.6(2)
N2-Co1-O1	114.62(9)	N2-C6-N4	117.1(2)
N2-Co1-N3	119.28(10)	N2-C6-C7	124.2(2)
N2-Co1-N1	87.17(9)	N4-C10-C9	124.5(3)
N3-Co1-Co2'	88.78(7)	N5-C11-C12	119.0(2)
N3-Co1-N1	86.51(9)	N3-C11-N5	117.0(2)
N1-Co1-Co2'	170.47(6)	N3-C11-C12	124.0(2)
Co2'-O1-Co2	125.00(12)	N5-C15-C14	124.6(3)
Co1-O1-Co2	129.84(2)	C13-C12-C11	120.5(3)
Co1'-O1-Co2	83.479(16)	C10-C9-C8	117.5(3)
Co1-O1-Co2'	83.479(16)	C12-C13-C14	120.1(3)
Co1'-O1-Co2'	129.84(2)	C8-C7-C6	120.3(3)
Co1-O1-Co1'	110.40(12)	C15-C14-C13	117.4(3)
C6-N4-Co2'	123.39(17)	N3-C5-C4	109.5(2)

C10-N4-Co2'	117.72(18)	N1-C4-C5	112.1(2)
C10-N4-C6	118.9(2)	C7-C8-C9	120.2(3)
C11-N5-Co2'	124.31(17)	N2-C3-C2	106.8(2)
C15-N5-Co2'	117.30(18)	N1-C2-C3	110.5(2)



**Figure S19.** X-ray molecular structure of complex **5** drawn with 50% probability. Hydrogen atoms are omitted for clarity.

**Table S5.** Bond distances (Å) and angles (deg) for **5**.

Co2-Co1	2.3682(6)	N6-C17	1.478(4)
Co2-N8	1.917(2)	N6-C19	1.491(4)
Co2-N5	1.948(2)	N6-C16	1.471(4)
Co2-N4	1.976(3)	N1-C1	1.479(4)
Co2-N7	1.957(3)	N1-C4	1.481(4)
Co2-N6	2.302(3)	N1-C2	1.483(4)
Co1-N10	1.973(2)	C11-C12	1.436(4)
Co1-N9	1.947(2)	C26-C27	1.434(4)
Co1-N3	1.956(2)	C21-C22	1.431(4)
Co1-N2	1.925(3)	C6-C7	1.441(4)



Co1-N1	2.295(3)	C30-C29	1.371(4)
N10-C26	1.376(4)	C25-C24	1.371(4)
N10-C30	1.348(4)	C12-C13	1.365(4)
N9-C21	1.380(4)	C5-C4	1.517(4)
N9-C25	1.341(4)	C15-C14	1.376(4)
N3-C11	1.322(4)	C22-C23	1.370(4)
N3-C5	1.462(4)	C10-C9	1.376(5)
N8-C26	1.328(4)	C3-C2	1.507(4)
N8-C20	1.445(4)	C23-C24	1.392(4)
N2-C6	1.321(4)	C13-C14	1.393(5)
N2-C3	1.454(4)	C27-C28	1.356(4)
N5-C11	1.373(4)	C17-C18	1.511(4)
N5-C15	1.345(4)	C20-C19	1.516(4)
N4-C6	1.375(4)	C9-C8	1.387(5)
N4-C10	1.342(4)	C7-C8	1.362(5)
N7-C21	1.324(4)	C28-C29	1.394(5)
N7-C18	1.451(4)		
N8-Co2-Co1	87.55(8)	C21-N7-Co2	124.1(2)
N8-Co2-N5	175.53(11)	C21-N7-C18	115.9(3)
N8-Co2-N4	87.23(10)	C18-N7-Co2	118.5(2)
N8-Co2-N7	92.97(10)	C17-N6-Co2	100.09(18)
N8-Co2-N6	82.77(10)	C17-N6-C19	111.5(3)
N5-Co2-Co1	90.10(7)	C19-N6-Co2	99.86(17)
N5-Co2-N4	88.97(10)	C16-N6-Co2	128.9(2)
N5-Co2-N7	90.62(10)	C16-N6-C17	107.4(2)
N5-Co2-N6	100.53(9)	C16-N6-C19	108.4(2)
N4-Co2-Co1	89.86(8)	C1-N1-Co1	128.6(2)
N4-Co2-N6	105.58(10)	C1-N1-C4	107.3(2)

N7-Co2-Co1	85.38(7)	C1-N1-C2	108.3(2)
N7-Co2-N4	175.22(10)	C4-N1-Co1	100.75(17)
N7-Co2-N6	79.18(10)	C4-N1-C2	111.5(2)
N6-Co2-Co1	161.27(7)	C2-N1-Co1	99.77(18)
N10-Co1-Co2	89.62(7)	N3-C11-N5	116.8(3)
N10-Co1-N1	106.14(10)	N3-C11-C12	125.2(3)
N9-Co1-Co2	90.54(7)	N5-C11-C12	118.0(3)
N9-Co1-N10	88.06(10)	N10-C26-C27	118.2(3)
N9-Co1-N3	90.42(10)	N8-C26-N10	117.3(2)
N9-Co1-N1	100.71(10)	N8-C26-C27	124.6(3)
N3-Co1-Co2	85.53(8)	N9-C21-C22	117.5(3)
N3-Co1-N10	174.91(10)	N7-C21-N9	116.8(3)
N3-Co1-N1	78.92(10)	N7-C21-C22	125.7(3)
N2-Co1-Co2	86.93(8)	N2-C6-N4	117.1(3)
N2-Co1-N10	87.78(10)	N2-C6-C7	124.8(3)
N2-Co1-N9	175.15(11)	N4-C6-C7	118.0(3)
N2-Co1-N3	93.50(11)	N10-C30-C29	125.0(3)
N2-Co1-N1	82.86(10)	N9-C25-C24	124.9(3)
N1-Co1-Co2	160.78(7)	C13-C12-C11	120.6(3)
C26-N10-Co1	118.31(19)	N3-C5-C4	110.7(2)
C30-N10-Co1	123.4(2)	N5-C15-C14	124.6(3)
C30-N10-C26	118.3(2)	C23-C22-C21	121.0(3)
C21-N9-Co1	118.0(2)	N4-C10-C9	124.9(3)
C25-N9-Co1	122.9(2)	N2-C3-C2	107.7(2)
C25-N9-C21	119.1(3)	C22-C23-C24	119.9(3)
C11-N3-Co1	124.0(2)	C12-C13-C14	120.0(3)
C11-N3-C5	116.1(2)	N1-C4-C5	111.9(3)
C5-N3-Co1	118.80(19)	C28-C27-C26	120.7(3)
C26-N8-Co2	122.4(2)	N6-C17-C18	112.0(2)

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C26-N8-C20	119.6(2)	N8-C20-C19	107.6(2)
C20-N8-Co2	113.66(19)	N6-C19-C20	109.7(3)
C6-N2-Co1	123.1(2)	C10-C9-C8	117.3(3)
C6-N2-C3	119.8(3)	C8-C7-C6	120.6(3)
C3-N2-Co1	113.3(2)	N7-C18-C17	111.0(3)
C11-N5-Co2	118.3(2)	N1-C2-C3	110.1(3)
C15-N5-Co2	122.7(2)	C25-C24-C23	117.1(3)
C15-N5-C11	119.0(3)	C27-C28-C29	120.1(3)
C6-N4-Co2	118.2(2)	C7-C8-C9	120.1(3)
C10-N4-Co2	123.0(2)	C30-C29-C28	117.1(3)
C10-N4-C6	118.8(3)	C15-C14-C13	117.2(3)

#### 4. Theoretical Calculations

All the geometry optimizations were performed using the Gaussian 16 package<sup>3</sup> with the TPSS functional<sup>4</sup> in the gas phase. The 6-31+g(d) basis set was used for C, H, O, and N atoms.<sup>5</sup> SDD was employed to describe Cl, Br, and Co atoms.<sup>6</sup> The wavefunction stability was assessed across all optimized structures to ensure their reliability. The relative mean deviation (RD) in Table S6 suggest that the TPSS-GD3BJ<sup>7</sup>/6-31+g(d)-SDD method provides well-optimized structural parameters for complexes **2**. The optimized structures on the local minimum geometry by frequency calculations (no imaginary frequency). The natural bond orbital (NBO) calculations<sup>8</sup> were carried out at TPSS-GD3BJ/6-31+g(d,p)-SDD//TPSS-GD3BJ/6-31+g(d)-SDD level<sup>9</sup>. The principal interacting orbital (PIO) analyses were performed with the PIO software.<sup>10</sup> To align the  $\alpha$  and  $\beta$  orbitals produced by the open-shell calculations, biorthogonalization was carried out using the canonical orbitals via the Multiwfn program<sup>11</sup>. Time dependent density functional theory (TD-DFT) was performed to calculate UV-vis spectra, under TD-DFT//TPSS-D3BJ/6-31++G(d,p)~SDD-SMD(THF)//TPSS-D3BJ/6-31+G(d)~SDD level including solvent effect in a SMD continuum model (solvent = THF).<sup>12</sup> The UV-Vis spectrum and spin density analysis and visualization were plotted with the help of Multiwfn<sup>11</sup> and VMD programs.<sup>13</sup>

**Table S6.** The relative free energy of **2** in possible spin states with DFT functional TPSS and B3LYP. The energy were given in kcal/mol.

	Multiplicity	TPSS- $\Delta G$ (kcal/mol)	B3LYP <sup>14</sup> - $\Delta G$ (kcal/mol)
Singlet	1	0.0	0.0
Triplet	3	-26.4	-36.9
Quintet	5	-22.0	-40.9
Septet	7	-35.6	-60.2
Nonet	9	25.8	4.6
--	11	91.3	70.4

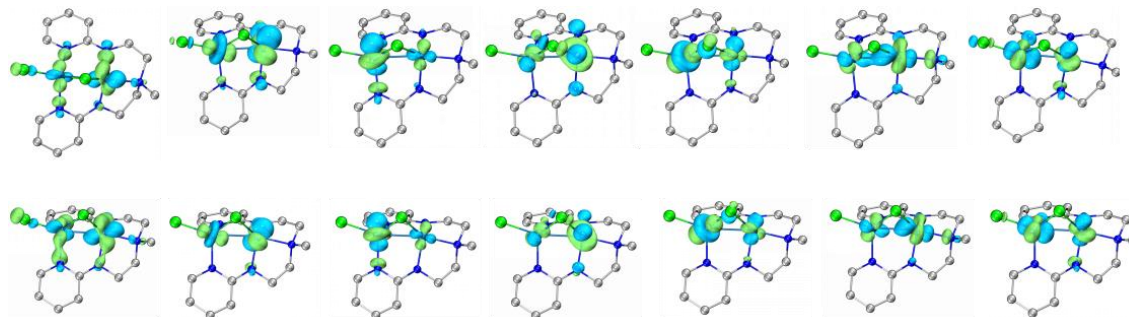
**Table S7.** Key distances (Å) of experiment and DFT calculation structures of **2**.

Bond length	Exp.	B3LYP		B3PW91 <sup>15</sup>		PBE0 <sup>16</sup>		TPSS	
		Cal.	RD	Cal.	RD	Cal.	RD	Cal.	RD
Co1-N1	2.062	2.101	1.89%	2.086	1.16%	2.087	1.21%	2.099	1.79%
Co1-N2	1.909	1.936	1.41%	1.923	0.73%	1.928	1.00%	1.926	0.89%
Co1-N3	1.906	1.949	2.26%	1.938	1.68%	1.942	1.89%	1.943	1.94%
Co1-Co2	2.618	2.772	5.88%	2.734	4.43%	2.76	5.42%	2.648	1.15%
Co1-Cl1	2.266	2.328	2.65%	2.312	1.94%	2.318	2.20%	2.309	1.81%
Co2-Cl1	2.336	2.459	5.27%	2.443	4.58%	2.441	4.49%	2.454	5.05%
Co2-N4	2.024	2.072	2.37%	2.055	1.53%	2.043	0.94%	2.044	0.99%
Co2-N5	2.030	2.052	1.08%	2.033	0.15%	2.066	1.77%	2.019	0.54%
Co2-Cl2	2.248	2.287	1.73%	2.275	1.20%	2.277	1.29%	2.288	1.78%
RD-Average		2.73%		1.93%		2.25%		1.77%	

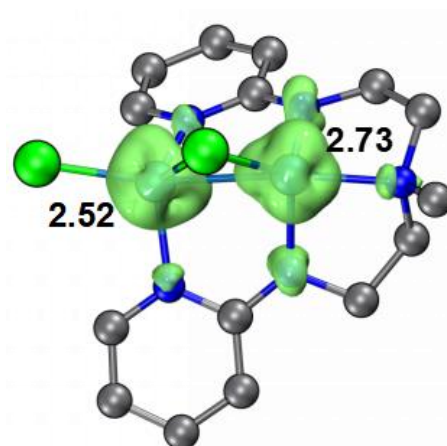
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$$RD = \sum_{i=1}^n \frac{|BL_{Exp} - BL_{DFT}|}{BL_{Exp}}$$

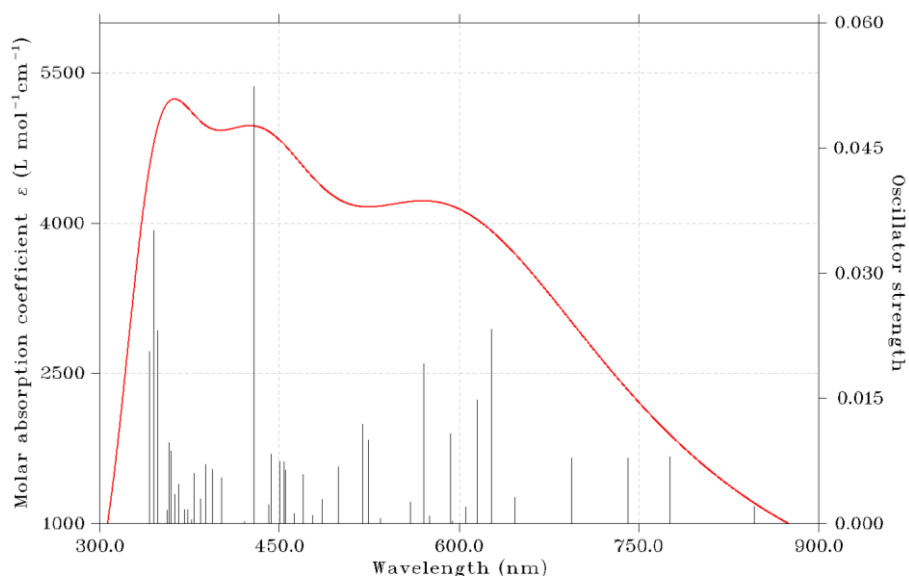
Where  $BL_{Exp}$  and  $BL_{DFT}$  represent the bond length measured by experiment and DFT calculation respectively.



**Figure S20.** The frontier molecular orbitals for complex **2** with wavefunction biorthogonalization.



**Figure S21.** Spin density populations for complex **2**.



**Figure S22.** Calculated and plotted UV-vis spectrum of Complex **2** at the TD-DFT//TPSS-D3BJ/6-311++G(d,p)~SDD-SMD(THF)//TPSS-D3BJ/6-31+G(d)~SDD level.

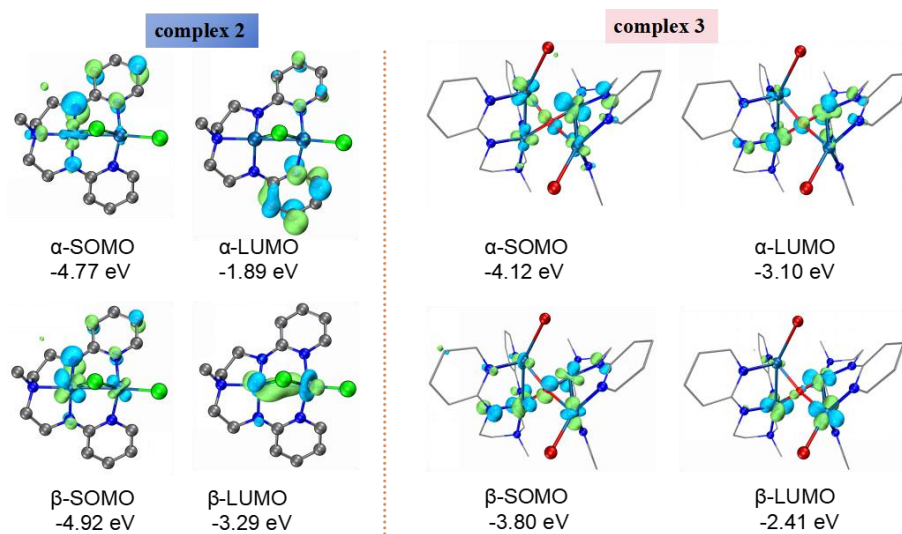
**Table S8.** Calculated UV absorption properties of **2**, including energy(eV), wavelength (nm), oscillator strength (f) and the Transition with absolute contribution.

Energy/eV	Wavelength/nm	Oscillator strength/f	Transition with absolute contribution
1.98	627.23	0.0233	SOMO-1 ( $\beta$ ) $\rightarrow$ LUMO+2 ( $\beta$ ) (46.5%) SOMO-2 ( $\beta$ ) $\rightarrow$ LUMO+1 ( $\beta$ ) (22.6%) SOMO( $\beta$ ) $\rightarrow$ LUMO+1 ( $\beta$ ) (10.8%) SOMO-1 ( $\beta$ ) $\rightarrow$ LUMO+1 ( $\beta$ ) (7.2%)
2.89	429.04	0.0524	SOMO-2 ( $\beta$ ) $\rightarrow$ LUMO+4 ( $\beta$ ) (21.3%) SOMO-1 ( $\beta$ ) $\rightarrow$ LUMO ( $\beta$ ) (19.1%) SOMO-3 ( $\beta$ ) $\rightarrow$ LUMO+4 ( $\beta$ ) (12.5%) SOMO-3 ( $\beta$ ) $\rightarrow$ LUMO+1 ( $\beta$ ) (16.0%)
3.59	345.47	0.0351	SOMO( $\alpha$ ) $\rightarrow$ LUMO+2 ( $\alpha$ ) (21.4%) SOMO( $\alpha$ ) $\rightarrow$ LUMO+3 ( $\alpha$ ) (14.9%) SOMO-2 ( $\beta$ ) $\rightarrow$ LUMO+7 ( $\beta$ ) (10.2%) SOMO( $\beta$ ) $\rightarrow$ LUMO+9 ( $\beta$ ) (7.9%) SOMO-3 ( $\beta$ ) $\rightarrow$ LUMO+7 ( $\beta$ ) (6.5%)

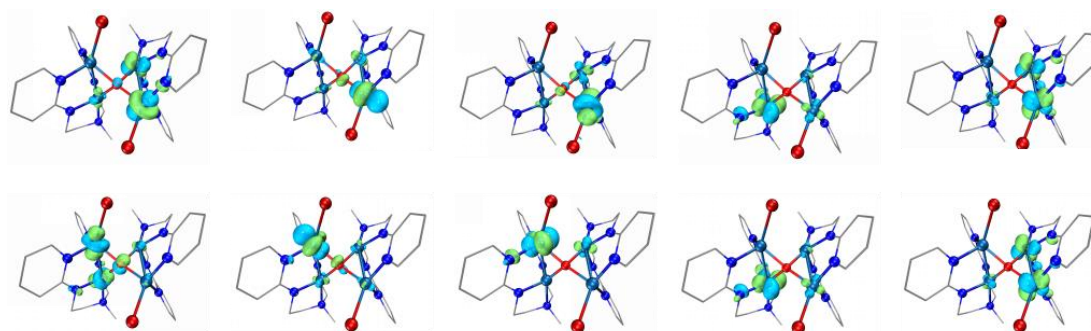
**Table S9.** The relative free energy of **3** in possible spin states with DFT functional TPSS. The energies were given in kcal/mol.

	Multiplicity	TPSS- $\Delta G$ (kcal/mol)
Singlet	1	0.0
Triplet	3	-66.74
Quintet	5	-56.83
Septet	7	-55.23

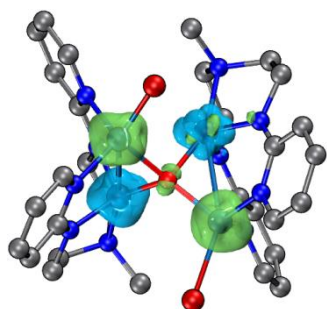
Nonet	9	-51.66
--	11	-61.11



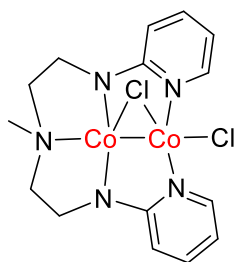
**Figure S23.** The frontier molecular orbitals for complexes **2** and **3**.



**Figure S24.** The frontier molecular orbitals for complex **3** from SOMO to SOMO-4 with wavefunction biorthogonalization.



**Figure S25.** Spin density populations for complex **3**.

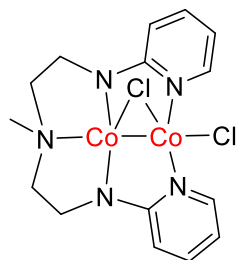


2-B3LYP (0 1)

E = -2069.15613605 au

Co	-1.01888900	-0.22791400	1.10650500
Co	1.01524300	0.25581900	0.38916800
Cl	1.11711100	-1.22190700	2.16160700
Cl	-1.32330300	1.24158800	2.76478800
N	-1.78712900	0.97925700	-0.16914800
N	-1.04184500	-1.75466400	-0.09718800
N	2.89374700	0.79526300	-0.30708400
N	0.37644700	1.73187000	-0.53262000
N	1.01118500	-1.08683300	-0.90562700
C	-0.94236200	1.83733100	-0.82834800
C	-2.07815700	-2.61541900	-0.05888200
H	-2.90561300	-2.32580300	0.58541700
C	0.05336400	-2.03203400	-0.87348000
C	1.36514500	2.51228400	-1.25648600
H	1.16441800	3.59198200	-1.18709400
H	1.37729100	2.26330800	-2.33191800
C	-3.11343200	1.04978000	-0.37066100
H	-3.71554400	0.35736600	0.21000600
C	0.09475000	-3.26190300	-1.59453000
H	0.97001600	-3.51413800	-2.18141400
C	2.73151400	2.24391100	-0.61248000
H	3.55235800	2.60504700	-1.25146900
H	2.78698200	2.77419300	0.34362000
C	-2.10950100	-3.80569100	-0.76456600
H	-2.96795100	-4.46439100	-0.69643200
C	-1.49279000	2.77359500	-1.74438000
H	-0.83518700	3.44754700	-2.28093500
C	3.07161800	-0.02870200	-1.54079900
H	4.14086200	-0.16801900	-1.75269500
H	2.62989400	0.51352300	-2.37981700
C	-3.70457200	1.95011800	-1.24464500

H	-4.78197700	1.96755200	-1.36537000
C	-0.98155500	-4.12586000	-1.54219100
H	-0.94803900	-5.05935100	-2.09883200
C	-2.86211500	2.82664800	-1.94345300
H	-3.27789600	3.54873700	-2.64185000
C	2.34975100	-1.36938000	-1.39236900
H	2.33597400	-1.86067300	-2.37569200
H	2.89483100	-2.03405800	-0.70050100
C	3.99033400	0.56400100	0.65649200
H	3.76617900	1.07627000	1.59510300
H	4.94899300	0.93112800	0.25837800
H	4.06935000	-0.50455300	0.86596700



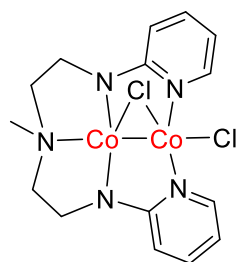
2-B3LYP (0 3)

E = -2069.21005235 au

Co	1.43847300	-0.20827600	0.69677800
Co	-1.18410200	0.18945300	0.64494800
Cl	0.02847600	0.23168500	2.63306900
Cl	3.56755800	-0.61637100	1.42979500
N	0.88659300	-1.91705600	-0.30518900
N	1.51971400	1.51794900	-0.37562400
N	-3.21475300	0.50543200	0.22541700
N	-1.40662300	-1.55209100	-0.14680900
N	-0.79188100	1.65458600	-0.55521400
C	-0.39566900	-2.30820100	-0.62019300
C	2.75684600	2.00708400	-0.62258100
H	3.57207200	1.41706900	-0.21798800
C	0.40994500	2.19611900	-0.82625000
C	-2.76839100	-1.83610000	-0.56628100
H	-3.08287500	-2.85999500	-0.31021300
H	-2.87171400	-1.74808600	-1.66146900
C	1.93307400	-2.65526000	-0.74267900
H	2.90851100	-2.29841900	-0.43015500
C	0.59549800	3.41561800	-1.53951400



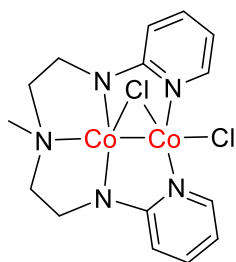
H	-0.26930200	3.97700900	-1.87075900	N	1.58390200	1.42513400	-0.05019600
C	-3.74271200	-0.87879000	0.14082400	N	0.64139600	-1.75313400	-0.50359900
H	-4.72453300	-0.89681200	-0.35803600	C	0.67202300	2.29081500	-0.54255500
H	-3.88455200	-1.21378400	1.17318300	C	-2.92528300	-1.84443200	-0.57431700
C	2.98607000	3.17617400	-1.32574400	H	-3.69791800	-1.17603600	-0.20994300
H	3.99973600	3.52156600	-1.49315600	C	-0.60440000	-2.20952800	-0.75425500
C	-0.58685800	-3.46893000	-1.42316300	C	2.96732000	1.58131400	-0.47406800
H	-1.59150800	-3.77933000	-1.68170700	H	3.39488800	2.55041400	-0.17329000
C	-3.11696900	1.18446000	-1.09324700	H	3.05552600	1.53360300	-1.57318100
H	-4.08565400	1.62826400	-1.36917400	C	-1.59493900	2.89320600	-0.77811300
H	-2.86733000	0.42550100	-1.83796100	H	-2.61896300	2.63148100	-0.53492400
C	1.79834000	-3.79335400	-1.51866700	C	-0.87304800	-3.44332600	-1.41376400
H	2.67711200	-4.34383200	-1.83457200	H	-0.05071400	-4.08257100	-1.71035700
C	1.86881800	3.89128700	-1.78535400	C	3.81733500	0.48986900	0.17932200
H	1.99862300	4.82502900	-2.32687900	H	4.79041500	0.38681200	-0.32337300
C	0.50054500	-4.19865900	-1.86379900	H	4.00173000	0.75444200	1.22489000
H	0.34354300	-5.08503100	-2.47346700	C	-3.23879000	-3.02957700	-1.21781100
C	-2.00469400	2.24502700	-1.10202600	H	-4.27483800	-3.30832300	-1.37261600
H	-1.87490400	2.56376300	-2.14662000	C	1.02725300	3.45315500	-1.28971200
H	-2.31415500	3.13976600	-0.53589500	H	2.07016100	3.67063900	-1.48002700
C	-3.96998200	1.31429300	1.19507100	C	2.95473000	-1.44063700	-1.13727700
H	-3.92118000	0.84198700	2.17926900	H	3.89209700	-1.93951100	-1.42469900
H	-5.02435600	1.41870400	0.89462700	H	2.75072500	-0.64389900	-1.85545300
H	-3.52264800	2.30817600	1.26922500	C	-1.29997100	4.03687800	-1.49861600



**2-B3LYP (0 5)**

E = -2069.21698216 au

Co	-1.45801500	0.37626400	0.62376600	C	3.69815900	-1.73935800	1.17530400
Co	1.20200800	-0.32183700	0.66932500	H	3.69098300	-1.28021500	2.16642600
Cl	-0.15813100	-0.15303300	2.56144300	H	4.73336200	-1.98323900	0.89479300
Cl	-3.60168600	0.98929700	1.18429900	H	3.11226500	-2.65948200	1.21534200
N	-0.65959300	2.02874900	-0.31921200				
N	-1.65859800	-1.42728700	-0.35132000				
N	3.09617400	-0.80849500	0.20066600				

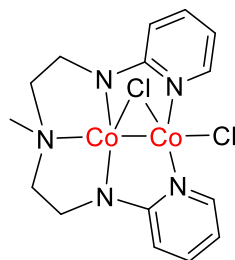


2-B3LYP (0 7)

E = -2069.24699780 au

Co	-1.50882600	0.27264200	0.67426200
Co	1.21544700	-0.23817700	0.70597800
Cl	-0.10517500	-0.25677300	2.62320300
Cl	-3.64331100	0.75752800	1.33711100
N	-0.80499900	1.94685300	-0.32359700
N	-1.58146500	-1.48855700	-0.37653200
N	3.22431900	-0.61342000	0.21905400
N	1.47850300	1.50830100	-0.08706500
N	0.73566700	-1.64881500	-0.55103100
C	0.50196000	2.29664600	-0.58332200
C	-2.81967000	-1.97561400	-0.61811300
H	-3.63318200	-1.37580500	-0.22326100
C	-0.47571300	-2.17823100	-0.81737100
C	2.85321500	1.76746900	-0.48385600
H	3.19708900	2.77006400	-0.18434400
H	2.96113400	1.72170600	-1.58086000
C	-1.80772200	2.72405500	-0.79639000
H	-2.80722700	2.39931800	-0.52672400
C	-0.66939400	-3.40128000	-1.52338900
H	0.19073600	-3.97174100	-1.85067900
C	3.79750700	0.75366000	0.18293100
H	4.77673000	0.75883200	-0.32154900
H	3.95778200	1.04444800	1.22625600
C	-3.05788400	-3.15108600	-1.30840200
H	-4.07368200	-3.49205500	-1.47211800
C	0.75851800	3.46098600	-1.36497600
H	1.78093400	3.74736900	-1.57560300
C	3.06803300	-1.23052800	-1.12296100
H	4.01292000	-1.69422300	-1.44527400
H	2.82311500	-0.43338600	-1.82791500
C	-1.60812900	3.86292200	-1.55623300

H	-2.45600600	4.44279000	-1.90235800
C	-1.94511800	-3.87437000	-1.76377300
H	-2.07899600	-4.81209200	-2.29746800
C	-0.28516400	4.22972700	-1.84233800
H	-0.07390800	5.11742800	-2.43339300
C	1.92216500	-2.25293400	-1.14209900
H	1.76140600	-2.53091900	-2.19417900
H	2.21730300	-3.17667500	-0.61567200
C	3.97465900	-1.48892800	1.13260100
H	3.97066000	-1.05759300	2.13687600
H	5.01637000	-1.61718400	0.79899700
H	3.49457800	-2.46916300	1.17780700

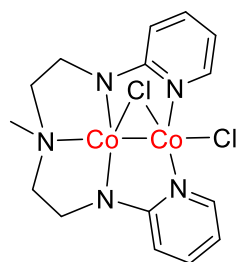


2-B3LYP (0 9)

E = -2069.13709661 au

Co	-1.52974200	0.23011000	0.67092800
Co	1.21723400	-0.22128700	0.70260200
Cl	-0.03261800	-0.21439400	2.63174300
Cl	-3.66484400	0.49529500	1.43254900
N	-0.90311900	1.88782500	-0.29738600
N	-1.49786400	-1.54376600	-0.40289900
N	3.24305400	-0.47370000	0.24037800
N	1.39053700	1.56695800	-0.19820700
N	0.82482500	-1.64327700	-0.54467900
C	0.37541900	2.32778100	-0.63751800
C	-2.71846200	-2.05366200	-0.67822500
H	-3.55365600	-1.48032100	-0.28922900
C	-0.37290300	-2.20264100	-0.83559500
C	2.76637700	1.85634700	-0.58269400
H	3.05116600	2.88778600	-0.33674100
H	2.87385400	1.75329400	-1.67163300
C	-1.96060900	2.68850300	-0.72344300
H	-2.94716200	2.36875000	-0.41520600
C	-0.52040500	-3.42257100	-1.55208500

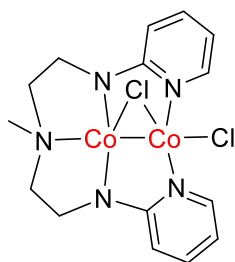
H	0.35880300	-3.97139600	-1.86538000	N	1.37271600	1.56235400	-0.24055400
C	3.74220400	0.92013300	0.15083700	N	0.83253400	-1.68263000	-0.55367900
H	4.72905000	0.95667200	-0.33621000	C	0.34753700	2.30781900	-0.68427800
H	3.86815100	1.26743000	1.18155400	C	-2.70775600	-2.10866800	-0.62054600
C	-2.91610800	-3.22621700	-1.38922700	H	-3.56159300	-1.57806700	-0.22056100
H	-3.92099200	-3.58594400	-1.57841000	C	-0.35886500	-2.22904800	-0.84628800
C	0.59156500	3.49840200	-1.40789700	C	2.74856600	1.86932500	-0.61145100
H	1.60609900	3.80194800	-1.63143000	H	3.01267000	2.90796000	-0.37459900
C	3.15116900	-1.16160800	-1.07609500	H	2.87652800	1.75380200	-1.69701900
H	4.12411800	-1.59844200	-1.34583800	C	-1.98918900	2.62816800	-0.78937500
H	2.89676100	-0.41127000	-1.82747700	H	-2.97311500	2.29390300	-0.48792700
C	-1.77808200	3.85612400	-1.49194500	C	-0.47728400	-3.43374200	-1.58477600
H	-2.66936100	4.40914200	-1.77888700	H	0.41938700	-3.94583300	-1.90939700
C	-1.78103300	-3.92201000	-1.82576300	C	3.72592900	0.95958400	0.15297400
H	-1.88269800	-4.85734500	-2.37035700	H	4.71792800	0.99199800	-0.32194000
C	-0.51808100	4.29633600	-1.87369300	H	3.83487200	1.32624800	1.17861400
H	-0.36057100	5.19153000	-2.46152500	C	-2.86119200	-3.30622000	-1.34748800
C	2.04600800	-2.22898000	-1.08004300	H	-3.87411800	-3.67165500	-1.49873900
H	1.92396200	-2.55220700	-2.12365700	C	0.55376700	3.47525700	-1.46518600
H	2.35992100	-3.11958800	-0.50969600	H	1.56522100	3.78471600	-1.69474600
C	4.02395500	-1.26401000	1.20770600	C	3.15910500	-1.14202500	-1.04956100
H	3.97025800	-0.79301400	2.19233900	H	4.14013100	-1.56075200	-1.31487400
H	5.07784200	-1.34219600	0.89990100	H	2.89224100	-0.40430200	-1.80898300
H	3.60091800	-2.26822400	1.28325600	C	-1.81982400	3.79392700	-1.56521200



**2-B3LYP (0 11)**

E=-2069.02515171 au

Co	-1.56025400	0.20623800	0.66447400	C	4.02989900	-1.20983300	1.24244400
Co	1.21553300	-0.18382600	0.71018200	H	3.97469600	-0.72237100	2.21860500
Cl	0.01228700	-0.13617600	2.64188300	H	5.08220600	-1.28097200	0.93025800
Cl	-3.64582500	0.54270700	1.50886000	H	3.61824700	-2.21691200	1.33777600
N	-0.92172900	1.85387900	-0.34029000				
N	-1.46580800	-1.53958400	-0.35866400				
N	3.23841900	-0.44070000	0.26366800				

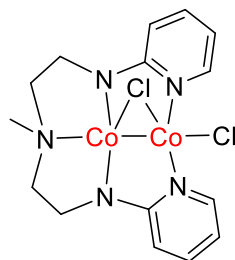


**2-TPSS (0 1)**

E = -2069.21644735 au

Co	0.97452400	0.11773900	1.13738600
Co	-1.05736700	-0.16996200	0.36160200
Cl	-0.94055500	1.35027500	2.09966100
Cl	0.92994000	-1.43130300	2.73720400
N	1.68432400	-1.11984000	-0.08321800
N	1.21914100	1.59007300	-0.04840600
N	-2.93006000	-0.51452600	-0.36866300
N	-0.52729800	-1.68380400	-0.53832400
N	-0.87748500	1.15550600	-0.92433700
C	0.79013100	-1.88249700	-0.81366800
C	2.36306600	2.31205900	0.00272200
H	3.13737700	1.91191900	0.65707600
C	0.17477200	2.00558900	-0.84782800
C	-1.55538100	-2.33003700	-1.34928700
H	-1.44724200	-3.42682700	-1.33905500
H	-1.50435200	-2.00646300	-2.40551500
C	3.01324300	-1.28708200	-0.25391300
H	3.64677100	-0.66799700	0.37749200
C	0.28845800	3.24258700	-1.54782100
H	-0.54894300	3.60717300	-2.13669900
C	-2.90760700	-1.96985700	-0.71677700
H	-3.74974800	-2.22734300	-1.38109700
H	-3.02149600	-2.51733100	0.22663000
C	2.54602200	3.49854200	-0.69810800
H	3.48251700	4.04404800	-0.61963900
C	1.29383100	-2.81380900	-1.76164500
H	0.59547700	-3.40099000	-2.35262500
C	-3.03041300	0.35433300	-1.58779400
H	-4.08483800	0.59079300	-1.79858800
H	-2.62005200	-0.20676200	-2.43393000
C	3.55440900	-2.19813600	-1.15777500

H	4.63267700	-2.29881800	-1.24874900
C	1.46880900	3.96925900	-1.47852500
H	1.55482400	4.90925700	-2.02241500
C	2.66583000	-2.97180600	-1.92631300
H	3.04512100	-3.69125200	-2.65084500
C	-2.18692200	1.61406900	-1.37776400
H	-2.11985800	2.15969400	-2.33209000
H	-2.65182000	2.28463900	-0.63254100
C	-4.00103500	-0.19749500	0.60814200
H	-3.82365700	-0.76599700	1.52656000
H	-4.99527500	-0.44597400	0.19888500
H	-3.95389300	0.86951600	0.84651900

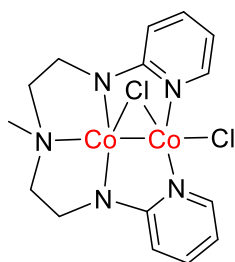


**2-TPSS (0 3)**

E = -2069.25446883 au

Co	-1.36224800	0.27775500	0.64984900
Co	1.09904100	-0.22538400	0.53361400
Cl	-0.01129900	-0.23806100	2.56595200
Cl	-3.51168700	0.73483000	1.33457700
N	-0.80198400	1.99352800	-0.31018200
N	-1.55006500	-1.48095200	-0.38206100
N	3.08411000	-0.62873300	0.24384000
N	1.46009900	1.47298000	-0.19694000
N	0.75052600	-1.70960700	-0.56798900
C	0.50026100	2.33873500	-0.61221000
C	-2.80935000	-1.93679800	-0.59856000
H	-3.59711300	-1.28983500	-0.21790400
C	-0.47754200	-2.23826700	-0.80630800
C	2.85162300	1.71698500	-0.57221000
H	3.18922700	2.73099600	-0.29834800
H	2.98412600	1.62083300	-1.66599500
C	-1.81059000	2.82205400	-0.68286800
H	-2.80280100	2.49277700	-0.38113100
C	-0.70472000	-3.48759000	-1.45166900

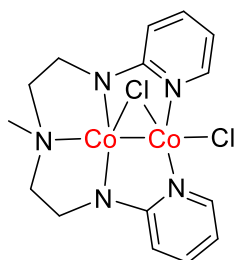
H	0.14162100	-4.09888100	-1.75412600	N	2.04490800	0.46309800	-0.21450600
C	3.73447800	0.71313700	0.18412200	N	-0.33761900	-1.85284500	-0.62173700
H	4.73998400	0.64479700	-0.26553100	C	1.73012000	1.72975200	-0.59773200
H	3.84115100	1.04314200	1.22439400	C	-3.40821000	-0.06195200	-0.57372700
C	-3.08810100	-3.13873200	-1.24504900	H	-3.68305400	0.92452500	-0.20618100
H	-4.11908300	-3.44919700	-1.39336000	C	-1.66680900	-1.62597000	-0.80930500
C	0.76140600	3.53906800	-1.33489100	C	3.33353100	-0.12825500	-0.57125100
H	1.78514300	3.80456200	-1.58478500	H	4.18209300	0.51926700	-0.29392900
C	3.07948100	-1.34383800	-1.06634400	H	3.39952000	-0.29688900	-1.66198500
H	4.06100700	-1.80944700	-1.26006700	C	0.04356400	3.37428300	-0.63627800
H	2.88162800	-0.59558100	-1.84184100	H	-0.97532300	3.61907800	-0.34361000
C	-1.60997200	4.00649100	-1.38693700	C	-2.57231200	-2.55824700	-1.38129700
H	-2.45974200	4.62649100	-1.66029800	H	-2.22213200	-3.54852700	-1.66269500
C	-2.00448500	-3.92721800	-1.67225700	C	3.47066700	-1.44265600	0.21075000
H	-2.17599600	-4.88384500	-2.16499800	H	4.26316300	-2.08558800	-0.20713900
C	-0.29034100	4.36150600	-1.71966800	H	3.72019600	-1.21138400	1.25232900
H	-0.08595200	5.27730400	-2.27371700	C	-4.33598200	-0.92084400	-1.16135000
C	1.94469000	-2.37917500	-1.08222000	H	-5.36746400	-0.60052500	-1.28405100
H	1.80485600	-2.72182900	-2.12052600	C	2.61708300	2.62025500	-1.26070800
H	2.20772200	-3.26807000	-0.48042500	H	3.62825500	2.29847000	-1.49721600
C	3.68031300	-1.46297400	1.31516900	C	1.80949500	-2.85622100	-1.02662100
H	3.56198200	-0.94602200	2.27256600	H	2.37573700	-3.79632400	-1.13608000
H	4.75049000	-1.65068000	1.12141600	H	2.08726300	-2.17566400	-1.83981000
H	3.14738800	-2.41743100	1.36689800	C	0.86788900	4.28878300	-1.28917800



**2-TPSS (0 5)**

E = -2069.24696242 au

Co	-0.92238900	0.93360600	0.62032200	C	2.11884700	-3.11361700	1.40620000
Co	0.75565500	-0.73423800	0.35608500	H	2.26040300	-2.54409500	2.32886200
Cl	-0.05456500	-0.32227000	2.50198600	H	2.90048900	-3.88605500	1.31034100
Cl	-2.46821500	2.48065200	1.39060000	H	1.13407500	-3.58801400	1.44184600
N	0.44259700	2.12095200	-0.30280100				
N	-2.10285300	-0.38644200	-0.39935700				
N	2.16602200	-2.17485000	0.25624100				

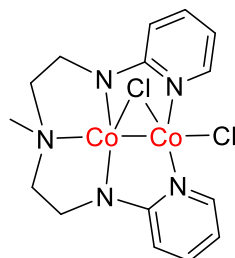


**2-TPSS (0 7)**

E = -2069.26833657 au

Co	-1.39537000	0.39591600	0.66391900
Co	1.14409100	-0.35125100	0.71511000
Cl	-0.13954500	-0.35248200	2.63453100
Cl	-3.43261400	1.13526200	1.39697200
N	-0.59453400	1.98623900	-0.33892600
N	-1.75531000	-1.30635700	-0.36040300
N	3.09417100	-0.92712100	0.19451900
N	1.63391400	1.35623400	-0.02824200
N	0.53366100	-1.64488000	-0.60003800
C	0.74826100	2.23716400	-0.55771400
C	-3.04346700	-1.68245700	-0.55846600
H	-3.78275400	-1.01541100	-0.11870000
C	-0.72584500	-2.08150400	-0.85463900
C	3.04684300	1.51145700	-0.36690500
H	3.46791300	2.45932000	0.01147000
H	3.18858800	1.51959300	-1.46361400
C	-1.52223500	2.83883400	-0.84843800
H	-2.55268700	2.58669000	-0.60499400
C	-1.04160800	-3.26520500	-1.58623800
H	-0.23997100	-3.89333800	-1.96549100
C	3.84670100	0.35790800	0.26619800
H	4.83791100	0.26653800	-0.21167100
H	3.99915800	0.55921800	1.33436500
C	-3.40148300	-2.82715300	-1.26357200
H	-4.44967500	-3.08320400	-1.39329700
C	1.12602300	3.38280600	-1.32093000
H	2.17955600	3.59184200	-1.48542600
C	2.88294700	-1.41397600	-1.19916100
H	3.78280800	-1.93426400	-1.57072100
H	2.69955200	-0.53570200	-1.82701400
C	-1.20370800	3.96241300	-1.60337600

H	-1.99330700	4.60713000	-1.98016900
C	-2.36781500	-3.62833700	-1.78451600
H	-2.60052900	-4.53874600	-2.33642700
C	0.15724600	4.23237600	-1.83777600
H	0.45698100	5.10601200	-2.41606700
C	1.64611300	-2.32324600	-1.27013100
H	1.42959400	-2.50508700	-2.33628600
H	1.85602400	-3.30772600	-0.81249800
C	3.72311500	-1.96313200	1.04383600
H	3.77065700	-1.59888200	2.07574700
H	4.74161100	-2.20382000	0.69244800
H	3.10999400	-2.86988100	1.02161300

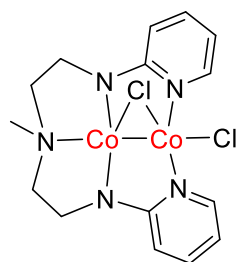


**2-TPSS (0 9)**

E = -2069.16398156 au

Co	-1.42282300	0.23632200	0.75395700
Co	1.21161900	-0.22296900	0.75079400
Cl	0.03451700	-0.28658800	2.70600900
Cl	-3.44059000	0.79014700	1.64732400
N	-0.86029200	1.84411900	-0.35748700
N	-1.58216000	-1.43715900	-0.29619400
N	3.19194400	-0.57778400	0.19927900
N	1.42704300	1.45385700	-0.15581100
N	0.70380100	-1.58921200	-0.61668200
C	0.42913500	2.21589400	-0.69219300
C	-2.85590100	-1.94370300	-0.51437000
H	-3.65651600	-1.41627400	-0.00400000
C	-0.51664500	-2.10840600	-0.91288500
C	2.81029500	1.80487100	-0.46725000
H	3.07073800	2.81897900	-0.11905000
H	2.97527100	1.79598700	-1.56010100
C	-1.90354300	2.56618400	-0.86008600
H	-2.88656500	2.23801300	-0.52881200
C	-0.71919200	-3.23396400	-1.74039800

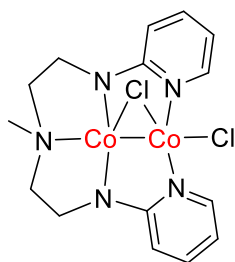
H	0.13913300	-3.74337700	-2.16999100	N	1.60375800	1.34389900	-0.13040000
C	3.75716100	0.80494600	0.22294900	N	0.60753100	-1.64842500	-0.64663300
H	4.75644600	0.83189300	-0.24453900	C	0.69373100	2.20015500	-0.67459500
H	3.86684800	1.06723200	1.28293200	C	-2.97570100	-1.78640100	-0.42375000
C	-3.09421200	-3.05909500	-1.33115000	H	-3.73656200	-1.19586800	0.07780800
H	-4.12504300	-3.38959000	-1.45445500	C	-0.65465000	-2.10268300	-0.89023200
C	0.65057200	3.32958300	-1.54171200	C	3.02876000	1.55081300	-0.36465800
H	1.66703300	3.62683200	-1.78563500	H	3.36054000	2.52439700	0.02990700
C	3.03492500	-1.12464400	-1.18179800	H	3.23184100	1.56147400	-1.44854600
H	3.98313800	-1.56264100	-1.53593400	C	-1.61517000	2.51962800	-1.19263800
H	2.76812000	-0.29096600	-1.83899800	H	-2.63611900	2.16363400	-1.08678800
C	-1.73879700	3.65797200	-1.70812700	C	-0.94335700	-3.24306200	-1.65364100
H	-2.61273400	4.19317900	-2.07143000	H	-0.12177400	-3.81471100	-2.07888600
C	-2.04143500	-3.73604300	-1.97298500	C	3.81573900	0.43335400	0.34128900
H	-2.21048800	-4.60353100	-2.60391200	H	4.83143600	0.34447000	-0.07922100
C	-0.43368600	4.04995600	-2.05402500	H	3.90643900	0.65981700	1.41110700
H	-0.26107200	4.90523000	-2.70531400	C	-3.29054500	-2.92244400	-1.17204700
C	1.90184300	-2.16203000	-1.23555100	H	-4.33993700	-3.20952000	-1.23548000
H	1.72953000	-2.42443700	-2.28966500	C	1.03510900	3.35049500	-1.39556400
H	2.18553600	-3.08888700	-0.70804900	H	2.08417900	3.61444500	-1.50726300
C	3.97770800	-1.49038100	1.06245400	C	2.96501200	-1.37329500	-1.14740500
H	3.98239600	-1.09866000	2.08505300	H	3.89363800	-1.88410000	-1.45112200
H	5.01504800	-1.58448300	0.69895200	H	2.81132800	-0.50808700	-1.79986000
H	3.50721600	-2.47911400	1.06904300	C	-1.30944800	3.68212700	-1.90300500



**2-TPSS (0 11)**

E = -2069.05361013 au

Co	-1.45045500	0.40447800	0.66556700	C	3.67641600	-1.87912500	1.15520900
Co	1.07745400	-0.33500000	0.73861700	H	3.66105700	-1.49919800	2.18263200
Cl	-0.03844400	0.00447200	2.69835000	H	4.71575200	-2.10574800	0.86522700
Cl	-3.37363000	1.08934900	1.61346400	H	3.08130700	-2.79698700	1.11036400
N	-0.64547100	1.78458900	-0.49035100				
N	-1.66697500	-1.31863400	-0.27448500				
N	3.08315100	-0.86334500	0.25136200				

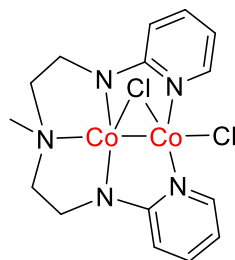


**2-B3PW91 (0 7)**

E = -2068.87842283 au

Co	-1.47590600	0.30584900	0.67375300
Co	1.19672000	-0.26813500	0.70287200
Cl	-0.10951800	-0.28585400	2.61014800
Cl	-3.57519900	0.85761100	1.35623700
N	-0.74350700	1.94486700	-0.32583700
N	-1.62089000	-1.43322100	-0.36927400
N	3.17898500	-0.69396800	0.21348600
N	1.51880500	1.46392000	-0.06725900
N	0.68094500	-1.63732200	-0.56746300
C	0.56678700	2.26983300	-0.57231000
C	-2.86929600	-1.88828000	-0.59486200
H	-3.66259100	-1.27092000	-0.18241400
C	-0.53960600	-2.13937900	-0.82702500
C	2.89682900	1.69653800	-0.44155500
H	3.26292600	2.68410800	-0.11736700
H	3.01876600	1.67081600	-1.53842500
C	-1.72645300	2.73196400	-0.81131400
H	-2.73425400	2.42275900	-0.54822200
C	-0.76560800	-3.34765600	-1.54164500
H	0.07903300	-3.93263600	-1.88616900
C	3.79734500	0.64545700	0.21506000
H	4.78469400	0.62919800	-0.27381200
H	3.95060100	0.91023000	1.26709400
C	-3.14219900	-3.05091100	-1.29060200
H	-4.16739400	-3.36921100	-1.44288400
C	0.85298400	3.42595300	-1.34932700
H	1.88378900	3.69569500	-1.54562000
C	3.00588200	-1.26433500	-1.13803500
H	3.93936800	-1.73632800	-1.48247000
H	2.77005700	-0.44064100	-1.81655300
C	-1.50116700	3.86307000	-1.57231900

H	-2.33606000	4.45476300	-1.93064700
C	-2.05282000	-3.79072500	-1.76802600
H	-2.21385300	-4.72027800	-2.30920600
C	-0.17132000	4.20808600	-1.84157300
H	0.06115700	5.09155600	-2.43166400
C	1.84146100	-2.25536000	-1.17820100
H	1.66728000	-2.50173500	-2.23674900
H	2.11592500	-3.20074300	-0.67873000
C	3.88616100	-1.61581200	1.10396300
H	3.89677000	-1.20809000	2.11834100
H	4.92302000	-1.78142100	0.77128800
H	3.36476400	-2.57585500	1.12785900



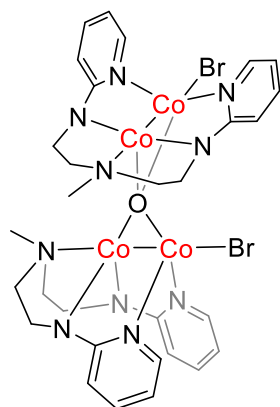
**2-PBE0 (0 7)**

E = -2067.74331567 au

Co	-1.49612000	0.30234600	0.66848500
Co	1.20558000	-0.26287500	0.70800100
Cl	-0.12263000	-0.25612600	2.60748000
Cl	-3.61568000	0.83821800	1.30543500
N	-0.74801200	1.95250500	-0.32382000
N	-1.60901300	-1.45540300	-0.36781800
N	3.19055700	-0.67933600	0.21670200
N	1.51391400	1.47205800	-0.07459100
N	0.69289500	-1.65084700	-0.55056200
C	0.55978400	2.27758300	-0.57273800
C	-2.85158900	-1.91965500	-0.59866100
H	-3.65227500	-1.30340900	-0.19786400
C	-0.52299700	-2.15944600	-0.81160600
C	2.88666300	1.70366400	-0.45941900
H	3.25471200	2.69421500	-0.14575800
H	3.00211500	1.67068000	-1.55718000
C	-1.72962000	2.74517700	-0.79883500
H	-2.73777200	2.43670000	-0.53439900
C	-0.73763400	-3.37459000	-1.51655700



H	0.11259100	-3.95856400	-1.84913000	Co	10.59684000	5.92389100	5.97642500
C	3.79620400	0.66336800	0.19865300	O	10.49345200	5.46504900	4.07711100
H	4.78004200	0.64896400	-0.29775800	N	12.70112500	3.59224800	6.26016800
H	3.95738400	0.94000200	1.24678200	N	13.15276800	5.74203100	4.61252000
C	-3.11489300	-3.08811800	-1.28559500	N	11.74459900	5.35572700	7.47008700
H	-4.13760100	-3.41186700	-1.44216000	C	12.40530000	4.17534300	7.48558700
C	0.84423900	3.43579500	-1.34589900	C	13.45377500	2.46788200	6.19810700
H	1.87462700	3.70380900	-1.54701700	H	13.61685500	2.09165600	5.19002800
C	3.01244000	-1.26458900	-1.12569600	N	11.69031700	7.35944800	5.40854100
H	3.94818900	-1.73184800	-1.47115900	C	14.36280900	5.35863000	4.13919100
H	2.76585400	-0.44981900	-1.81201200	H	14.43432900	4.30611200	3.87836900
C	-1.50740200	3.88009200	-1.55268700	N	9.84249700	7.33489600	7.29520400
H	-2.34340700	4.47513400	-1.90240400	C	15.22806600	7.58998100	4.34414300
C	-2.01950600	-3.82582500	-1.74807100	H	16.03924500	8.31168800	4.25117600
H	-2.17160400	-4.76099500	-2.28203300	C	13.99439700	7.99953000	4.83355500
C	-0.17964000	4.22251600	-1.82761700	H	13.82773500	9.03333100	5.12815500
H	0.05217600	5.10829000	-2.41443700	C	12.83004100	3.49736600	8.67323000
C	1.85747100	-2.26522000	-1.15157100	H	12.54932000	3.89128200	9.64586700
H	1.68724000	-2.52638600	-2.20741500	C	12.92737200	7.06103100	4.96945700
H	2.14144200	-3.20252400	-0.64141000	C	15.42597700	6.24319300	3.98139300
C	3.91903700	-1.58273000	1.10486400	H	16.37574900	5.88247200	3.59590700
H	3.93654600	-1.16821200	2.11654000	C	13.94052600	1.81632500	7.32474400
H	4.95435100	-1.73534800	0.76145300	H	14.53369100	0.91141300	7.22012100
H	3.41352800	-2.55107400	1.14192600	C	13.59760700	2.34559400	8.58624300



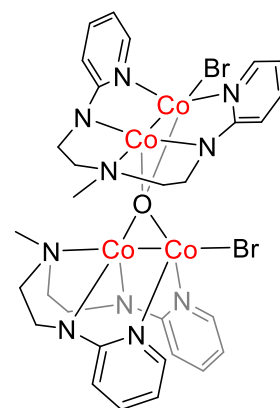
**3-TPSS (0 1)**

E = -2399.65664807 au

Br	12.11404800	2.79653400	3.00355400
Co	11.82940900	4.42554200	4.77077700

C 10.76612500 7.29668100 8.47829200

H	10.2616000	7.7308040	9.3560460
H	11.6460820	7.9035940	8.2468160
Br	9.0318320	4.0431730	6.5003030
Co	8.6805690	5.5052240	4.4588220
Co	9.7144150	6.9099710	3.1725110
N	8.0602940	4.4474630	3.0154100
N	7.1359310	6.6218510	4.5958630
N	9.2078210	5.9311130	1.6603400
C	8.6621130	4.6989110	1.7977330
C	7.3678200	3.3012790	3.2137680
H	6.9456470	3.1847620	4.2096440
N	8.3617810	8.1922360	3.3728960
C	5.9816610	6.2183850	5.1851510
H	6.0546630	5.2722230	5.7199540
N	10.5995850	8.2562080	1.8459020
C	4.7937160	8.1530390	4.4057810
H	3.8821910	8.7436030	4.3197520
C	5.9606080	8.5866170	3.7863240
H	5.9665790	9.5074400	3.2074460
C	8.6286090	3.6879010	0.7928330
H	9.1910530	3.8224700	-0.1267950
C	7.1583990	7.8241680	3.8921520
C	4.7964800	6.9447020	5.1319610
H	3.9053470	6.5732160	5.6320800
C	7.2284830	2.3270390	2.2327810
H	6.6520660	1.4276220	2.4328380
C	7.9000970	2.5272440	1.0080950
H	7.8706320	1.7602450	0.2349370
C	10.0740820	6.2376190	0.5268650
H	9.6336960	5.8905870	-0.4215050
H	11.0667340	5.7644860	0.6336090
C	8.4616740	9.3604630	2.5045340
H	8.0894130	10.2792940	2.9909530
H	7.8705400	9.2237870	1.5801900
C	12.0745280	8.3578170	1.9193070
H	12.3632560	8.6668130	2.9264110
H	12.4618670	9.0867150	1.1845010
H	12.5104420	7.3731890	1.7220790
C	9.9519440	9.5597180	2.1825220

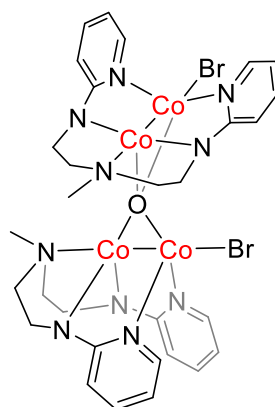


**3-TPSS (0 3)**

E = -2399.75320943 au

Br	12.9945560	3.7285490	2.5435620
Co	12.3230320	4.8868090	4.5872730
Co	10.6095610	6.3577400	6.0844770
O	10.4880490	5.3555670	4.5028950
N	12.4649380	3.6827580	6.1852280
N	13.3386680	6.6601260	4.4937130
N	11.4010740	5.3030200	7.4846400
C	11.9516510	4.0651400	7.4088960
C	13.0218830	2.4556440	6.0395900
H	13.3759590	2.2339090	5.0337990
N	11.6215690	7.9065850	5.5048210
C	14.5608730	6.6042160	3.9083460
H	14.8655700	5.6080490	3.5920300
N	9.9035710	7.5488810	7.5361890
C	14.8710140	8.9709520	4.0807980
H	15.4562710	9.8757870	3.9163670
C	13.6198980	9.0614860	4.6756780
H	13.2280600	10.0319650	4.9685270
C	12.0428500	3.1605790	8.5092660
H	11.6104830	3.4364140	9.4671720
C	12.8346080	7.8837510	4.9043530

C	15.37059700	7.71426800	3.68765000	C	8.52749500	3.14921000	0.68463500
H	16.34409800	7.59879900	3.21838400	H	8.91967300	3.38823000	-0.30034900
C	13.13957300	1.54124700	7.08119100	C	7.61937200	7.81648200	4.13615800
H	13.59821900	0.57087200	6.90942800	C	5.18638700	7.36819200	5.46808700
C	12.63272100	1.91547300	8.34134900	H	4.25823800	7.15000000	5.98998100
H	12.68298000	1.22485100	9.18296000	C	7.43256900	1.61323400	2.20574700
C	11.08193100	5.82582100	8.81511100	H	6.94556800	0.66636100	2.42396200
H	11.91306000	5.65906500	9.52039900	C	7.90034700	1.93375000	0.91464100
H	10.18431100	5.34567200	9.24453100	H	7.78411200	1.22420900	0.09548700
C	11.23956500	9.15214400	6.17173800	C	9.74205000	5.76508200	0.32761500
H	11.06446300	9.98057300	5.46027500	H	9.00676600	5.56772200	-0.47117300
H	12.04298900	9.48772100	6.85344600	H	10.68748600	5.27343700	0.03811900
C	8.51902100	7.22728000	7.97690100	C	9.10921400	9.15153200	2.75840800
H	7.83711500	7.38460600	7.13860300	H	9.11449200	10.05750700	3.39248500
H	8.22945000	7.87756800	8.82006300	H	8.34563900	9.32209900	1.97630600
H	8.46076600	6.17618600	8.26960900	C	12.20787200	7.45878500	1.29295700
C	9.93598200	8.91688000	6.94065300	H	12.80217400	7.75041400	2.16161500
H	9.09017600	8.95448700	6.24434800	H	12.50021600	8.07620400	0.42564200
H	9.78516500	9.68687600	7.71680100	H	12.39973200	6.40176200	1.08400000
C	10.87097900	7.33514200	8.65203600	C	10.51205800	9.02260700	2.12970400
H	10.50315900	7.80596100	9.57988200	H	11.27237400	9.18966400	2.90211900
H	11.82020500	7.79829200	8.36022100	H	10.64815100	9.77983500	1.33739200
Br	8.14853300	3.72081300	6.66791600	C	9.91802100	7.29056600	0.42760100
Co	8.59224900	4.93962900	4.60968800	H	10.35522500	7.70825300	-0.49550600
Co	9.92387100	6.42901700	3.05068300	H	8.93061700	7.73988400	0.58549800
N	8.24326400	3.74253800	3.01721300				
N	7.34816600	6.58049500	4.70496800				
N	9.27332600	5.29621000	1.63052600				
C	8.69482500	4.08299300	1.75288900				
C	7.64050700	2.54444900	3.21681700				
H	7.33789300	2.35337800	4.24525500				
N	8.81165200	7.94104700	3.51718600				
C	6.16427700	6.38640500	5.33861500				
H	6.03809500	5.39467900	5.77031100				
N	10.76942500	7.64820200	1.60651100				
C	5.44974300	8.63434300	4.90783900				
H	4.71568100	9.43621800	4.98663200				
C	6.65065900	8.86199000	4.24913700				
H	6.86252800	9.83336800	3.80848600				



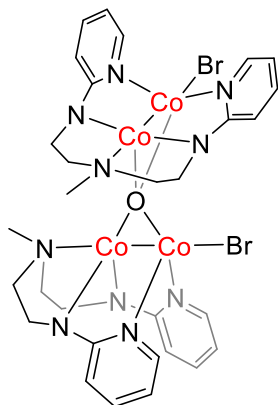
**3-TPSS (0 5)**

E = -2399.73817614 au

Br 12.80636600 3.75514400 2.43049900

Co	12.19958200	4.94324500	4.48011500	C	10.80226700	7.36104400	8.58713700
Co	10.56873100	6.43788300	5.99321600	H	10.42867500	7.82886600	9.51424200
O	10.32125400	5.26165400	4.56692500	H	11.78569500	7.77694400	8.34050000
N	12.32953300	3.72094100	6.07447400	Br	7.89488700	3.65952900	6.70237900
N	13.30676900	6.65048300	4.38905400	Co	8.45644700	4.87150100	4.65369500
N	11.27625200	5.33792900	7.38797000	Co	10.02952300	6.42663500	3.13977700
C	11.78244300	4.08255500	7.28957300	N	8.37407500	3.64413500	3.05985300
C	12.86290600	2.48531100	5.91638700	N	7.28695300	6.53621500	4.74654000
H	13.24553000	2.27946900	4.91777800	N	9.36647100	5.29860200	1.74552200
N	11.67274300	7.95257900	5.45309300	C	8.90836700	4.02499800	1.84491300
C	14.51784700	6.53966700	3.78783600	C	7.88731400	2.38947700	3.21846600
H	14.75377700	5.54024900	3.42639000	H	7.51181400	2.17023000	4.21691700
N	9.88773900	7.65799700	7.44631100	N	8.86897900	7.89848300	3.67917300
C	14.98470600	8.87079900	4.06638700	C	6.08167000	6.38005800	5.34935300
H	15.62817900	9.74129500	3.93844000	H	5.88452600	5.37279700	5.71226600
C	13.74854300	9.01561000	4.68192400	N	10.66397900	7.67061100	1.68580100
H	13.42696000	9.99412200	5.02828600	C	5.52582200	8.69130100	5.06856000
C	11.80033900	3.14348300	8.36386700	H	4.84970200	9.53675100	5.19610200
H	11.32851600	3.40137300	9.30796600	C	6.75484000	8.88240300	4.45134400
C	12.88686700	7.88423200	4.85897700	H	7.03829400	9.87202000	4.10322300
C	15.39512900	7.60427100	3.60669700	C	8.92723100	3.08483400	0.77158300
H	16.35428000	7.44768500	3.12011100	H	9.39017100	3.35938800	-0.17221400
C	12.92035500	1.54081400	6.93597900	C	7.65895200	7.78455000	4.27466600
H	13.36313000	0.56480900	6.75450700	C	5.16463100	7.41063000	5.53038200
C	12.36791400	1.89000000	8.18418300	H	4.21275100	7.21813700	6.01835900
H	12.36352100	1.17335900	9.00520400	C	7.86640100	1.44261000	2.19967500
C	10.92505100	5.83888900	8.71830800	H	7.46027300	0.45087100	2.38156800
H	11.71495400	5.60890100	9.45234300	C	8.40684100	1.81111800	0.95177600
H	9.98518700	5.39584700	9.09282400	H	8.43911000	1.09439200	0.13144900
C	11.35635700	9.19948300	6.15363800	C	9.69938000	5.81129200	0.41499500
H	11.25576900	10.05998100	5.46593400	H	8.91989900	5.54991000	-0.31966600
H	12.16501200	9.45854100	6.86202900	H	10.65627200	5.40476900	0.04213400
C	8.47344900	7.39302600	7.83039300	C	9.13681500	9.15572100	2.97679300
H	7.82299400	7.67657800	7.00067100	H	9.20407000	10.02037200	3.66334800
H	8.20513800	7.98151600	8.72441400	H	8.31860300	9.38224500	2.26823300
H	8.33745700	6.32496500	8.02435200	C	12.08774800	7.45948800	1.30350700
C	10.02269000	9.03422600	6.89013300	H	12.72591500	7.76788200	2.13389900
H	9.19573000	9.14688100	6.17963700	H	12.33458000	8.05727200	0.40946300
H	9.90960300	9.79449100	7.68225600	H	12.26433700	6.39723100	1.11045600

C	10.47576700	9.04128200	2.24025000	C	15.44181800	7.56618800	3.60153900
H	11.29787800	9.18700200	2.95037000	H	16.39656200	7.39155400	3.11244900
H	10.55913700	9.80429600	1.44708600	C	12.75908200	1.52852800	6.90922500
C	9.76268800	7.33723600	0.54462600	H	13.17956200	0.54181800	6.73260500
H	10.11853100	7.81829200	-0.38270200	C	12.18026400	1.88373400	8.14409200
H	8.76362000	7.71479900	0.79012500	H	12.13125700	1.16079500	8.95808800

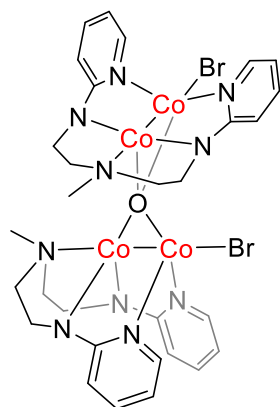


**3-TPSS (0 7)**

E = -2399.73524363 au

Br	12.78871600	3.77799700	2.41988500	H	9.26424600	9.25732800	6.14773800
Co	12.19114500	4.97061400	4.46541000	H	9.98575200	9.86230700	7.66406600
Co	10.56051300	6.50316500	5.93789600	C	10.78983400	7.39635100	8.54630400
O	10.28979300	5.27255100	4.56131000	H	10.42417700	7.87363000	9.47181300
N	12.25187600	3.72939800	6.04933900	H	11.78985800	7.77737700	8.31041200
N	13.32944300	6.65556100	4.37152500	Br	7.85650500	3.56625100	6.71713600
N	11.21147300	5.36687800	7.34330200	Co	8.46489800	4.78031500	4.68836900
C	11.68071100	4.09739100	7.25062800	Co	10.07536000	6.43074900	3.14809000
C	12.75638300	2.48121700	5.89589900	N	8.44833200	3.59551200	3.06046200
H	13.16109200	2.27183100	4.90686500	N	7.32284400	6.46812100	4.78482400
N	11.72661100	7.98567500	5.44457500	N	9.39855100	5.29724900	1.76401900
C	14.53840600	6.52185300	3.76950100	C	8.96585200	4.01266500	1.84951300
H	14.74982900	5.52119500	3.39679700	C	7.99955400	2.32363800	3.19785000
N	9.89676900	7.73104800	7.39937300	H	7.63520600	2.07572800	4.19392500
C	15.06465800	8.83653200	4.07955500	N	8.93922000	7.87060500	3.80029200
H	15.73101700	9.69145300	3.96440000	C	6.10409600	6.30320600	5.35763100
C	13.83283400	9.00483500	4.69723700	H	5.89579700	5.28830800	5.69170200
H	13.53767400	9.98591900	5.05934800	N	10.62511900	7.68449000	1.71401800
C	11.64185600	3.15048800	8.31764800	C	5.55638400	8.61917600	5.11743700
H	11.14699900	3.41333100	9.24841000	H	4.88030800	9.46407800	5.24884500
C	12.94079700	7.89434000	4.85638600	C	6.80040000	8.82087400	4.53386100
				H	7.09302300	9.81974700	4.22265000

C	8.99099800	3.09567200	0.75613500	Co	10.40353300	6.15456500	6.02251200
H	9.43487700	3.40161600	-0.18726500	O	10.26571600	5.14362800	4.51008700
C	7.70954600	7.72642400	4.35625100	N	12.30464800	3.51039500	6.04231900
C	5.18385300	7.33029800	5.54300200	N	13.16058200	6.35728700	4.37585800
H	4.22200700	7.12778000	6.00672200	N	11.42808300	5.22497500	7.37238600
C	7.99471100	1.39586200	2.16168100	C	11.97752700	3.98950900	7.29890600
H	7.61764500	0.39007600	2.32841900	C	12.83674500	2.26954200	5.91050100
C	8.50694300	1.80501600	0.91471700	H	13.04472800	1.97169500	4.88335800
H	8.54729700	1.10710500	0.07862300	N	11.34081200	7.67044800	5.11023600
C	9.65148200	5.84692900	0.43043000	C	14.44388200	6.24523500	3.95768200
H	8.84112900	5.58352800	-0.26924400	H	14.73590900	5.24113100	3.65486900
H	10.59605600	5.47460100	-0.00526900	N	9.89035100	7.42523400	7.45058200
C	9.17374500	9.14229500	3.10433700	C	14.85020600	8.58110600	4.25850800
H	9.26648200	9.99746900	3.79976600	H	15.49437800	9.45858700	4.20647100
H	8.32338400	9.37233000	2.43684500	C	13.52985300	8.72323900	4.67544800
C	12.03860900	7.45976700	1.29466000	H	13.15016100	9.71182200	4.91626800
H	12.69995600	7.74927600	2.11372900	C	12.25447200	3.17180400	8.43871200
H	12.26919400	8.06530600	0.40210400	H	11.98660500	3.52787900	9.42994300
H	12.19647000	6.39779300	1.08569100	C	12.66456500	7.58842500	4.74094800
C	10.47227900	9.04656000	2.30206000	C	15.33306600	7.31501400	3.88913000
H	11.32946300	9.17624600	2.97217500	H	16.35370600	7.15994000	3.54943200
H	10.51705800	9.82305400	1.51960200	C	13.11471000	1.43436200	6.98631900
C	9.68998100	7.37119000	0.59402700	H	13.54269000	0.44911700	6.82076800
H	10.00889300	7.88194800	-0.33059200	C	12.81486000	1.91320100	8.27798000
H	8.69534900	7.72751800	0.88464000	H	13.00379400	1.29219900	9.15353700



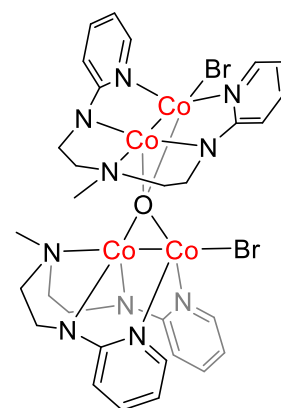
**3-TPSS (0 9)**

E = -2399.73275233 au

Br	12.80837900	3.55115500	2.32083700
Co	12.09252900	4.61468400	4.37461800

H	8.87017100	8.65939200	6.12566200
H	9.69053100	9.56611900	7.42935300
C	11.00024100	7.33327600	8.44852900

H	10.73016700	7.86314600	9.37730300
H	11.88565200	7.80347500	8.00704900
Br	7.82965400	3.87369300	6.69523400
Co	8.30575000	5.10909200	4.63522200
Co	10.09593200	6.61050800	3.33004600
N	8.24583600	3.85971400	3.08393000
N	7.16283600	6.76081400	4.71292400
N	9.40694600	5.50014800	1.89021800
C	8.94745600	4.22157200	1.95452600
C	7.72497600	2.61594700	3.19793200
H	7.22419200	2.41535400	4.14370800
N	8.71683700	8.09063500	3.58191100
C	5.94931900	6.60843100	5.30713300
H	5.79709800	5.63777400	5.77789600
N	10.72714500	7.87524300	1.81369000
C	5.26673000	8.82422600	4.71169300
H	4.53175000	9.62945100	4.70367600
C	6.49676600	9.01361900	4.10273200
H	6.72366100	9.96212000	3.62297000
C	9.10880700	3.26032800	0.91121900
H	9.72119500	3.50231100	0.04776000
C	7.48582400	7.97009900	4.10273400
C	4.97251700	7.59519300	5.34098300
H	4.02165000	7.40974400	5.83371900
C	7.82237700	1.65711500	2.19515000
H	7.37640700	0.67485100	2.32888000
C	8.54243100	1.99925400	1.03316600
H	8.68439000	1.26750600	0.23814100
C	9.86768800	5.95639800	0.57691400
H	9.16384300	5.64520800	-0.21216000
H	10.86060800	5.54939700	0.31505900
C	9.00954500	9.32664500	2.86288700
H	8.95752500	10.21936200	3.51622100
H	8.27723300	9.50138400	2.05179300
C	12.16786300	7.72283400	1.47581700
H	12.77273700	8.11472400	2.29584100
H	12.40579200	8.28140500	0.55413300
H	12.40358600	6.66276000	1.33875800
C	10.42980700	9.25193400	2.28043100



**3-TPSS (0 11)**

E = -2399.74425451 au

Br	12.60188100	3.92576300	2.37983100
Co	12.13868200	5.09169400	4.46804300
Co	10.58053000	6.55750400	5.92688000
O	10.17871000	5.22186900	4.60375400
N	12.43416500	3.87135900	6.03450700
N	13.29016100	6.77436900	4.43573400
N	11.31561400	5.42640900	7.35707200
C	11.89383100	4.20753700	7.26294200
C	13.04655300	2.67506800	5.86450300
H	13.41769300	2.49173300	4.85716200
N	11.73918700	8.09038200	5.57541500
C	14.50628900	6.62294900	3.84912000
H	14.67301100	5.64511700	3.39883000
N	9.77482100	7.76176900	7.44743600
C	15.15443100	8.87010600	4.37206800
H	15.87365500	9.68866000	4.34716300
C	13.92072300	9.05530800	4.97999300
H	13.66866800	10.01314900	5.42847200
C	11.98643400	3.26477000	8.33288200
H	11.52308600	3.49296600	9.28876200

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C	12.96458300	7.99145900	5.02019200	C	6.08315400	6.34879600	5.22911100
C	15.46805800	7.62531500	3.78920700	H	5.79178800	5.34612400	5.53735300
H	16.42210400	7.43961600	3.30261700	N	10.67269400	7.46714900	1.63134600
C	13.18081800	1.73561300	6.88036300	C	5.71585900	8.70184600	5.02153500
H	13.67835900	0.78818400	6.68990300	H	5.10115400	9.59273800	5.15025800
C	12.62474700	2.04882600	8.13769000	C	6.99234700	8.82158400	4.48607700
H	12.67932500	1.33205400	8.95690700	H	7.36953000	9.80312900	4.21349900
C	10.85563600	5.88161100	8.66932200	C	8.59309000	3.07112900	0.65420600
H	11.60255200	5.68047200	9.45641700	H	8.96255200	3.39332900	-0.31556900
H	9.91901400	5.37694500	8.96557400	C	7.82166100	7.66565500	4.30961800
C	11.40032700	9.30046700	6.31840000	C	5.23332900	7.43711000	5.40393500
H	11.38316300	10.20076500	5.67593500	H	4.24360300	7.29818200	5.83085700
H	12.15051500	9.49734500	7.10675700	C	7.62962600	1.36600900	2.07923700
C	8.35022000	7.54023900	7.79893300	H	7.21625300	0.37382100	2.24093900
H	7.72208000	7.85530700	6.96228600	C	8.05775700	1.80025700	0.80888200
H	8.07572800	8.12130800	8.69706500	H	7.98922100	1.13616800	-0.05269700
H	8.17995300	6.47386200	7.97879400	C	9.43411600	5.77089900	0.37961700
C	9.99893700	9.14382400	6.94224800	H	8.56012800	5.61008000	-0.27378900
H	9.23116400	9.30780600	6.17640000	H	10.30905100	5.32477000	-0.12770200
H	9.85294400	9.89160300	7.74251000	C	9.40759600	9.00056700	3.12188200
C	10.66294000	7.40280700	8.59288800	H	9.59249700	9.81947600	3.84020100
H	10.25056200	7.80382700	9.53512700	H	8.56863600	9.32560700	2.48081200
H	11.64109300	7.86200200	8.41125500	C	12.02984800	7.20470500	1.07486100
Br	7.68702100	3.54614100	6.68550600	H	12.76139100	7.27644700	1.88274500
Co	8.36231800	4.67566000	4.63897100	H	12.25775300	7.94652400	0.29095200
Co	10.12021000	6.23499800	3.07514000	H	12.07205100	6.19344500	0.66710600
N	8.26715500	3.50491800	3.01123300	C	10.66938600	8.81050500	2.28370900
N	7.32817600	6.43481200	4.69910800	H	11.55122400	8.82503800	2.93352800
N	9.21608700	5.20135100	1.71051800	H	10.77301100	9.61020100	1.53049500
C	8.71204700	3.94455800	1.77884000	C	9.63049400	7.27749800	0.57717100
C	7.76232600	2.25353600	3.14165300	H	9.92802100	7.78676200	-0.35499500
H	7.45820800	1.98995700	4.15395600	H	8.69753900	7.71415000	0.94978800
N	9.07834200	7.73313500	3.78774800				



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