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Supplementary Material

Hybrid Pyrazolyl-1,2,3-Triazolyl Tripodal Tetraamine Ligands: Click Synthesis and Cobalt(III) Complexes.

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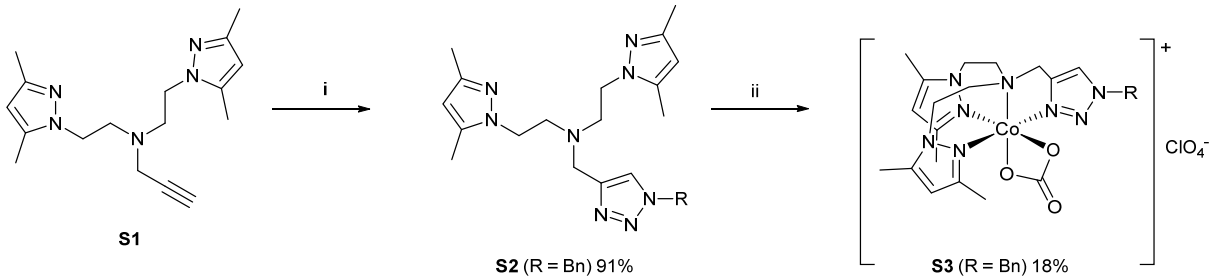
1. Synthetic Information



Scheme S1 (i) NaN_3, benzyl bromide, $CuSO_4 \cdot 5H_2O$, sodium ascorbate, DMF:H_2O (4:1), (ii) $Na_3[Co(CO_3)_3] \cdot 3H_2O$, HCl then $NaClO_4$.

2-(3,5-(Dimethyl)-1*H*-pyrazol-1-yl)-*N*-[2-(3,5-(dimethyl)-1*H*-pyrazol-1-yl)ethyl]ethanamine (**S0**)

Compound **S0** was synthesised by a modification of the method for synthesis of bis(pyrazolylethyl)amine described by Sorrell, *et al*.[1] Dry DMF (350 mL) was poured into a three neck flask in a glovebox, and then 60% sodium hydride (20.6 g, 0.515 mol) was added while purging the flask with N_2. 3,5-dimethylpyrazole (33.0 g, 0.343 mol) was slowly added, with stirring. The solution was stirred for 2 h, and then bis(2-chloroethyl)amine hydrochloride (28.7 g, 0.161 mol) was added. The resulting solution was heated at 60 °C for two days. The solvent was removed (rotary evaporation) and the resulting solid dissolved in boiling water (800 mL) and crystallized on standing at 4 °C. This was collected by filtration, dissolved in methanol (250 mL) and washed with hexane (2 × 600 mL). Solvent was removed, and the resulting white solid was dissolved in boiling water (1 L). White needle-shaped crystals formed on cooling to room temperature, and were collected by filtration (48.5 g, 91%).

Anal. Calc. for $C_{14}H_{23}N_5 \cdot 4H_2O$: C: 50.4%, H: 9.4%, N: 21.0%; Found C: 50.8%, H: 9.4%, N: 21.1%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.75 (s, 1H, H_b), 4.01 (t, J = 6.1 Hz, 2H, H_d), 2.97 (t, J =

6.1 Hz, 2H, H_e), 2.20 (s, 3H, H_a or H_c), 2.18 (s, 3H, H_a or H_c). ^{13}C NMR ($CDCl_3$): 147.5, 139.1 , 104.9, 49.2, 48.3, 13.4, 11.0. ESMS (m/z) ($CHCl_3$): 262.2003 ([H**S0**]$^+$, calc. 262.2026). FT-IR (ν/cm^{-1}): 3242 (s, br, ν H_2O and ν NH), 2975 (w, ν C-H_{sat}), 2920 (w, ν C-H_{sat}), 2859 (w, ν C-H_{sat}), 776 (s, γ pz), 640 (s, pz).

N,*N*-Bis[2-(3,5-dimethyl-1*H*-pyrazol-1-yl)ethyl]prop-2-yn-1-amine (**S1**)

Compound **S0** (4.81 g, 14.4 mmol) was dissolved in 25 mL CH_3CN. K_2CO_3 (7.99 g, 57.8 mmol) was added, and then 3-bromopropyne (80% w/w in toluene, 1.6 mL, 15 mmol) was added dropwise. The resulting yellow suspension was refluxed overnight, over which time it became dark brown. K_2CO_3 was filtered off, and the resulting dark brown solution was run through a plug of basic alumina. Solvent was removed to yield a brown oil (3.05 g, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.74 (s, 2H, H_b), 3.89 (t, J = 6.9 Hz, 4H, H_d), 3.36 (d, J = 2.3 Hz, 2H, H_e), 2.91 (m, 4H, H_f), 2.19 (s, 6H, H_a or H_c), 2.18 (s, 7H, H_a or H_c and H_g). ^{13}C NMR ($CDCl_3$): 147.4, 139.1, 104.8, 78.7, 72.9, 54.2, 47.1, 43.3, 13.4, 11.0. ESMS (m/z) (CH_3CN): 322.2033 ([Na**S1**]$^+$, calc. 322.2002). FT-IR (ν/cm^{-1}): 2922 (w, ν C-H_{sat}), 2863 (w, ν C-H_{sat}), 2039 (w, ν C≡C), 776 (s, γ pz), 628 (s, pz).

N-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methyl]-2-(3,5-dimethyl-1*H*-pyrazol-1-yl)-*N*-[2-(3,5-dimethyl-1*H*-pyrazol-1-yl)ethyl]ethanamine (**S2**)

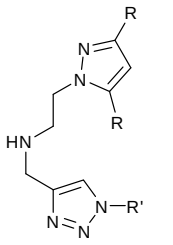
Benzyl bromide (1.13 mL, 1.62 g, 9.46 mmol), NaN_3 (0.635 g, 9.76 mmol), $CuSO_4{\cdot}5H_2O$ (0.872 g, 3.49 mmol), and sodium ascorbate (1.71 g, 8.64 mmol) were combined in 25 mL DMF:H_2O (4:1). Compound **S1** (2.58 g, 8.60 mmol) was added and the resulting brown solution was stirred at room temperature for 20 h. An aqueous solution of 0.1 M EDTA/1 M NH_4OH (50 mL) was then added and the resulting green solution was stirred at room temperature for 1 h. The product was extracted with $CHCl_3$ (3 × 25 mL) and washed with water (5 × 150 mL) and brine (150 mL), dried with $MgSO_4$ and filtered. Solvent was removed to yield a yellow oil (3.39 g, 91%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, J = 5.7 Hz, 3H, H_i and H_k), 7.25 (m, 2H, H_j), 7.15 (s, 1H, H_g), 5.70 (s, 2H, H_b), 5.47 (s, 2H, H_h), 3.90 (t, J = 6.7 Hz, 4H, H_d), 3.72 (s, 2H, H_f), 2.87 (t, J = 6.7 Hz, 4H, H_e), 2.16 (s, 6H, H_a), 2.11 (s, 6H, H_c). ^{13}C NMR ($CDCl_3$): 147.3, 145.1, 139.2,

134.7, 129.1, 128.7, 128.0, 122.4, 104.7, 54.1, 49.4, 47.1, 13.4, 11.0. ESMS (m/z) (CH_3CN): 455.2610 ([Na**S2**]$^+$ calc. 455.2642). FT-IR (ν/cm^{-1}): 2954 (w, ν C-H_{sat}), 2919 (w, ν C-H_{sat}), 2859 (m, ν C-H_{sat}), 776 (s, γ pz), 628 (s, pz).

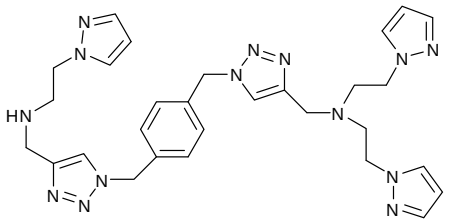
[Co(**S2**)O_2CO]ClO_4 (**S3**)

Ligand **S2** (0.447 g, 1.03 mmol) was dissolved in 25 mL H_2O, and the resulting solution was adjusted to *ca*. pH 1 with conc. HCl. $Na_3[Co(CO_3)_3]\cdot 3H_2O$ (0.414 g, 1.14 mmol) was added, resulting in evolution of CO_2. The mixture was heated to 60 °C for 0.5 h, during which time more CO_2 evolved, and the dark red solution was allowed to cool to room temperature and filtered through Celite. The filtrate was diluted to 800 mL and loaded onto a Sephadex SP C-25 cation exchange column, and eluted with 0.1 M $NaClO_4$ solution. The main band was collected as a fraction of 250 mL and concentrated to 200 mL. On standing at 4 °C, purple crystals (0.130 g, 18%) formed, which were collected by filtration, washed with isopropanol and diethyl ether and air-dried. Anal. Calc. for $[Co(C_{24}H_{32}N_8)(O_2CO)](ClO_4)\cdot 0.5H_2O$: C: 45.5%, H: 5.0%, N: 17.0%. Found: C 45.2%, H: 5.1%, N: 17.0%. ^{1}H NMR (400 MHz, CD_3CN) δ 8.01 (s, 1H, H_g), 7.42 (m, 3H, H_i and H_k), 7.34 (m, 2H, H_j), 6.12 (s, 1H, H_b), 6.03 (s, 1H, H_b), 5.63 (m, 2H, H_h), 5.05 (m, 1H, H_d or H_e), 4.80 (d, J = 15.6 Hz, 1H, H_f), 4.43 (dt, J = 15.0, 2.7 Hz, 1H, H_d or H_e), 4.08 (m, 2H, H_d or H_e and H_f), 3.47 (ddd, J = 14.5, 12.2, 2.3 Hz, 1H, H_d or H_e), 3.36 (m, 2H, H_d or H_e), 3.02 (dd, J = 13.8, 4.8 Hz, 1H, H_d or H_e), 2.90 (s, 3H, H_a or H_c), 2.53 (dd, J = 13.9, 10.5 Hz, 1H, H_d or H_e), 2.41 (s, 3H, H_a or H_c), 2.21 (s, 3H, H_a or H_c), 1.79 (s, 3H, H_a or H_c). ^{13}C NMR (CD_3CN): 158.5, 155.0, 146.0, 145.6, 145.5, 133.9, 129.1, 128.6, 124.7, 109.7, 109.2, 58.7, 58.6, 57.1, 55.9, 43.5, 42.9, 13.4, 11.3, 11.0, 10.7. ESMS (m/z) (CH_3CN): 551.1896 ([Co(**S2**)O_2CO]$^+$, calc. 551.1924), 507.1996 ([Co(**S2**)O]$^+$, calc. 507.2031). FT-IR (ν/cm^{-1}): 3532 (w, br, H_2O), 3133 (w, ν pz), 1672 (s, ν CO_3), 1084 (s, br, ClO_4), 747 (s, γ pz), 623 (s, pz). UV-Vis (CH_3CN) [λ_{max}, nm (ε, L mol^{-1} cm^{-1})]: 524 (153).

2. Ligand Mass Spectra



4a: R = H, R' = Bn
4b: R = H, R' = Ph
4c: R = H, R' = pyr
S4: R = Me, R' = Bn



4d

Figure S1. Mass spectral fragmentation products of ligands **2a-d** and **S2** observed in the mass spectra of complexes **3a-d** and **S3**.

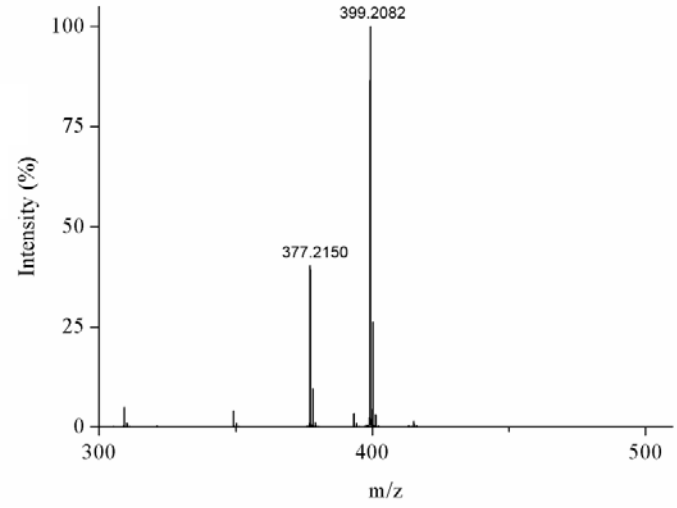


Figure S2. The mass spectrum of ligand **2a** in CH_2Cl_2. Assigned peaks (m/z): 399.2082 = $[Na(\mathbf{2a})]^+$ (calc. 399.2075), 375.2150 = $[H(\mathbf{2a})]^+$(calc. 377.2197).

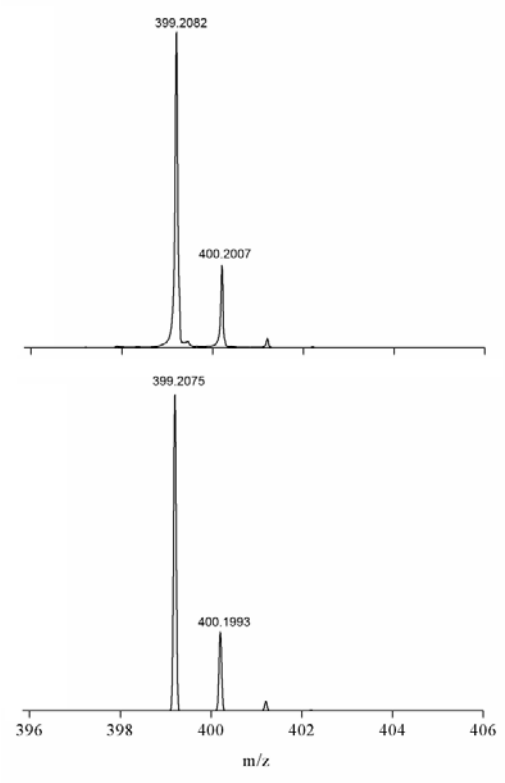


Figure S3. The observed (top) and calculated (bottom) isotopic patterns for the $[Na(\mathbf{2a})]^+$ ion with exact masses indicated.

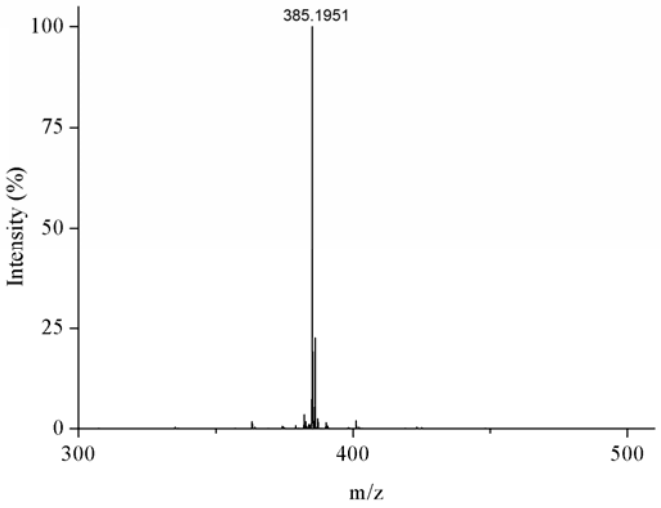


Figure S4. The mass spectrum of ligand **2b** in CH_2Cl_2. Assigned peaks (m/z): 385.1951 = $[Na(\mathbf{2b})]^+$ (calc. 385.1861).

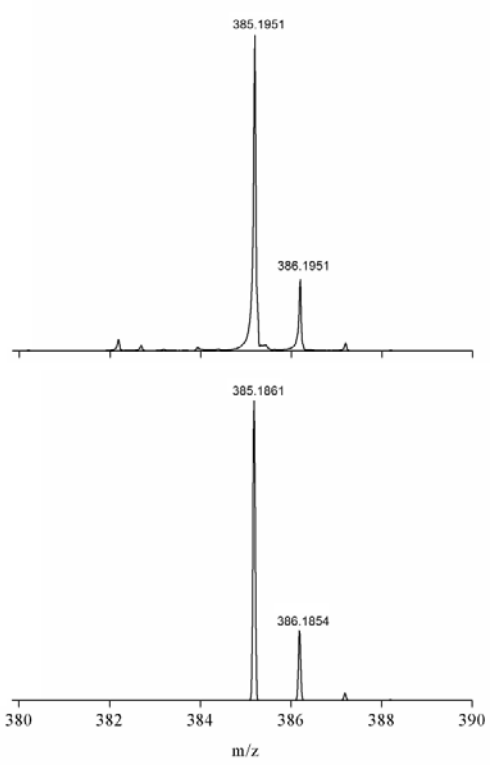


Figure S5. The observed (top) and calculated (bottom) isotopic patterns for the $[Na(\mathbf{2b})]^+$ ion with exact masses indicated.

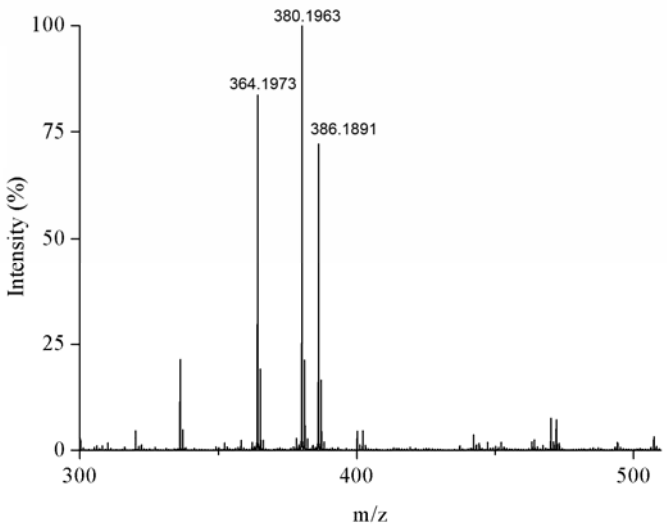


Figure S6. The mass spectrum of ligand **2c** in CH_2Cl_2. Assigned peaks (m/z): 386.1981 = $[Na(\mathbf{2c})]^+$ (calc. 386.1912), 380.1963 = $[H_3O(\mathbf{2c})]^+$ - H_2 (calc. 380.1955), 364.1973 = $[H(\mathbf{2c})]^+$ (calc. 364.1993).

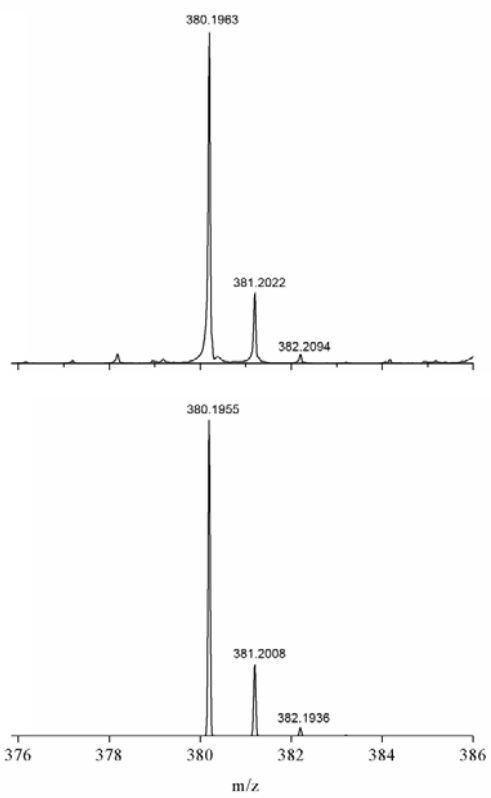


Figure S7. The observed (top) and calculated (bottom) isotopic patterns for the $[H_3O(\mathbf{2c}) - H_2]^+$ ion with exact masses indicated.

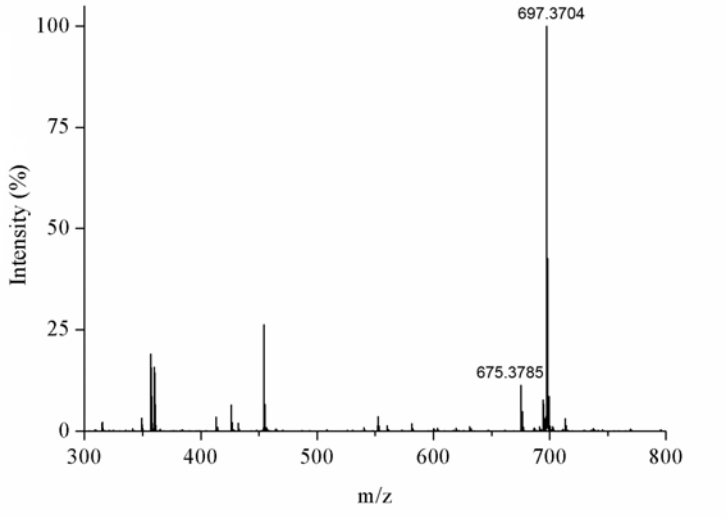


Figure S8. The mass spectrum of ligand **2d** in CH_2Cl_2. Assigned peaks (m/z): 697.3704 = $[Na(\mathbf{2d})]^+$ (calc. 697.3671), 675.3785 = $[H(\mathbf{2d})]^+$(calc. 675.3851).

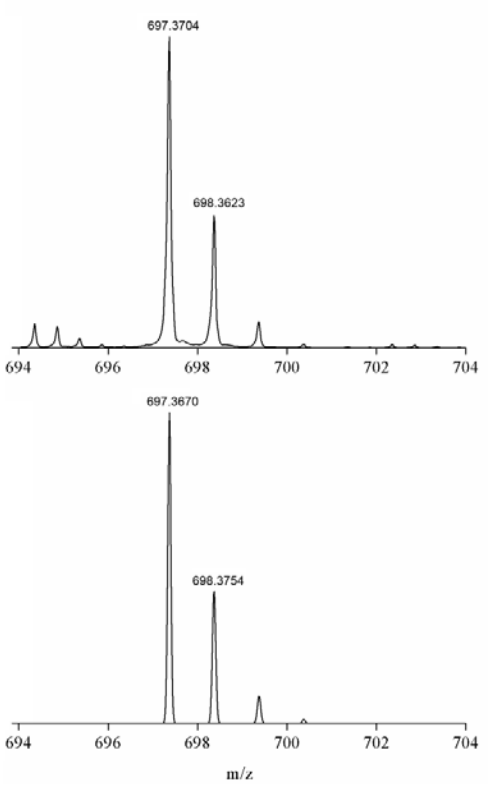


Figure S9. The observed (top) and calculated (bottom) isotopic patterns for the $[Na(\mathbf{2d})]^+$ ion with exact masses indicated.

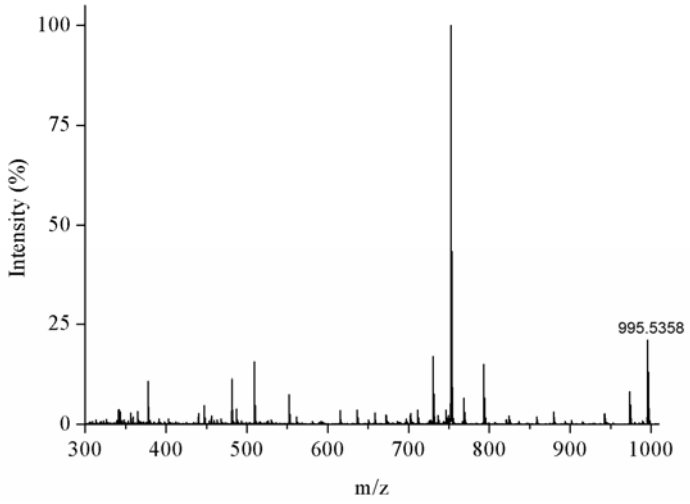


Figure S10. The mass spectrum of ligand **2e** in CH_2Cl_2. Assigned peaks (m/z): 995.5358 = $[Na(\mathbf{2e})]^+$ (calc. 995.5306).

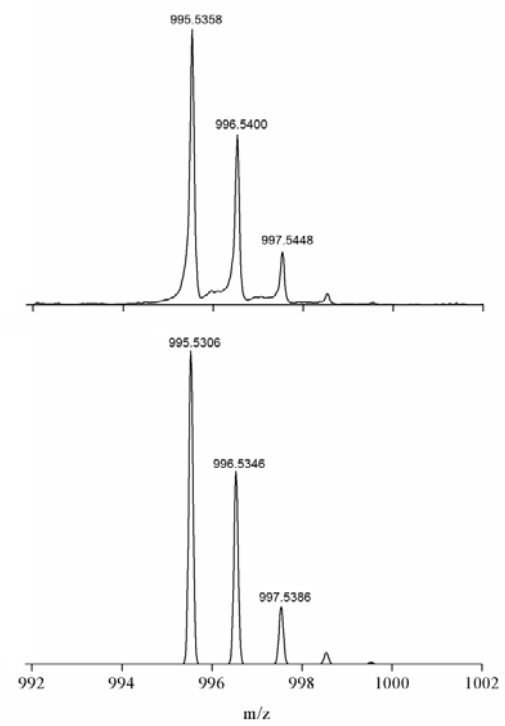


Figure S11. The observed (top) and calculated (bottom) isotopic patterns for the $[Na(\mathbf{2e})]^+$ ion with exact masses indicated.

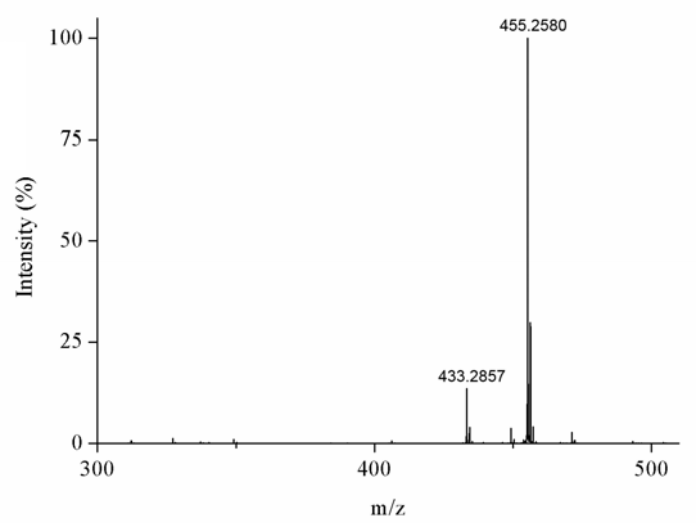


Figure S12. The mass spectrum of ligand **S2** in CH_2Cl_2. Assigned peaks (m/z): 455.2580 = $[Na(\mathbf{S2})]^+$ (calc. 455.2615), 433.2857 = $[H(\mathbf{S2})]^+$ (calc. 433.2823).

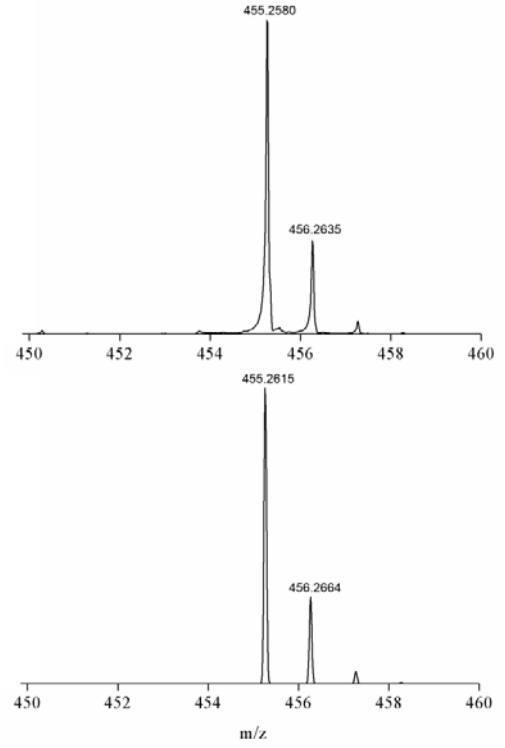


Figure S13. The observed (top) and calculated (bottom) isotopic patterns for the $[Na(\mathbf{S2})]^+$ ion with exact masses indicated.

3. Complex Mass Spectra

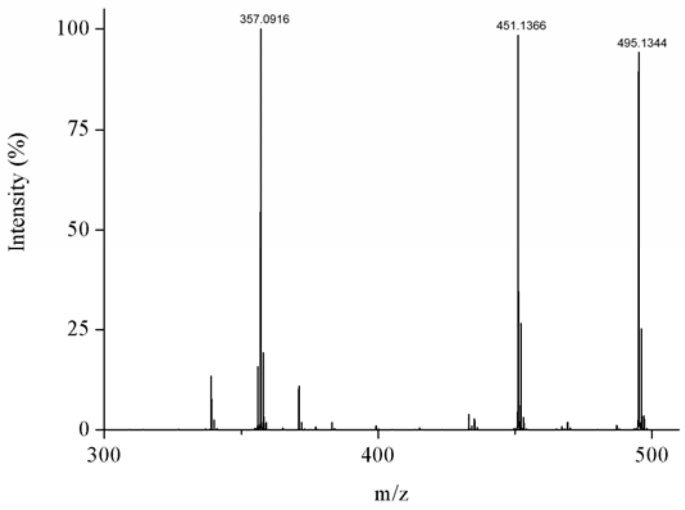


Figure S14. The mass spectrum of complex **3a** in CH_3CN. Assigned peaks (m/z): 495.1344 = $[Co(\mathbf{2a})CO_3]^+$ (calc 495.1298), 451.1366 = $[Co(\mathbf{2a})O]^+$ (calc 451.1400), 357.0916 = $[Co(\mathbf{4a})OH]^+$ (calc 357.0921).

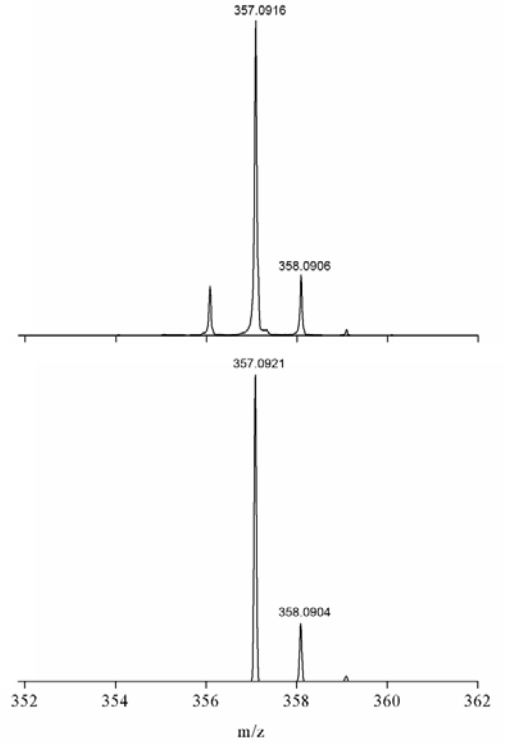


Figure S15. The observed (top) and calculated (bottom) isotopic patterns for the $[Co(\mathbf{4a})OH]^+$ ion with exact masses indicated.

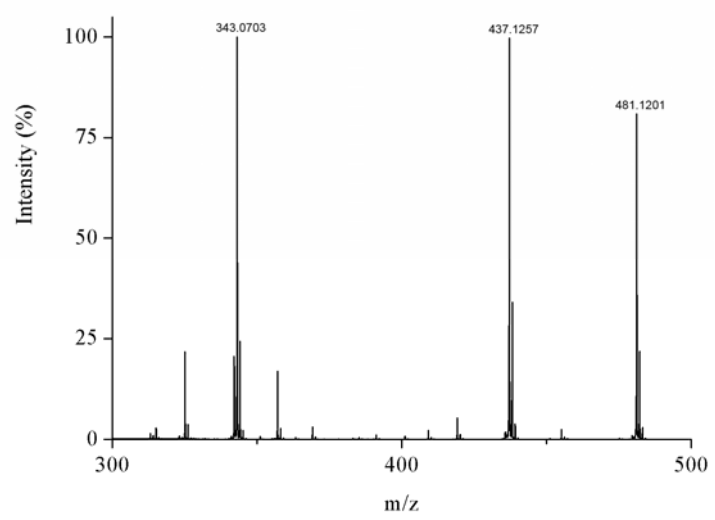


Figure S16. The mass spectrum of complex **3b** in CH_3CN. Assigned peaks (m/z): 481.1201 = $[Co(\mathbf{2b})CO_3]^+$ (calc 481.1141), 437.1257 = $[Co(\mathbf{2b})O]^+$ (calc 437.1224), 343.0703 = $[Co(\mathbf{4b})OH]^+$ (calc 343.0718).

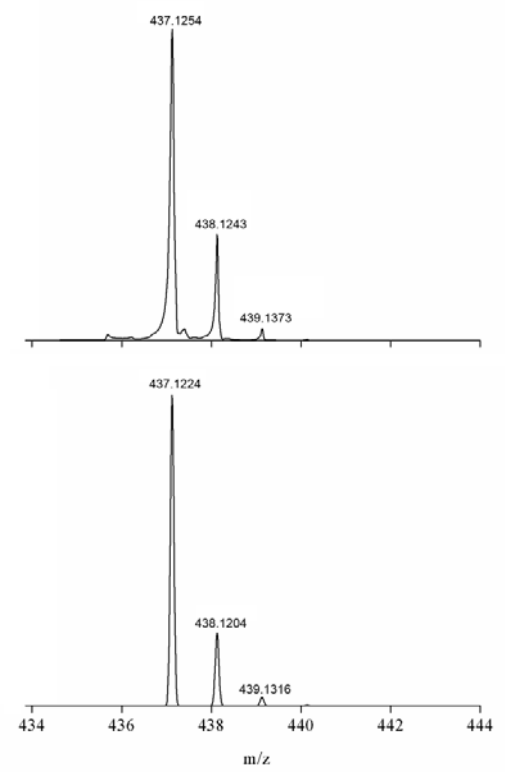


Figure S17. The observed (top) and calculated (bottom) isotopic patterns for the $[Co(\mathbf{2b})O]^+$ ion with exact masses indicated.

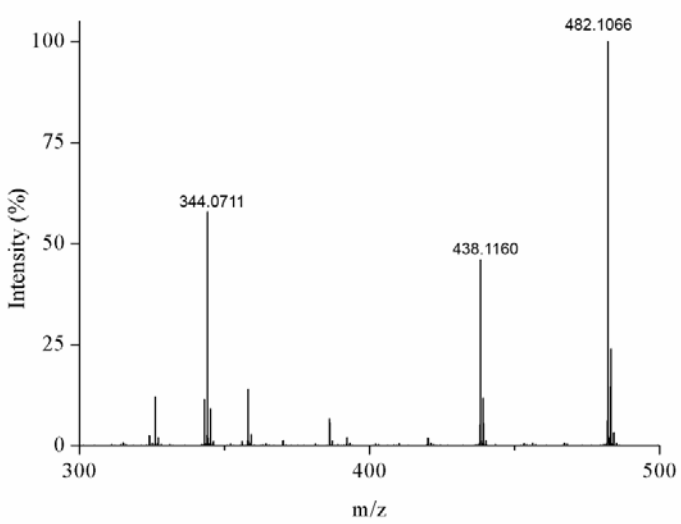


Figure S18. The mass spectrum of complex **3c** in CH_3CN. Assigned peaks (m/z): 482.1066 = $[Co(\mathbf{2c})CO_3]^+$ (calc 482.1016), 438.1160 = $[Co(\mathbf{2c})O]^+$ (calc 438.1201), 344.0711 = $[Co(\mathbf{4c})OH]^+$ (calc 344.0670).

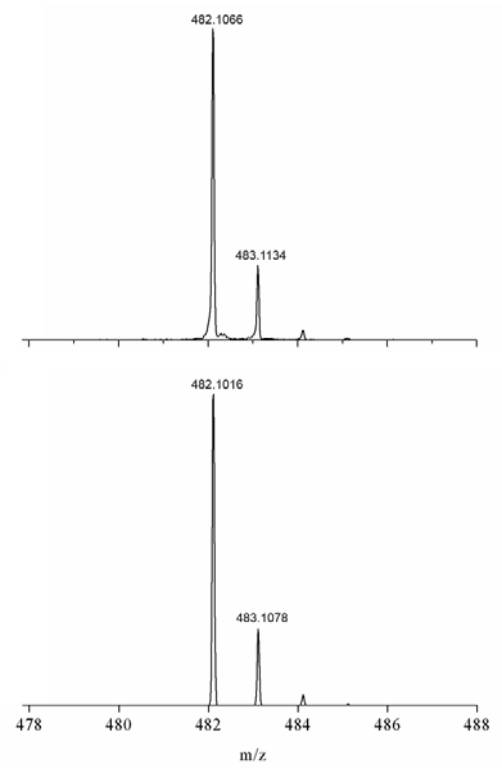


Figure S19. The observed (top) and calculated (bottom) isotopic patterns for the $[Co(\mathbf{2c})O_2CO]^+$ ion with exact masses indicated.

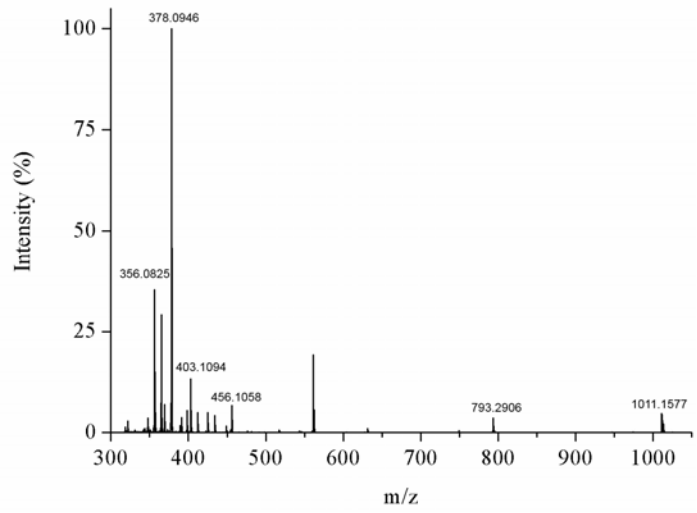


Figure S20. The mass spectrum of complex **3d** in CH_3CN. Assigned peaks (m/z): 1011.1577 = $[Co_2(\mathbf{2d})(CO_3)_2ClO_4]^+$ (calc 1011.1577), 793.2906 = $[Co(\mathbf{2d})CO_3]^+$ (calc 793.2952), 456.1058 = $[Co_2(\mathbf{2d})(CO_3)_2]^{2+}$ (calc 456.1063), 403.1094 = $[Co_2(\mathbf{2d})O - H_2]^{2+}$ (calc 403.1112), 378.0946 = $[Co(\mathbf{4d})CO_3]^+$ (calc 378.0796), 356.0825 = $[Co(\mathbf{4d})CO_3]^+$ (calc 356.0847).

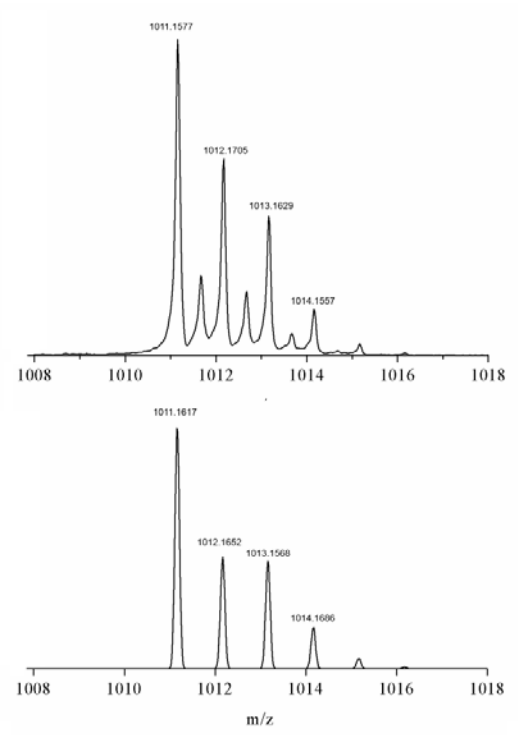


Figure S21. The observed (top) and calculated (bottom) isotopic patterns for the $[Co_2(\mathbf{2d})(CO_3)_2ClO_4]^+$ ion with exact masses indicated.

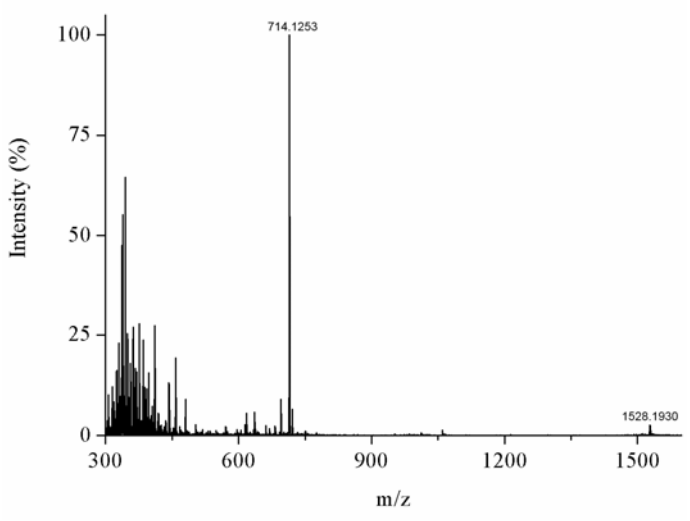


Figure S22. The mass spectrum of complex **3e** in CH_3CN. Assigned peaks (m/z): 1528.1930 = $[Co_3(\mathbf{2e})(O_2CO)_3(ClO_4)_2]^+$ (calc 1528.2014), 714.1253 = $[Co_3(\mathbf{2e})(CO_3)_3(ClO_4)]^{2+}$ (calc 714.1223).

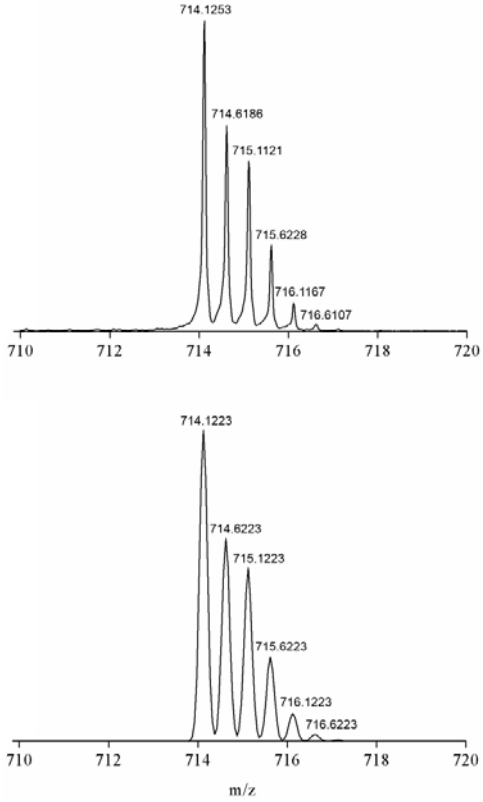


Figure S23. The observed (top) and calculated (bottom) isotopic patterns for the $[Co_3(\mathbf{2e})(O_2CO)_3(ClO_4)]^{2+}$ ion with exact masses indicated.

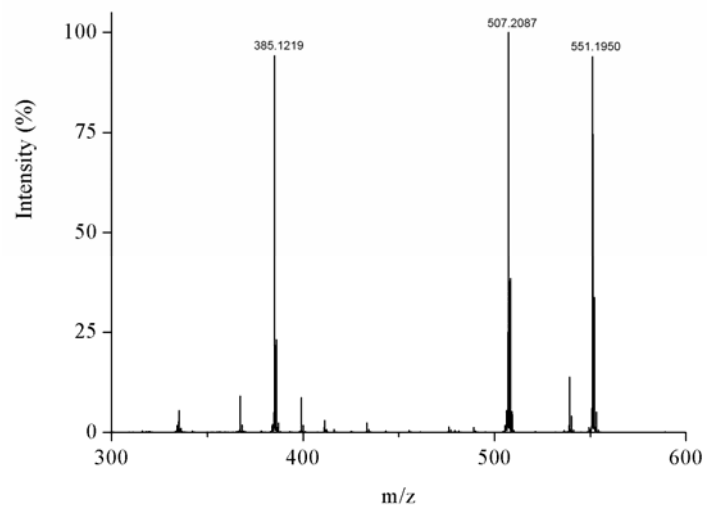


Figure S24. The mass spectrum of complex **S3** in CH_3CN. Assigned peaks (m/z): 551.1950 = $[Co(\mathbf{S2})(O_2CO)]^+$ (calc 551.1924), 507.2087 = $[Co(\mathbf{S2})(O)]^+$ (calc 507.2012), 385.1219 = $[Co(\mathbf{S4})(OH)]^+$ (calc 385.1182).

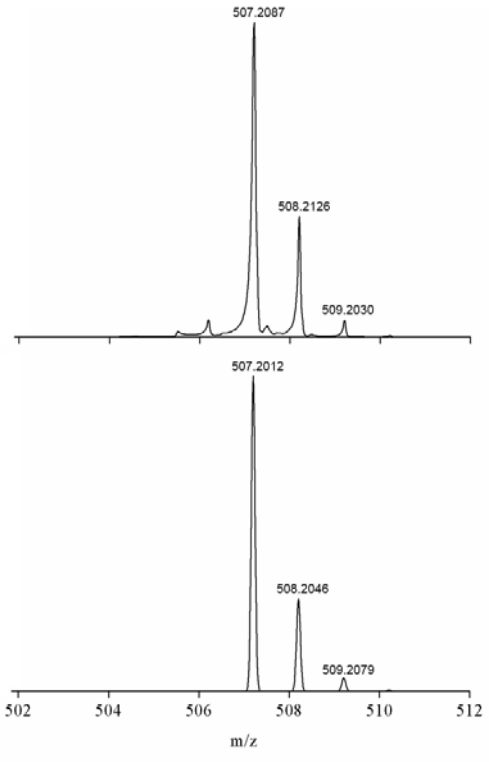


Figure S25. The observed (top) and calculated (bottom) isotopic patterns for the $[Co(\mathbf{S2})(O_2CO)]^+$ ion with exact masses indicated.

4. ^{1}H NMR Spectra

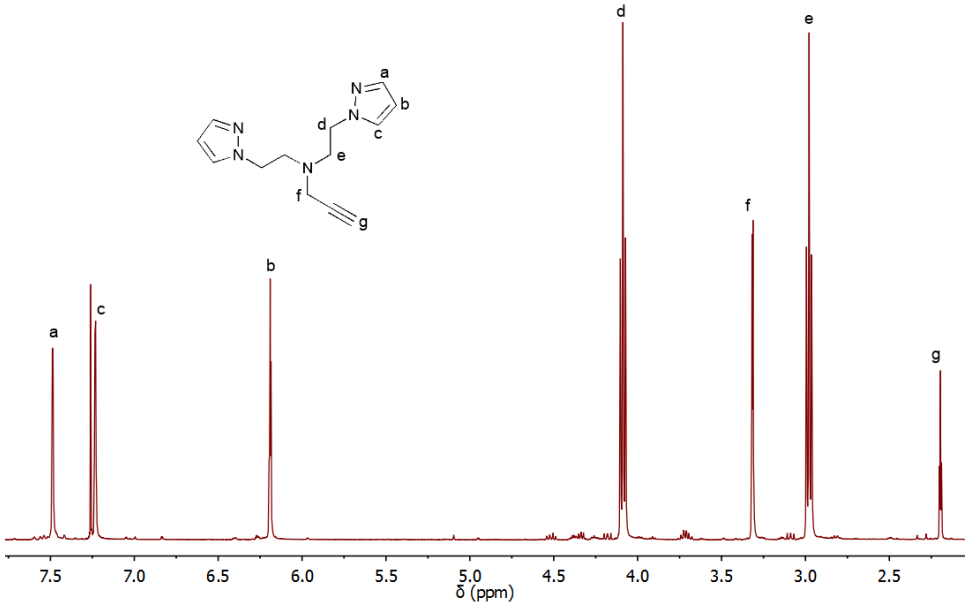


Figure S26. The ^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of compound **1** with peaks assigned.

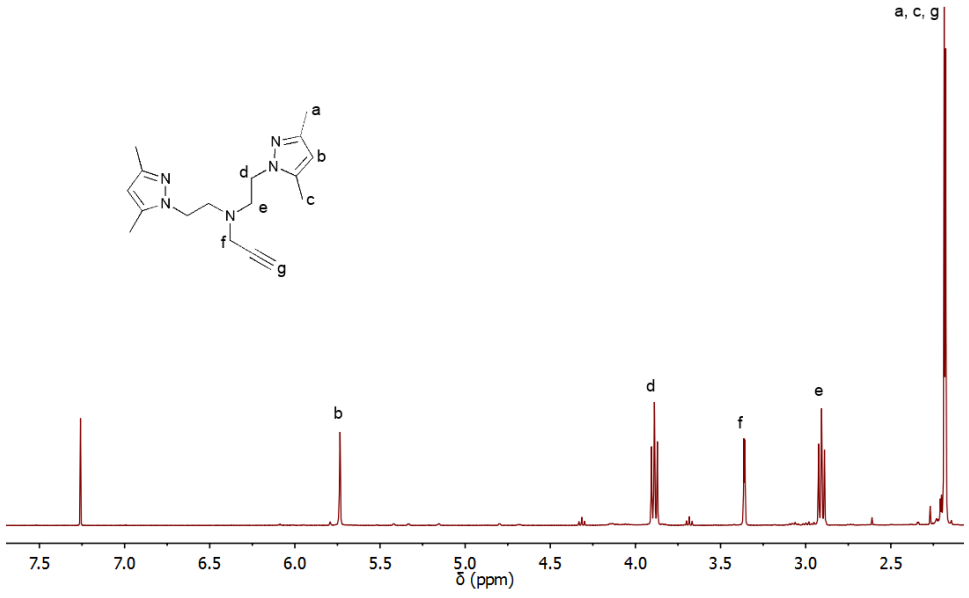


Figure S27. The ^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of compound **S1** with peaks assigned.

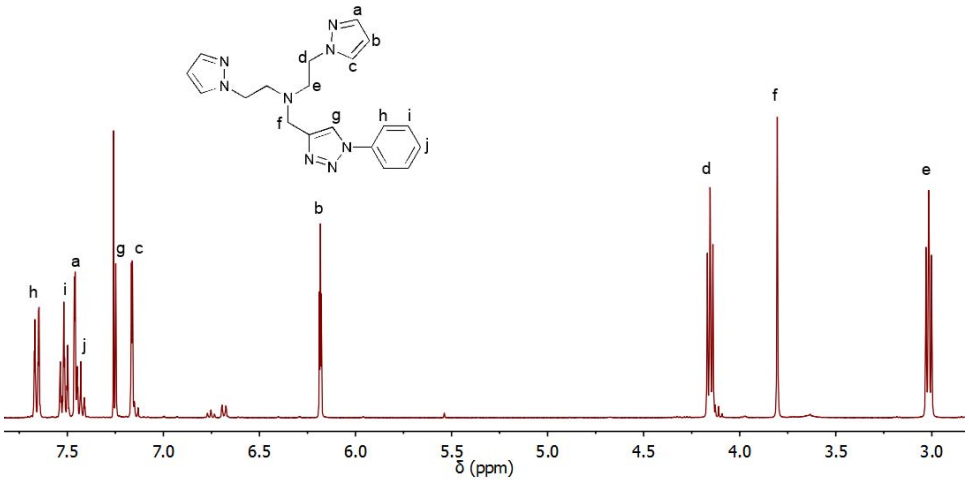


Figure S28. The ^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of ligand **2b** with peaks assigned.

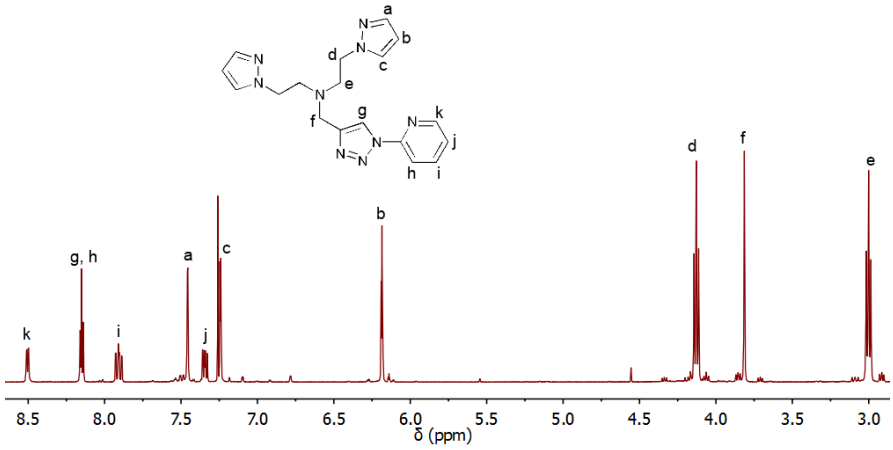


Figure S29. The ^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of ligand **2c** with peaks assigned.

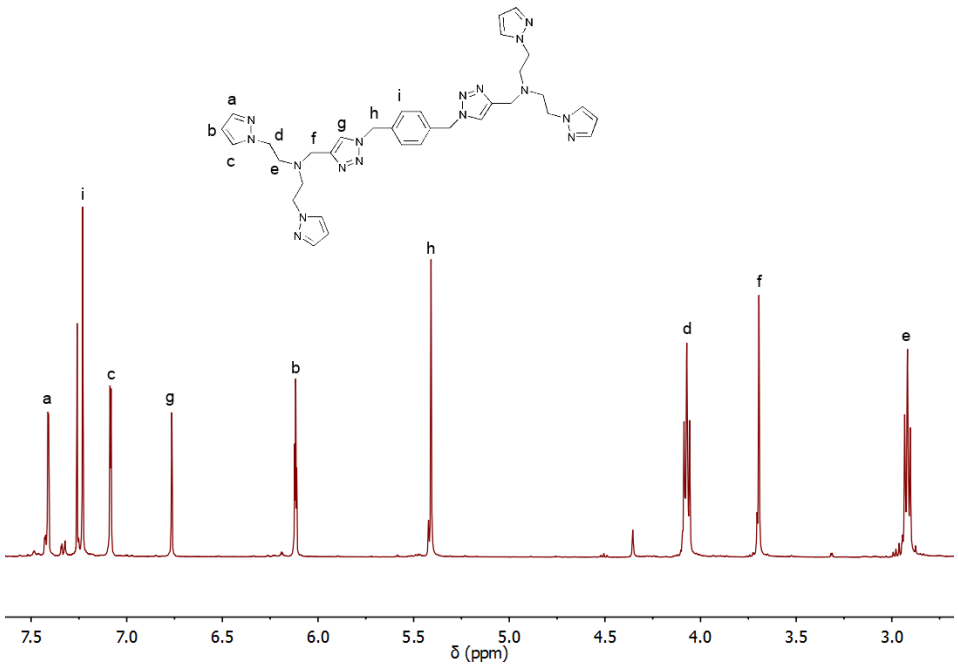


Figure S30. The ^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of ligand **2d** with peaks assigned.

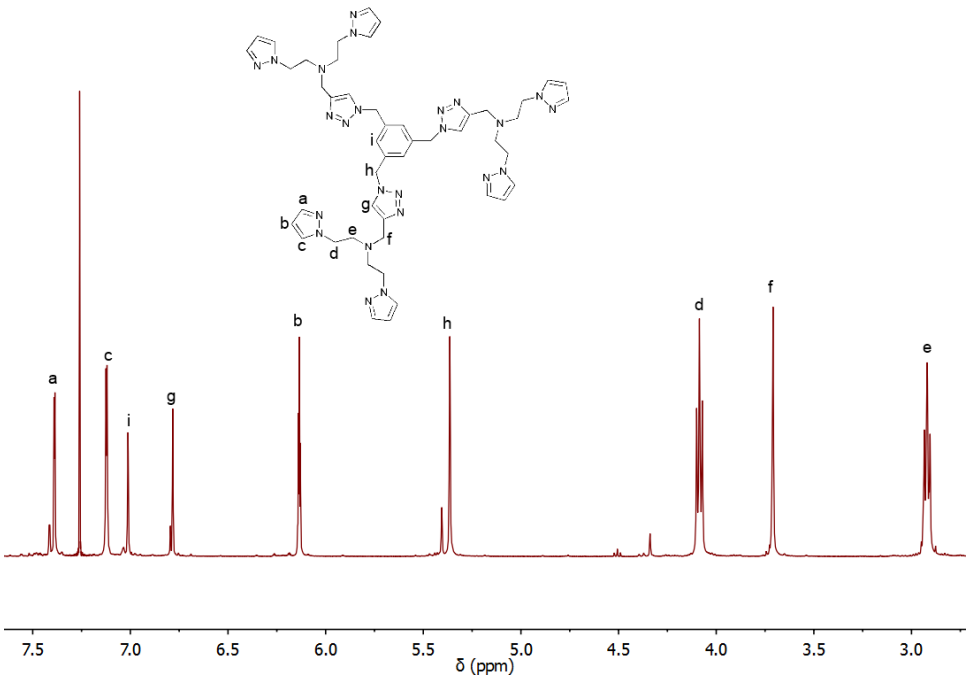


Figure S31. The ^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of ligand **2e** with peaks assigned.

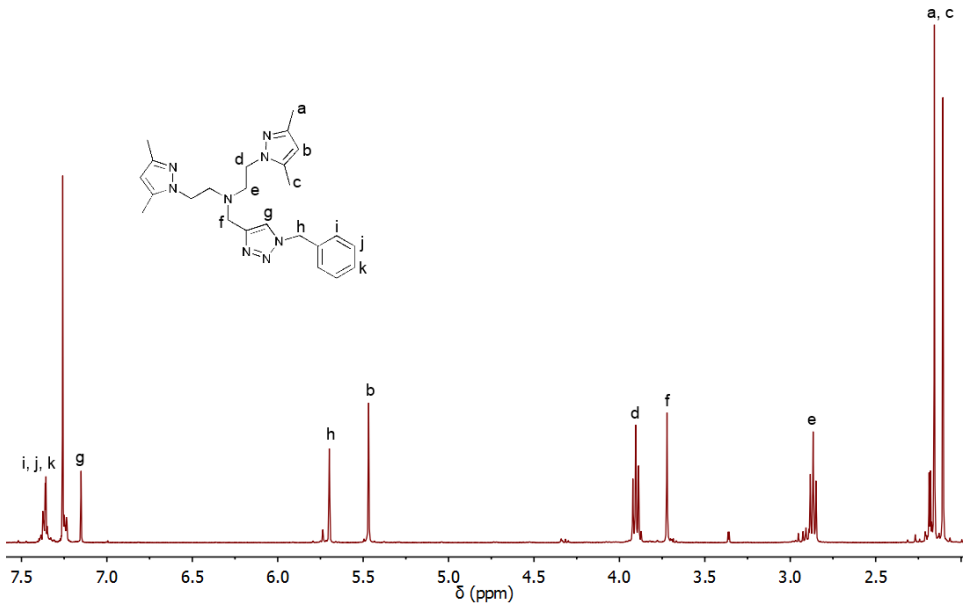


Figure S32. The ^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of complex **S2** with peaks assigned.

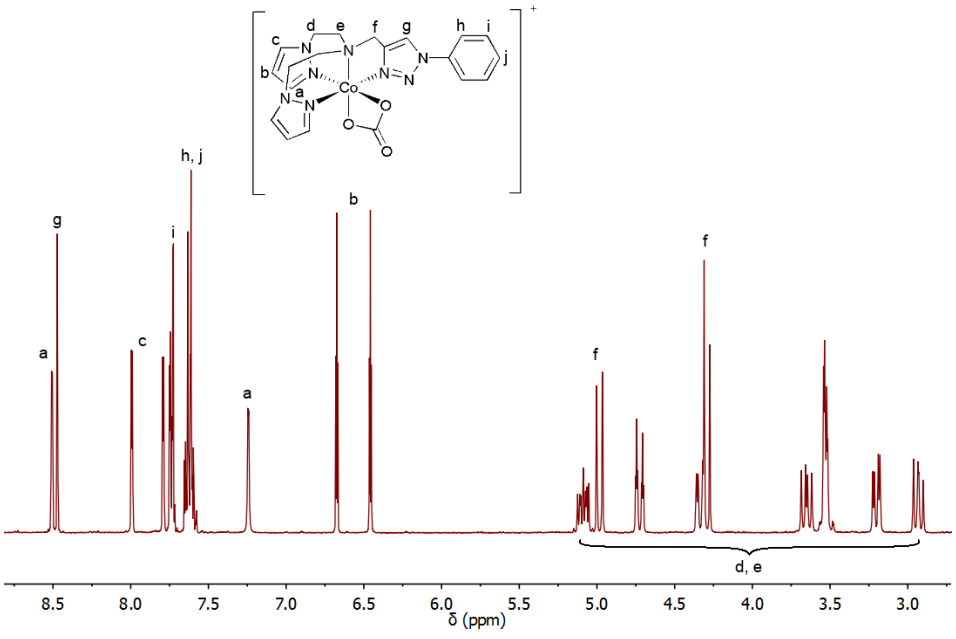


Figure S33. The ^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of complex **3b** with peaks assigned.

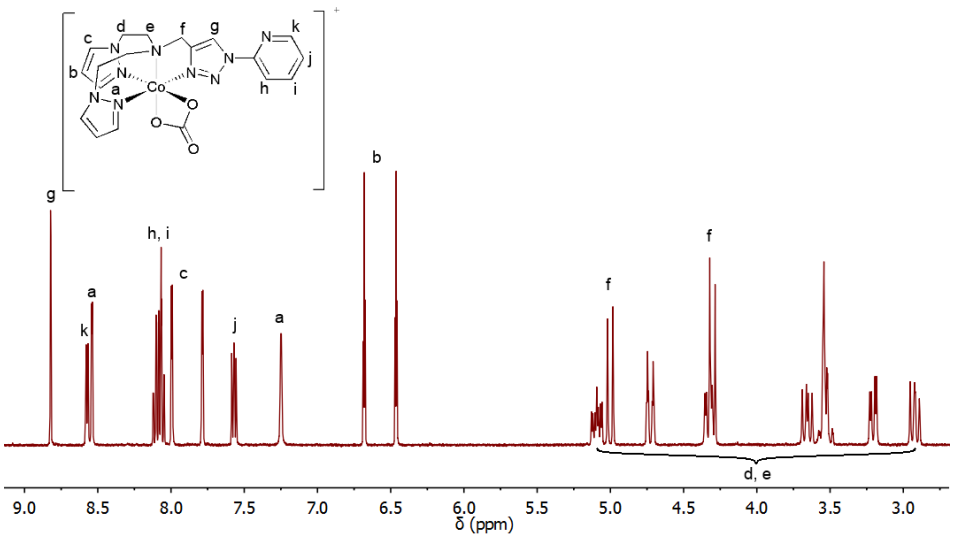


Figure S34. The ^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of complex **3c** with peaks assigned.

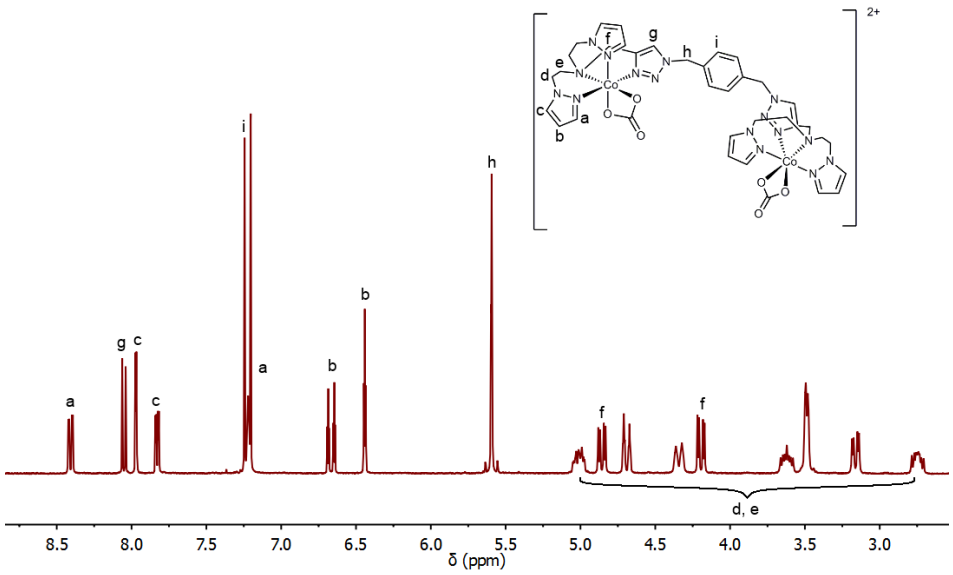


Figure S35. The ^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of complex **3d** with peaks assigned.

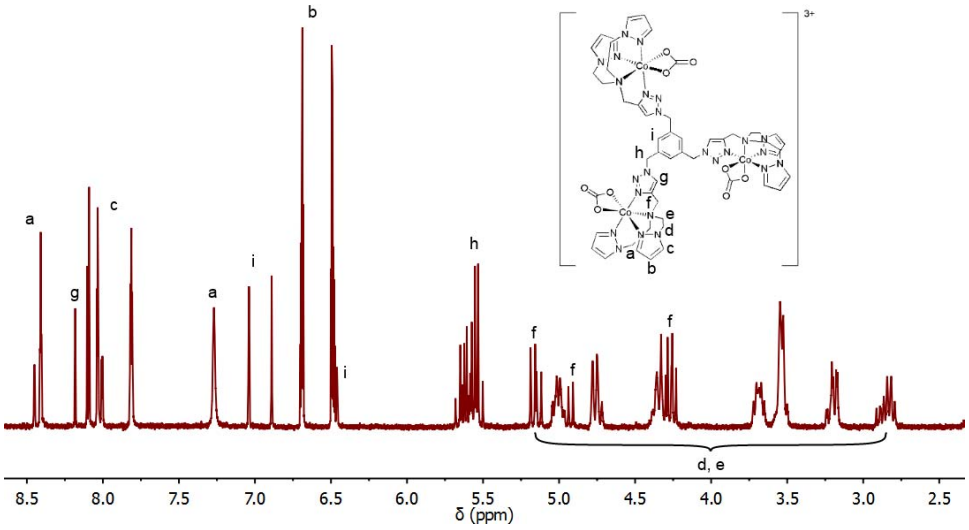


Figure S36. The ^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of complex **3e** with peaks assigned.

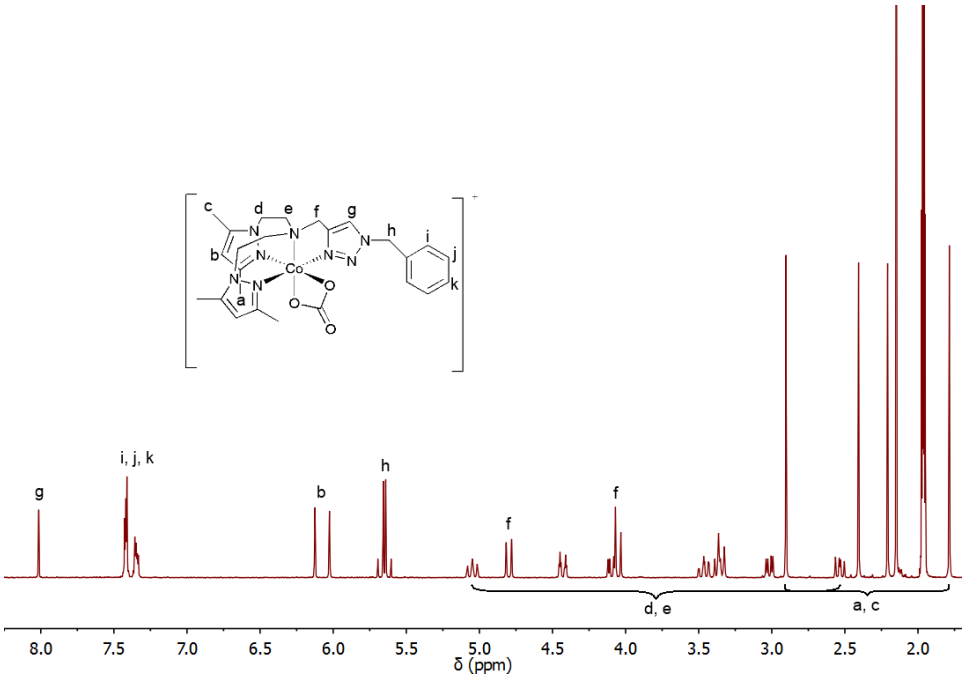


Figure S37. The ^{1}H NMR spectrum (400 MHz, 298 K, CD_3CN) of complex **S3** with peaks assigned.

5. Crystallographic Data

An ORTEP plot of the cation of complex **S3** is shown in Fig. S38, with selected bond lengths and angles provided in Tables S1 and S2. There is very little variation in bond lengths between complex **S3** and its non-methylated analogue **3a**, with the exception of the Co-O(1) bond length. This can be attributed to the increased steric crowding provided by the incorporation of the methylated pyrazole rings, a phenomenon which is reflected in an increase in some of the bond angles adjacent to the methylated pyrazole rings (especially N(6)-Co-O(1) and N(5)-Co-N(6)) and a corresponding decrease in bond angles remote from the methyl substituents (*e.g.* N(1)-Co-O(2)). We note that methyl substitution of pyrazole rings does not have any impact on CuAAC chemistry, although further steric bulk may impede coordination.

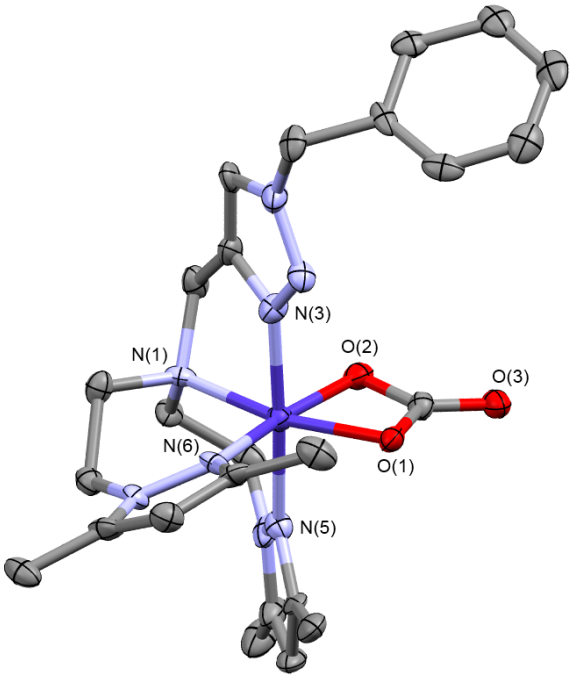


Figure S38. An ORTEP diagram of the solid state structure of complex **S3**. Ellipsoids are drawn at the 50% probability level and counter-anions and solvent molecules have been omitted for clarity. The Δ enantiomer is shown in each case.

Table S1. Selected bond lengths in the complex **S3**. Comparison to complex **3a** is provided.

Complex	Co-N(1)	Co-N(3)	Co-N(5)	Co-N(6)	Co-O(1)	Co-O(2)
3a	2.022(3)	1.919(3)	1.916(3)	1.925(3)	1.897(2)	1.890(2)
S3	2.012(6)	1.908(6)	1.929(7)	1.942(6)	1.918(5)	1.879(6)

Table S2. Selected bond angles in the complex **S3**. Comparison to complex **3a** is provided.

Complex	O(2)-Co(1)-O(1)	O(2)-Co(1)-N(5)	O(2)-Co(1)-N(3)	O(2)-Co(1)-N(1)	O(1)-Co(1)-N(5)	O(1)-Co(1)-N(3)
3a	69.59(9)	89.46(10)	87.16(10)	97.73(10)	90.64(10)	92.56(9)
S3	69.2(2)	90.8(3)	88.2(3)	93.0(2)	89.8(3)	94.3(2)

Complex	O(1)-Co(1)-N(6)	N(5)-Co(1)-N(6)	N(3)-Co(1)-N(6)	N(5)-Co(1)-N(1)	N(3)-Co(1)-N(1)	N(6)-Co(1)-N(1)
3a	96.00(10)	88.70(11)	95.74(11)	93.51(11)	82.32(10)	96.78(10)
S3	100.6(3)	91.8(3),	90.1(3)	92.5(3)	82.7(3)	97.1(3)

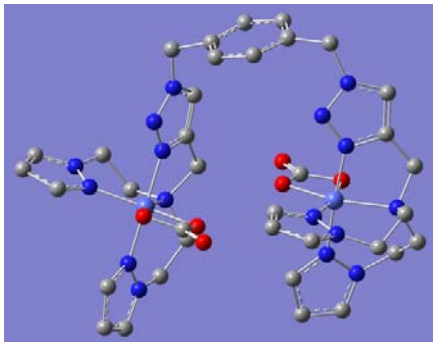
Complex	O(2)-Co(1)-N(6)	O(1)-Co(1)-N(1)	N(5)-Co(1)-N(3)
3a	165.45(10)	166.65(10)	174.22(11)
S3	169.4(3)	162.0(2)	175.0(3)

S3: Formula $C_{25}H_{36}ClCoN_8O_9$, M 687.00, orthorhombic, space group $P2_12_12_1$, Flack parameter 0.02(3), a 12.9002(10) Å, b 13.5454(10) Å, c 16.9813(12) Å, α 90°, β 90°, γ 90°, V 2967.3(4) Å^3, Z 4, crystal size 0.18 × 0.10 × 0.07 mm, colour red, collection temperature 93(2) K, $\lambda(Mo_{k\alpha})$ 0.71073 Å, $\mu(Mo_{k\alpha})$ 0.734 mm^{-1}, $T_{min,max}$ 0.8792, 0.9504, $2\theta_{max}$ 51.44, N 9704, N_{ind} 4794, N_{obs} 4794, R_{int} 0.0832, R_1 ($I > 2\sigma(I)$) 0.0792, $wR(F^2)$ ($I > 2\sigma(I)$) 0.1537, R_1 (all data) 0.1082, $wR(F^2)$ (all data) 0.1708, GooF (all) 1.058.

6. Density Functional Theory (DFT) Calculations

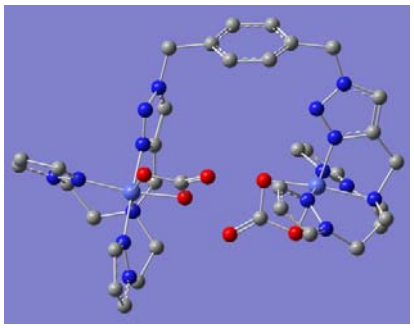
Calculations were conducted on the isomers using a B3LYP functional[2] with 6-31G(d) basis set on all atoms except Co for which a LANL2DZ effective core potential[3] was used. The calculations were implemented using Gaussian 09. [4]

Calculated structure of the *cis*, *cis*-isomer of **3d**



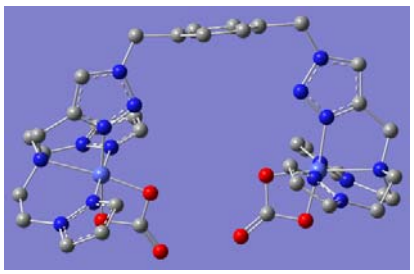
E(B3LYP) = -3013.43673841 hartrees 0 kJ mol^{-1}

Calculated structure of the *trans*, *cis*-isomer of **3d**



E(B3LYP) = -3013.42928201 hartrees +19.6 kJ mol^{-1} relative to the *cis*, *cis*-isomer

Calculated structure of the *trans*, *trans*-isomer of **3d**



E(B3LYP) = -3013. 41533523 hartrees +56.2 kJ mol^{-1} relative to the *cis*, *cis*-isomer

Cartesian coordinates for calculated structures

6,6 isomer

Symbol	X	Y	Z
H	-3.30049	-1.90672	-3.26541
C	-3.3656	-1.86961	-2.16897
H	-2.37948	-2.06512	-1.74292
C	-4.34769	-2.95002	-1.73059
H	-5.34691	-2.79843	-2.15279
N	-3.71651	-0.45515	-1.75182
C	-5.10655	-0.07772	-2.19553
H	-5.78982	-0.86909	-1.88572
H	-5.12448	-0.02216	-3.29316
C	-5.64	1.240986	-1.63108
H	-6.56579	1.483895	-2.15987
H	-4.94019	2.065794	-1.79669
N	-5.97923	1.155129	-0.20922
C	-5.65518	0.784446	1.919918
N	-5.1307	0.563868	0.699972
C	-7.03117	1.738975	0.445675
C	-6.85506	1.516187	1.803891
H	-7.80961	2.257177	-0.09074
H	-7.50361	1.833909	2.602648
H	-5.14203	0.428765	2.797737
C	-2.64868	0.457849	-2.35813
H	-1.70336	-0.0937	-2.41589
H	-2.94271	0.757035	-3.37075
C	-2.42824	1.610646	-1.44845
N	-2.45408	2.47303	0.612022
C	-1.97107	2.907895	-1.55866
N	-2.00798	3.403777	-0.27984
N	-2.69811	1.392746	-0.1246
H	-1.62077	3.476113	-2.40154
Co	-3.44596	-0.33717	0.274859
O	-2.67594	-0.38205	2.027502
H	6.981821	-1.76653	0.233832
C	6.000395	-1.36769	0.524758
H	6.145172	-0.34526	0.879492
C	5.429599	-2.21596	1.663182
H	6.22299	-2.40038	2.392382
H	5.080985	-3.1913	1.304289
N	5.119316	-1.31385	-0.70787
C	5.258142	-2.60862	-1.48711

H	5.504628	-3.4031	-0.77952
H	6.105974	-2.51095	-2.17755
C	4.008687	-3.01943	-2.27019
H	4.256174	-3.87288	-2.9064
H	3.631302	-2.20258	-2.89106
N	2.934916	-3.44499	-1.37211
N	4.345347	-1.54688	2.374227
C	2.868402	-0.8989	3.905285
N	3.278639	-1.005	1.691613
C	4.107812	-1.49422	3.722487
C	2.380636	-0.60765	2.613426
H	4.819292	-1.88321	4.433054
H	1.434664	-0.19302	2.306492
H	2.371396	-0.70765	4.840893
C	5.553956	-0.13617	-1.57927
H	6.642214	-0.14689	-1.71407
H	5.06888	-0.26114	-2.55122
C	5.055501	1.110558	-0.92627
N	3.511152	2.090237	0.351223
C	5.381149	2.454324	-0.87066
N	4.40548	3.02036	-0.08427
N	3.918541	0.951681	-0.17717
H	6.179433	3.024269	-1.31388
Co	3.141438	-0.79758	-0.2367
O	1.367719	-0.10651	-0.26258
C	1.367763	-0.02625	-1.62066
O	0.431481	0.332998	-2.34744
C	-1.59049	4.74717	0.19827
H	-2.05962	4.868631	1.175551
H	-2.021	5.480553	-0.48888
C	-0.08329	4.862547	0.277053
C	2.722265	4.754455	0.338779
C	0.664034	5.229648	-0.85298
C	0.583901	4.525877	1.463822
C	1.977707	4.480966	1.495898
C	2.059087	5.168021	-0.82578
H	0.161326	5.545996	-1.76254
H	0.015197	4.264652	2.350308
H	2.483264	4.180602	2.407416
H	2.625552	5.416736	-1.71819
C	4.202902	4.449356	0.309104
H	4.671021	4.598166	1.286273
H	4.736109	5.050714	-0.43053

N	-4.2221	-2.09809	0.626822
O	-1.73947	-1.15451	0.194873
C	-1.56026	-1.01052	1.542615
O	-0.58443	-1.40502	2.194678
H	-3.97734	-3.89876	-2.13139
N	-4.45295	-3.11327	-0.27798
C	-4.86418	-4.23981	0.379415
H	-5.10614	-5.14306	-0.15722
C	-4.89012	-3.95327	1.735856
H	-5.15671	-4.62117	2.537211
C	-4.47611	-2.61328	1.849298
H	-4.29991	-2.01756	2.727388
O	2.61165	-0.4302	-2.0435
N	2.449524	-2.57728	-0.4195
C	2.206612	-4.60029	-1.35741
H	2.429182	-5.41244	-2.03041
C	1.231484	-4.46683	-0.37556
H	0.493095	-5.19825	-0.0943
C	1.40738	-3.18423	0.185432
H	0.833222	-2.67239	0.947373

5,6 isomer

Symbol	X	Y	Z
H	2.003558	-2.82068	2.001767
C	2.556761	-2.42356	1.143254
H	1.834921	-2.21112	0.353968
C	3.54831	-3.48366	0.686216
H	4.263375	-3.74933	1.472483
N	3.16485	-1.08044	1.521782
C	4.296325	-1.23842	2.504177
H	5.01025	-1.95205	2.091652
H	3.897117	-1.65418	3.439819
C	5.052738	0.053952	2.818341
H	5.691629	-0.12355	3.687604
H	4.370159	0.872208	3.073076
N	5.931168	0.465856	1.723304
C	6.476176	0.995781	-0.32545
N	5.504078	0.431104	0.416015
C	7.168621	1.04785	1.795747
C	7.544546	1.392659	0.50502
H	7.678838	1.169681	2.737581
H	8.464362	1.863067	0.201316

H	6.344818	1.102512	-1.38941
C	2.032214	-0.23056	2.107912
H	1.081735	-0.69565	1.822229
H	2.083189	-0.26053	3.202837
C	2.117583	1.158281	1.57226
N	2.878779	2.611581	0.053307
C	1.500844	2.368732	1.833384
N	1.993832	3.230074	0.884533
N	2.933074	1.359469	0.490403
H	0.771053	2.662405	2.566739
Co	3.768598	-0.20493	-0.22636
O	3.887224	0.562719	-1.96717
H	-5.91589	-2.73839	-2.18594
C	-5.01299	-2.15312	-1.96801
H	-4.96731	-1.32068	-2.67455
C	-3.76648	-3.01976	-2.15628
H	-3.87627	-3.61399	-3.06664
H	-3.60115	-3.70354	-1.31826
N	-5.15758	-1.5643	-0.57598
C	-5.63681	-2.65494	0.364194
H	-4.78184	-3.31528	0.524002
H	-6.44045	-3.22319	-0.12308
C	-6.18357	-2.19524	1.711978
H	-6.37257	-3.09816	2.301347
H	-7.14581	-1.68228	1.597835
N	-5.2819	-1.33922	2.489559
C	-3.73876	0.144333	2.930242
N	-4.23812	-0.62396	1.937691
C	-5.43204	-1.00594	3.806045
C	-4.46378	-0.06211	4.117564
H	-6.2052	-1.45106	4.411744
H	-4.29673	0.402808	5.074261
H	-2.87227	0.752877	2.742402
N	-2.59708	-2.17033	-2.32578
C	-0.73885	-1.15133	-3.00592
N	-2.34045	-1.17521	-1.41174
C	-1.63875	-2.1667	-3.30202
C	-1.20661	-0.56152	-1.8163
H	-1.66895	-2.8733	-4.11567
H	-0.77536	0.231208	-1.23267
H	0.154981	-0.85659	-3.53417
C	-6.07927	-0.35204	-0.66872
H	-6.83566	-0.50483	-1.44628

H	-6.60414	-0.23423	0.280568
C	-5.23088	0.856757	-0.91531
N	-3.28899	1.920813	-0.64907
C	-5.38671	2.118084	-1.46713
N	-4.17567	2.740256	-1.27994
N	-3.94828	0.795466	-0.43615
H	-6.22128	2.597155	-1.95021
Co	-3.35084	-0.92358	0.215594
O	-1.68434	-0.57496	1.072709
O	-2.61871	-2.5565	0.875062
C	-1.50533	-1.90871	1.3306
O	-0.50459	-2.40509	1.864367
C	1.58022	4.622329	0.582798
H	2.356848	5.017759	-0.07486
H	1.593166	5.188397	1.517082
C	0.20979	4.641294	-0.0679
C	-2.36217	4.418264	-1.17884
C	-0.9079	5.109711	0.637241
C	0.042193	4.12601	-1.36487
C	-1.23491	4.018135	-1.91508
C	-2.18762	4.999694	0.084317
H	-0.78555	5.549264	1.622849
H	0.902264	3.781598	-1.93109
H	-1.35475	3.591395	-2.90605
H	-3.04842	5.342389	0.6507
C	-3.74989	4.118396	-1.69527
H	-3.79041	4.150129	-2.78801
H	-4.49184	4.814341	-1.29457
N	4.532501	-1.84985	-0.94776
O	2.151778	-0.53713	-1.17556
C	2.622198	0.145025	-2.27438
O	2.004246	0.342325	-3.32474
H	2.96574	-4.38457	0.470213
N	4.28084	-3.14306	-0.53811
C	4.874271	-4.02691	-1.39505
H	4.799346	-5.09105	-1.23929
C	5.514729	-3.29519	-2.38402
H	6.068836	-3.68005	-3.22313
C	5.271637	-1.94475	-2.07493
H	5.539132	-1.05482	-2.61626

5,5 isomer

Symbol	X	Y	Z
H	-6.42037	-1.73122	-2.72952
C	-5.41464	-1.49395	-2.35755
H	-4.93728	-0.81599	-3.06947
C	-4.58061	-2.77398	-2.2631
H	-4.76099	-3.38253	-3.15268
H	-4.82983	-3.37241	-1.38213
N	-5.56218	-0.74758	-1.04507
C	-6.52067	-1.51619	-0.15365
H	-5.97847	-2.4028	0.179252
H	-7.393	-1.82556	-0.74537
C	-7.05765	-0.77193	1.065312
H	-7.62384	-1.50123	1.653611
H	-7.76148	0.018048	0.77724
N	-6.03428	-0.19535	1.942835
C	-4.14273	0.692893	2.583782
N	-4.73936	0.0689	1.544036
C	-6.23803	0.273079	3.209778
C	-5.05201	0.846289	3.645785
H	-7.1933	0.16783	3.698747
H	-4.86343	1.293322	4.606955
H	-3.09588	0.934315	2.526458
N	-3.16217	-2.44593	-2.23872
C	-0.95992	-2.34137	-2.53915
N	-2.70422	-1.44857	-1.40935
C	-2.12105	-2.99751	-2.92948
C	-1.36502	-1.3845	-1.59016
H	-2.27794	-3.80029	-3.63164
H	-0.76573	-0.69136	-1.0276
H	0.055773	-2.54639	-2.84372
C	-5.99486	0.67908	-1.34589
H	-6.565	0.71356	-2.28125
H	-6.65973	1.023853	-0.55238
C	-4.78342	1.558079	-1.38666
N	-2.6758	1.999925	-0.8005
C	-4.51171	2.844867	-1.81615
N	-3.21518	3.082444	-1.43197
N	-3.64584	1.097016	-0.77478
H	-5.1118	3.576043	-2.33049
Co	-3.78002	-0.68418	0.003731
O	-2.26698	-0.89847	1.145985
O	-3.85921	-2.38267	0.831101
C	-2.6964	-2.14889	1.525041

O	-2.15091	-2.89738	2.334918
H	6.419932	-1.72376	2.733671
C	5.4144	-1.48731	2.360639
H	4.936586	-0.80799	3.070953
C	4.580398	-2.76746	2.268089
H	4.760195	-3.37443	3.158872
H	4.829936	-3.36745	1.388288
N	5.562702	-0.74354	1.046752
C	6.522506	-1.51359	0.157937
H	5.980866	-2.40101	-0.17387
H	7.394149	-1.82169	0.751309
C	7.060768	-0.77148	-1.06169
H	7.629083	-1.50132	-1.64727
H	7.762944	0.020167	-0.77416
N	6.038033	-0.19863	-1.94232
C	4.146203	0.685142	-2.58863
N	4.742191	0.065173	-1.54611
C	6.242907	0.266074	-3.21047
C	5.056762	0.836414	-3.64985
H	7.198953	0.160457	-3.69783
H	4.8689	1.280209	-4.61266
H	3.098967	0.925361	-2.53346
N	3.162095	-2.43908	2.242281
C	0.959758	-2.33308	2.541341
N	2.705127	-1.44275	1.411119
C	2.120382	-2.98919	2.933229
C	1.365807	-1.37785	1.59108
H	2.276548	-3.79091	3.636762
H	0.767106	-0.68534	1.027115
H	-0.05613	-2.53711	2.84601
C	5.993724	0.684064	1.345045
H	6.564491	0.72094	2.27993
H	6.657429	1.028474	0.550395
C	4.781115	1.561601	1.384968
N	2.674044	2.00163	0.795397
C	4.507654	2.848214	1.813841
N	3.211476	3.084621	1.427773
N	3.644778	1.09944	0.77147
H	5.106289	3.579906	2.329148
Co	3.781999	-0.68279	-0.00407
O	2.268993	-0.89891	-1.14602
O	3.857752	-2.38521	-0.82408
C	2.696056	-2.15179	-1.51975

O	2.149548	-2.90236	-2.32702
C	-2.42465	4.33046	-1.63468
H	-3.10097	5.158176	-1.39643
H	-2.16844	4.392661	-2.69612
C	-1.17481	4.376699	-0.78315
C	1.17025	4.377235	0.777022
C	0.086989	4.392326	-1.3956
C	-1.25415	4.411142	0.61687
C	-0.09161	4.394539	1.389482
C	1.24959	4.409467	-0.62298
H	0.163845	4.385388	-2.47834
H	-2.22142	4.422061	1.109083
H	-0.16836	4.389375	2.472241
H	2.216801	4.418986	-1.11531
C	2.420049	4.332315	1.628712
H	2.163714	4.39575	2.690052
H	3.095833	5.160217	1.389524

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