Electronic Supporting Information

Consecutive Introduction of Ag(I) to an Anionic Homoleptic Co(III) complex: Variable Ag(I) Coordination Mode

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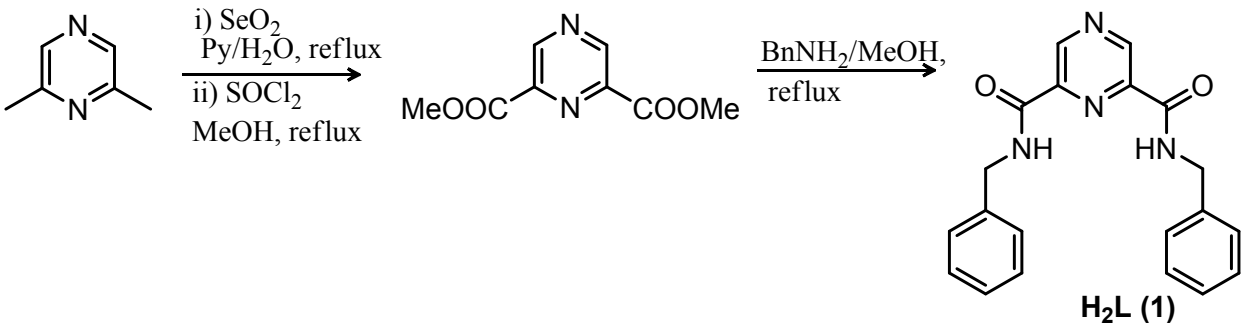
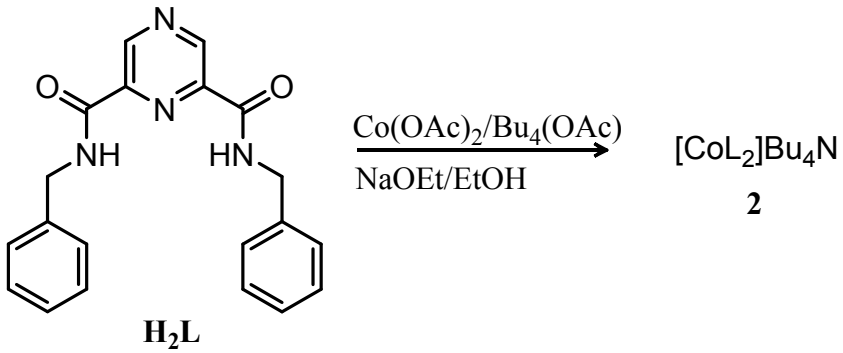
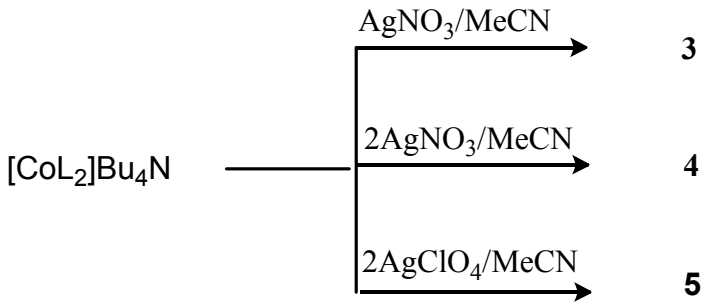


Scheme **S1**. Synthesis of ligand $\mathbf{H_2L}$

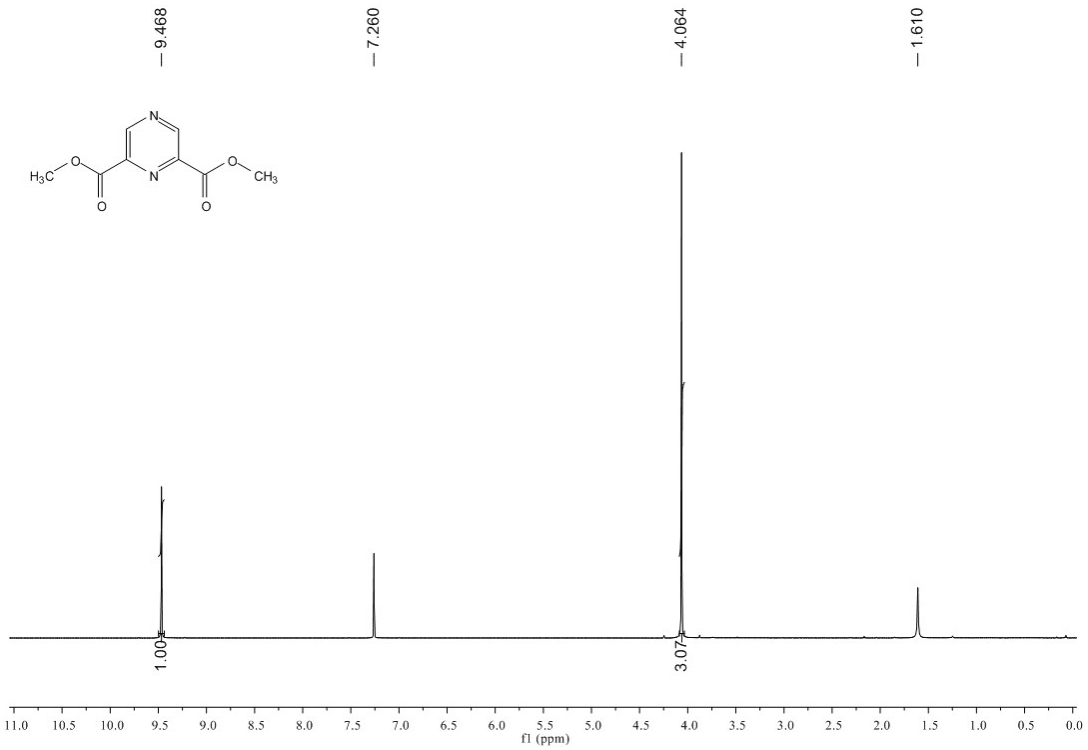


Scheme **S2**. Synthesis of Co(III) complex



Scheme **S3**. Synthesis of heterobimetallic Co(III), Ag(I) complexes

Fig. S1 ^{1}H NMR & ^{13}C NMR of Dimethyl pyrazine-2,6-dicarboxylate



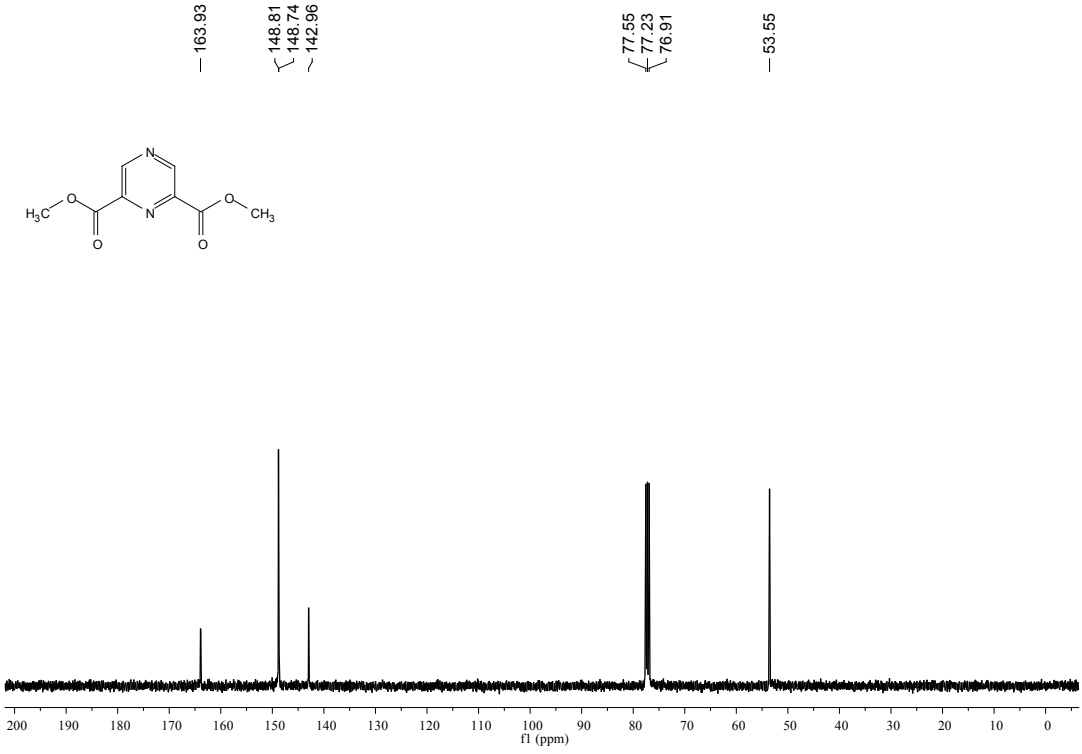
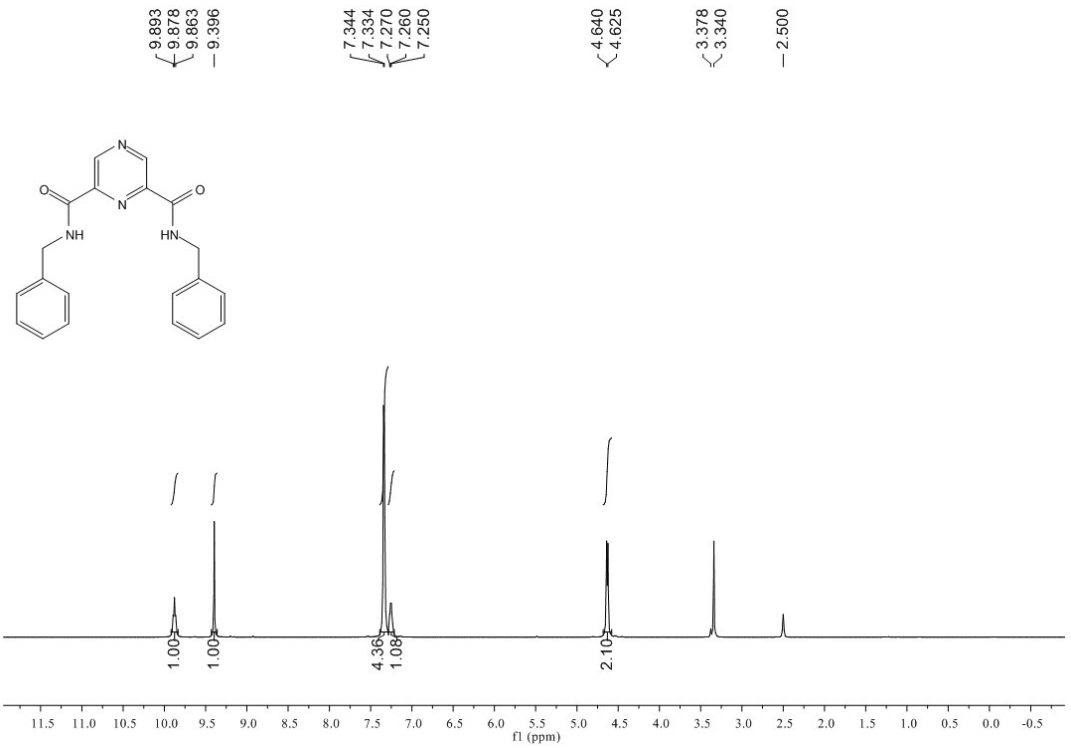


Fig. S2 ^{1}H NMR & ^{13}C NMR of Compound $\mathbf{H_2L}$



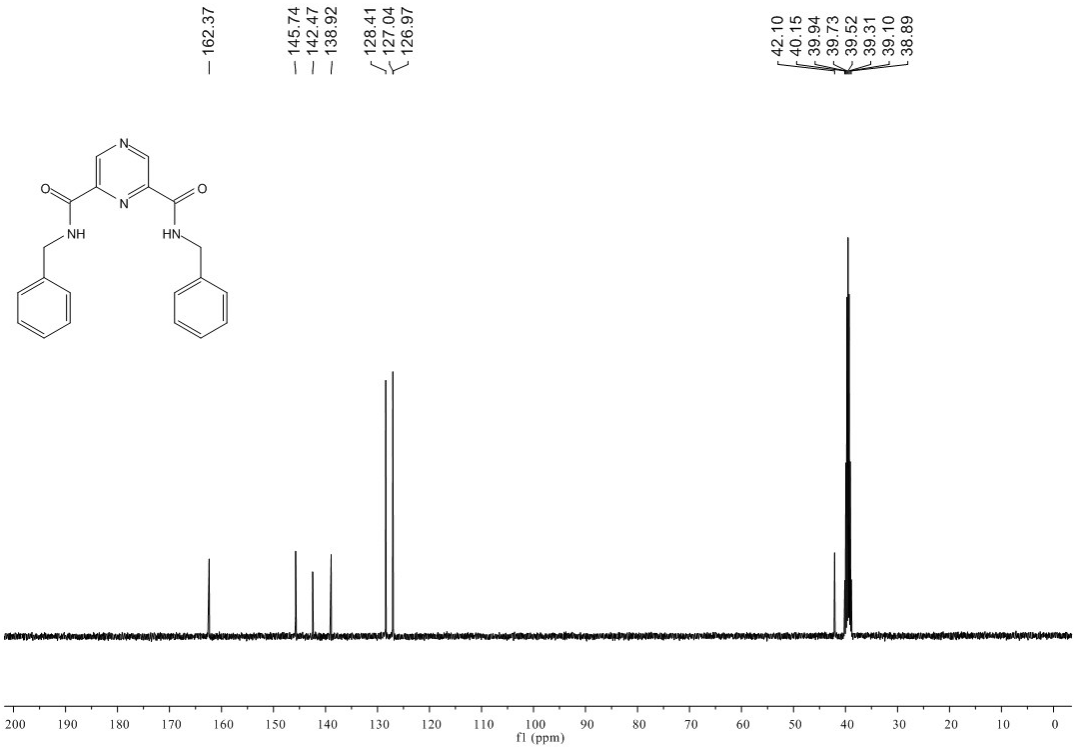
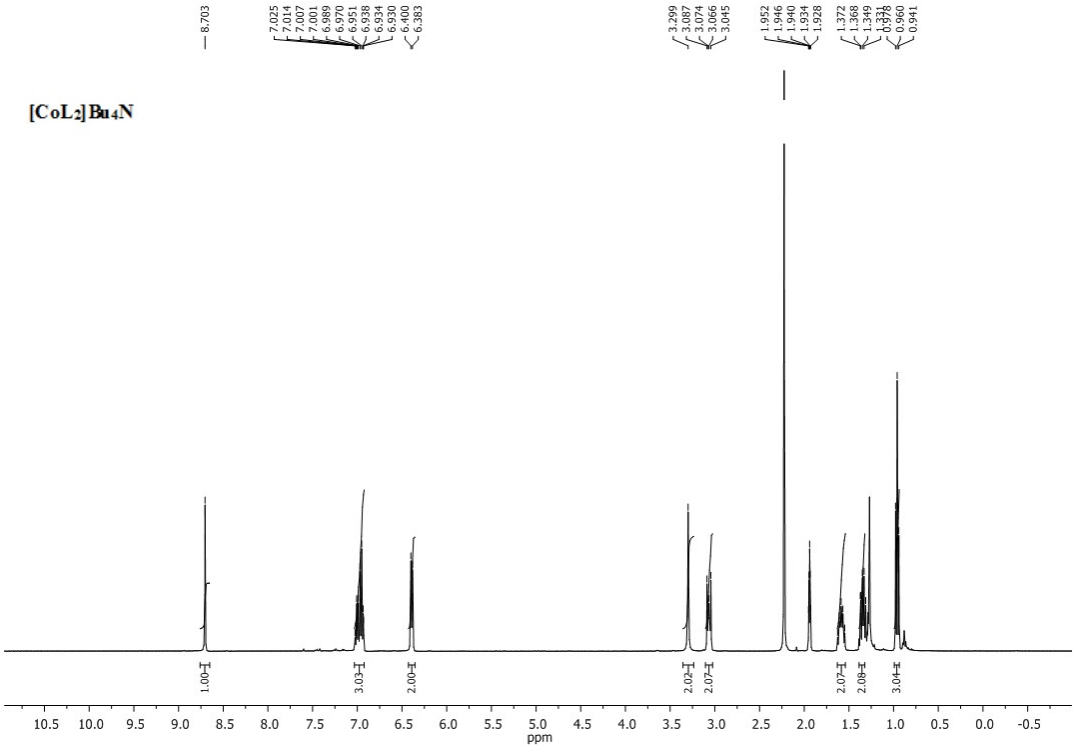


Fig. S3 ^{1}H NMR & ^{13}C NMR of $[CoL_2]Bu_4N$



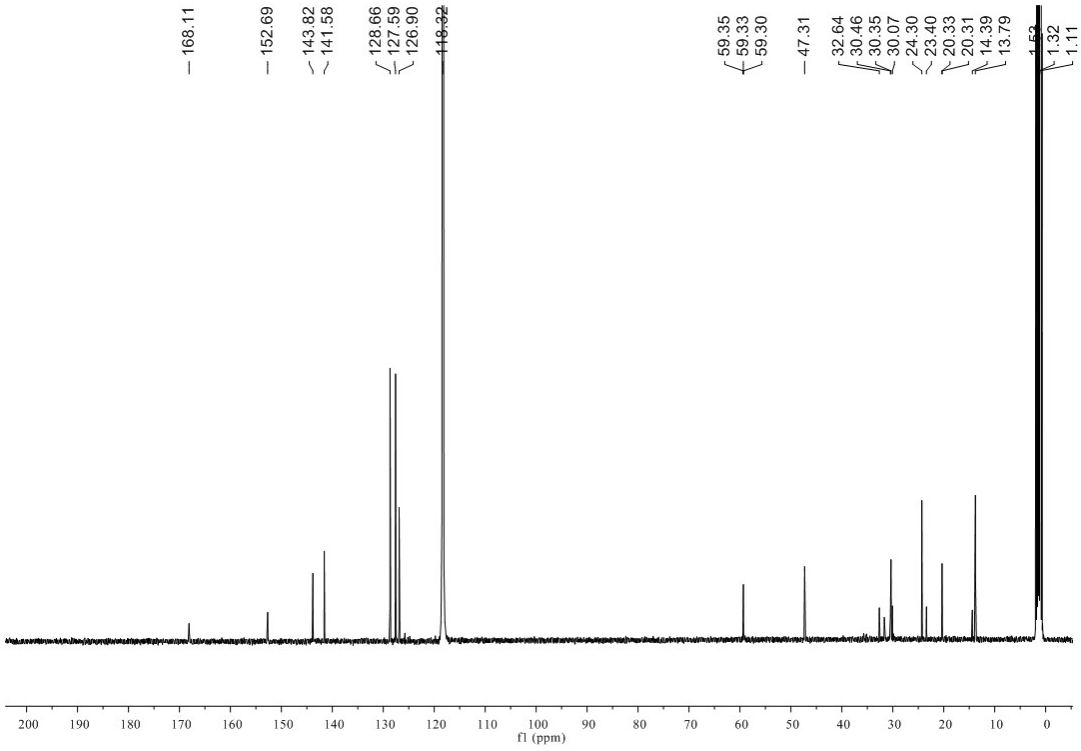


Fig. S4 ESI-MS spectrum of Dimethyl pyrazine-2,6-dicarboxylate

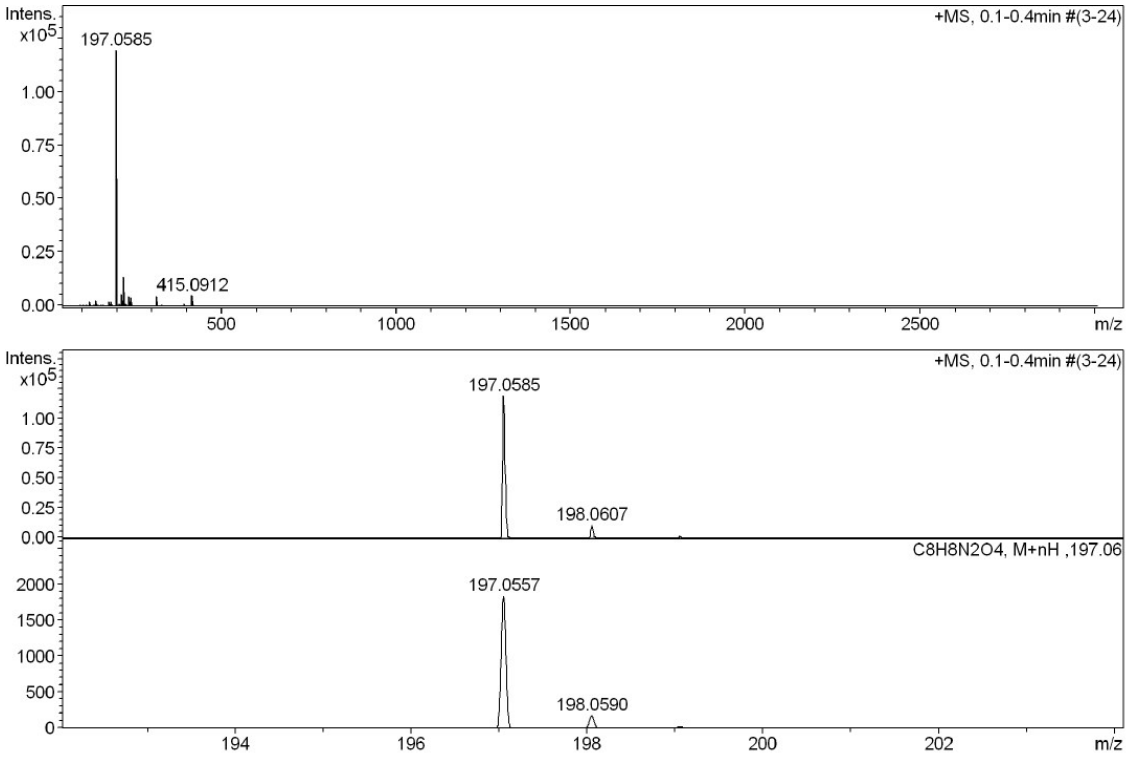


Fig. S5 ESI-MS spectrum of compound **1**

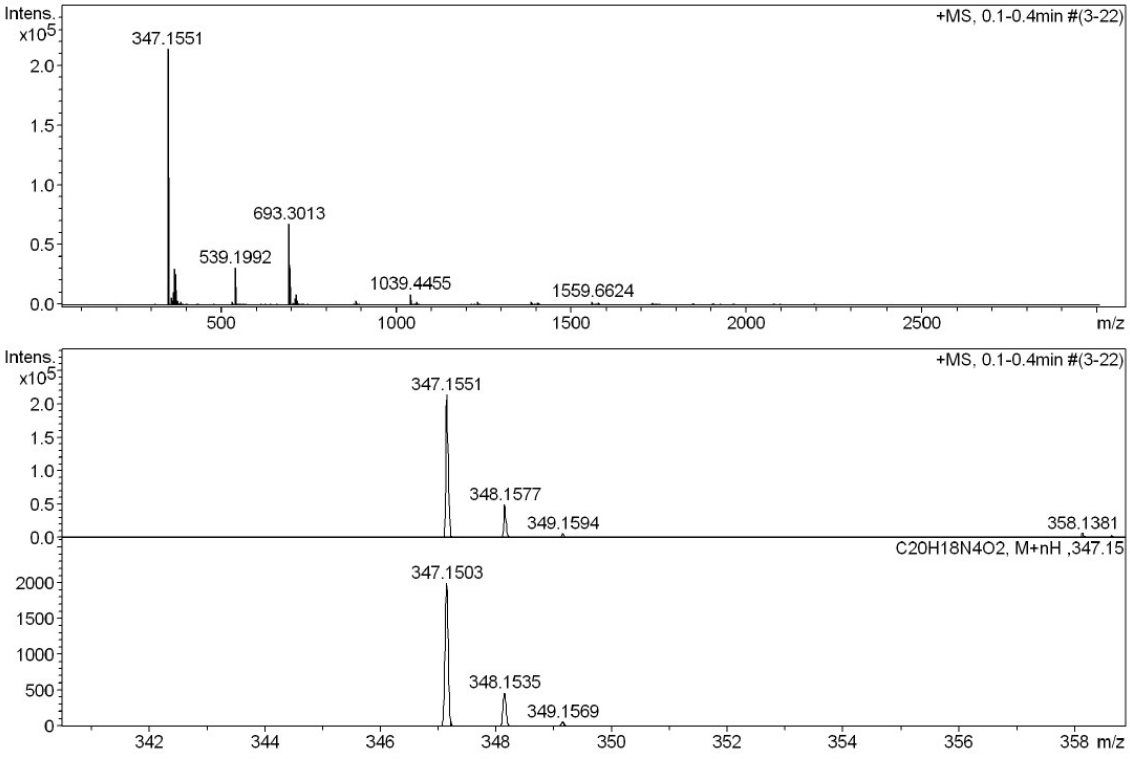


Figure S5. ESI-MS spectrum of $[CoL_2]Bu_4N$

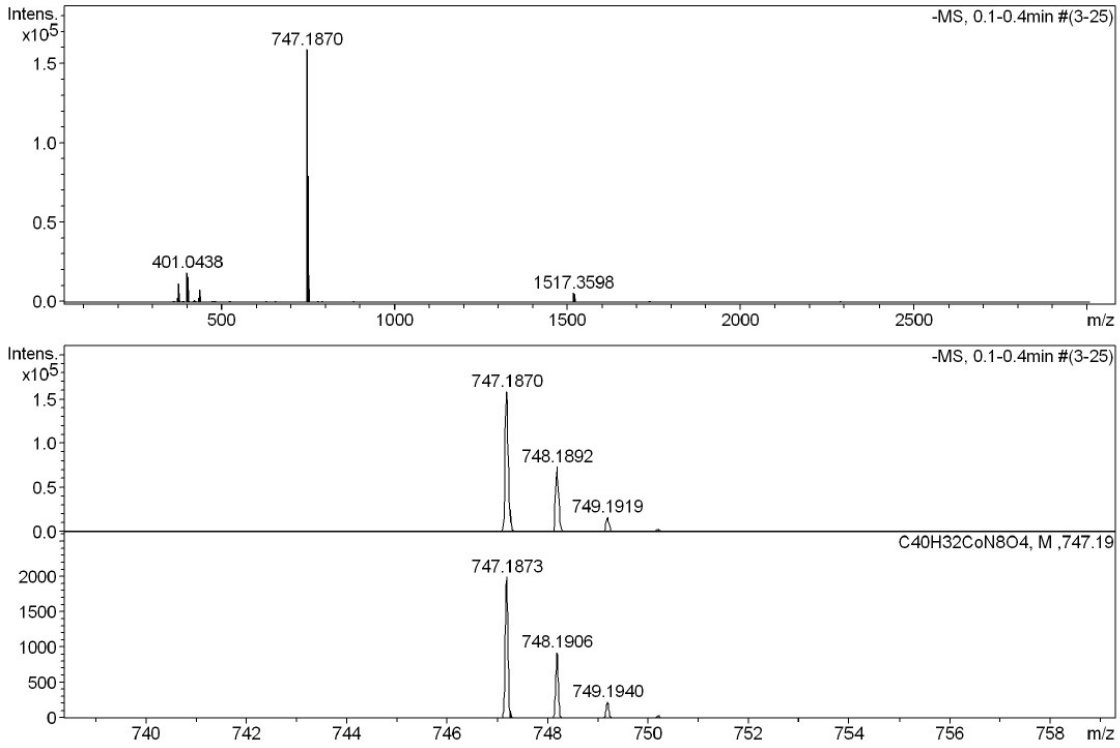


Table S2. Bond lengths and Bond angles of $[CoL_2]Bu_4N$, 3

Bond lengths		Bond angles	
C(1)-N(2)	1.354(5)	N(2)-C(1)-C(2)	121.1(4)
C(2)-N(1)	1.330(4)	N(1)-C(2)-C(3)	112.5(3)
C(2)-C(3)	1.515(6)	N(3)-C(3)-C(2)	110.0(3)
C(3)-O(1)	1.233(4)	N(3)-C(4)-C(5)	113.9(3)
C(5)-C(6)	1.377(7)	N(1)#5-Co(1)-N(3)#6	81.21(8)
C(5)-C(10)	1.390(7)	N(1)-Co(1)-N(3)#6	98.79(8)
C(6)-C(7)	1.381(7)	N(1)#5-Co(1)-N(3)#5	81.21(8)
C(7)-C(8)	1.343(13)	N(3)#6-Co(1)-N(3)#5	162.43(16)
C(8)-C(9)	1.415(14)	N(1)-Co(1)-N(3)	81.21(8)
C(9)-C(10)	1.404(9)	N(3)#5-Co(1)-N(3)	91.34(2)
C(11)-C(12)	1.485(8)	N(3)#6-Co(1)-N(3)#1	91.34(2)
C(11)-N(4)	1.518(5)	N(3)#5-Co(1)-N(3)#1	91.34(2)
C(12)-C(13)	1.461(9)	C(1)-C(2)-C(3)	128.2(4)
C(13)-C(14)	1.343(10)	C(6)-C(5)-C(10)	119.7(4)
N(1)-C(2)#1	1.330(4)	C(8)-C(7)-C(6)	121.7(7)
N(3)-Co(1)	1.959(3)	C(7)-C(8)-C(9)	118.9(6)
N(4)-C(11)#4	1.518(5)	C(10)-C(9)-C(8)	120.0(7)
Co(1)-N(3)#5	1.959(3)	C(5)-C(10)-C(9)	119.1(7)
C(1)#1-N(2)-C(1)	117.9(5)	C(13)-C(12)-C(11)	114.6(6)
C(11)#2-N(4)-C(11)#3	112.2(5)	C(14)-C(13)-C(12)	129.0(10)

C(11)#2-N(4)-C(11)#4	108.1(2)	C(2)-N(1)-C(2)#1	121.5(4)
C(11)-N(4)-C(11)#4	112.2(5)	C(2)-N(1)-Co(1)	119.3(2)
C(11)#3-N(4)-C(11)#4	108.1(2)	C(2)#1-N(1)-Co(1)	119.3(2)
O(1)-C(3)-N(3)	129.3(4)	C(1)#1-N(2)-C(1)	117.9(5)
O(1)-C(3)-C(2)	120.6(4)	C(3)-N(3)-C(4)	117.3(3)

Symmetry transformations used to generate equivalent atoms:

#1: -x+1,-y,z #2: -y+1/2,x+1/2,-z+1/2 #3: y-1/2,-x+1/2,-z+1/2 #4: -x,-y+1,z

#5: y+1/2,-x+1/2,-z+1/2 #6: -y+1/2,x-1/2,-z+1/2

Table S3. Bond lengths and Bond angles of 4

Bond lengths		Bond angles	
C(1)-N(1)	1.336(3)	N(1)-C(1)-C(2)	118.7(3)
C(1)-C(2)	1.379(4)	N(1)-C(1)-C(6)	111.8(2)
C(1)-C(6)	1.503(4)	N(2)-C(2)-C(1)	121.5(3)
C(3)-N(1)	1.334(3)	N(1)-C(3)-C(5)	113.0(2)
C(3)-C(4)	1.382(4)	N(2)-C(4)-C(3	121.7(3)
C(4)-N(2)	1.337(4)	N(6)-C(5)-C(3)	110.9(2)
C(5)-O(2)	1.249(3)	N(3)-C(7)-C(11)	112.2(2)
C(5)-N(6)	1.327(3)	N(3)-C(7)-C(10)	118.0(3)
C(6)-O(1)	1.237(3)	N(3)-C(8)-C(9)	118.1(3)
C(6)-N(5)	1.335(4)	N(3)-C(8)-C(12)	112.4(2)
C(7)-N(3)	1.331(4)	N(4)-C(9)-C(8)	121.9(3)
C(7)-C(11)	1.487(4)	N(4)-C(10)-C(7)	122.1(3)
C(8)-C(9)	1.387(4)	N(7)-C(11)-C(7)	112.3(2)
C(8)-C(12)	1.500(4)	N(8)-C(12)-C(8)	110.4(3)
C(9)-N(4)	1.338(4)	N(7)-C(14)-C(15)	117.8(2)
C(12)-O(3)	1.236(4)	N(5)-C(28)-C(29)	113.5(2)
C(14)-C(15)	1.504(4)	N(8)-C(35)-C(36)	114.0(3)
C(15)-C(20)	1.371(5)	N(1)-Co(1)-N(3)	175.58(10)
C(15)-C(16)	1.385(5)	N(1)-Co(1)-N(5)	81.39(10)
C(16)-C(17)	1.372(5)	N(3)-Co(1)-N(5)	102.34(10)
C(17)-C(18)	1.342(7)	N(3)-Co(1)-N(8)	81.08(10)
C(18)-C(119)	1.377(7)	N(1)-Co(1)-N(7)	96.22(10)
C(20)-C(119)	1.386(6)	N(5)-Co(1)-N(7)	89.93(10)
C(21)-N(6)	1.459(3)	N(1)-Co(1)-N(6)	81.34(10)
C(21)-C(22)	1.509(4)	N(3)-Co(1)-N(6)	95.03(10)
C(22)-C(23)	1.372(5)	N(7)-Co(1)-N(6)	94.39(10)
C(22)-C(27)	1.391(5)	N(2)#4-Ag(1)-C(32)	112.13(14)
C(23)-C(24)	1.387(5)	N(2)#4-Ag(1)-C(33)	89.16(12)
C(26)-C(27)	1.386(6)	C(9)-C(8)-C(12)	129.5(3)
C(29)-C(30)	1.382(4)	C(16)-C(15)-C(14)	118.9(3)
C(29)-C(34)	1.385(4)	C(17)-C(16)-C(15)	121.4(4)
C(31)-C(32)	1.366(6)	C(18)-C(17)-C(16)	119.3(4)
C(32)-Ag(1)	2.527(4)	C(17)-C(18)-C(119)	121.1(4)
C(33)-Ag(1)	2.658(5)	C(15)-C(20)-C(119)	119.9(4)
C(36)-C(41)	1.375(5)	C(27)-C(22)-C(21)	119.3(3)
C(36)-C(37)	1.383(5)	C(22)-C(23)-C(24)	120.9(4)
C(38)-C(39)	1.342(7)	C(25)-C(24)-C(23)	119.9(5)

N(2)-Ag(1)#1	2.381(2)	C(26)-C(27)-C(22)	120.0(4)
N(8)-Co(1)	1.952(2)	C(30)-C(29)-C(34)	118.4(3)
O(2)-Ag(1)#2	2.312(2)	C(30)-C(29)-C(28)	120.4(3)
O(4)-Ag(1)	2.269(2)	C(34)-C(29)-C(28)	121.1(3)
Ag(1)-N(2)#4	2.381(2)	C(32)-C(31)-C(30)	119.9(4)
		C(31)-C(32)-C(33)	120.0(4)
Bond Angles		C(31)-C(32)-Ag(1)	103.2(3)
C(36)-C(41)-C(40)	119.9(4)	C(34)-C(33)-Ag(1)	107.3(2)
C(18)-C(119)-C(20)	119.7(4)	C(29)-C(34)-C(33)	119.6(4)
C(1)-N(1)-Co(1)	119.62(19)	C(41)-C(36)-C(37)	119.3(3)
C(4)-N(2)-C(2)	118.1(3)	C(41)-C(36)-C(35)	121.1(3)
C(4)-N(2)-Ag(1)#1	112.83(19)	C(37)-C(36)-C(35)	119.6(3)
C(2)-N(2)-Ag(1)#1	127.22(19)	C(38)-C(37)-C(36)	119.9(4)
C(7)-N(3)-Co(1)	118.35(19)	C(39)-C(38)-C(37)	121.1(4)
C(6)-N(5)-Co(1)	116.49(18)	C(38)-C(39)-C(40)	119.9(4)
C(28)-N(5)-Co(1)	125.69(19)	O(2)-C(5)-N(6)	130.2(3)
C(5)-N(6)-C(21)	117.5(2)	O(2)-C(5)-C(3)	118.9(2)
C(5)-N(6)-Co(1)	115.81(18)	O(1)-C(6)-N(5)	127.9(3)
C(21)-N(6)-Co(1)	126.34(18)	O(1)-C(6)-C(1)	121.4(3)
C(11)-N(7)-C(14)	116.6(2)	O(4)-C(11)-N(7)	127.5(3)
C(11)-N(7)-Co(1)	114.93(19)	O(4)-C(11)-C(7)	120.1(3)
C(14)-N(7)-Co(1)	125.67(18)	O(3)-C(12)-N(8)	129.1(3)
C(12)-N(8)-C(35)	118.0(3)	O(3)-C(12)-C(8)	120.4(3)
C(12)-N(8)-Co(1)	116.69(19)	O(4)-Ag(1)-O(2)#3	106.73(8)
C(35)-N(8)-Co(1)	124.5(2)	O(4)-Ag(1)-N(2)#4	117.74(9)
C(5)-O(2)-Ag(1)#2	144.55(19)	O(2)#3-Ag(1)-N(2)#4	94.14(8)
C(11)-O(4)-Ag(1)	119.96(18)	O(4)-Ag(1)-C(32)	116.88(11)
C(32)-Ag(1)-C(33)	30.58(14)	O(2)#3-Ag(1)-C(32)	105.62(12)

Symmetry transformations used to generate equivalent atoms:

#:1 x-1/2,-y+1/2,z-1/2 #2: -x+3/2,y-1/2,-z+3/2 #3: -x+3/2,y+1/2,-z+3/2 #4: x+1/2,-y+1/2,z+1/2

Table S4. Bond lengths and Bond angles of 5

Bond lengths		Bond angles	
C(13)-N(5)	1.451(6)	N(5)-C(13)-C(14)	114.6(4)
C(15)-C(16)	1.365(10)	C(19)-C(14)-C(15)	119.4(6)
C(16)-C(17)	1.301(13)	C(15)-C(14)-C(13)	119.3(5)
C(18)-C(19)	1.424(13)	C(17)-C(16)-C(15)	120.1(8)
C(20)-N(7)	1.454(5)	C(16)-C(17)-C(18)	121.9(8)
C(22)-C(23)	1.382(9)	C(14)-C(19)-C(18)	117.9(9)
C(28)-C(29)	1.378(9)	C(26)-C(21)-C(22)	118.8(5)
C(28)-C(33)	1.385(8)	C(26)-C(21)-C(20)	120.8(5)
C(28)-C(27)	1.508(8)	C(22)-C(21)-C(20)	120.4(4)
C(29)-C(30)	1.382(10)	C(23)-C(22)-C(21)	120.4(5)
C(32)-C(33)	1.398(11)	C(23)-C(24)-C(25)	118.8(6)
C(34)-N(8)	1.461(6)	C(24)-C(25)-C(26)	121.0(6)
C(36)-C(37)	1.384(10)	C(29)-C(28)-C(33)	118.3(6)
C(37)-C(38)	1.366(13)	C(33)-C(28)-C(27)	121.2(6)

C(39)-C(40)	1.396(12)	C(31)-C(30)-C(29)	120.4(8)
C(41)-C(42)	1.409(16)	C(30)-C(31)-C(32)	120.2(8)
N(9)-O(8)	1.238(7)	N(8)-C(34)-C(35)	113.8(4)
O(5)-Ag(3)	2.375(7)	C(36)-C(35)-C(40)	119.3(6)
O(5)-Ag(2)#2	2.469(7)	C(36)-C(35)-C(34)	119.6(5)
O(8)-Ag(1)	2.575(5)	C(40)-C(35)-C(34)	121.0(6)
O(9)-Ag(2)#3	2.446(5)	C(35)-C(36)-C(37)	120.1(7)
C(1)-C(5)	1.492(6)	C(38)-C(37)-C(36)	120.2(9)
C(3)-N(3)	1.338(6)	C(39)-C(38)-C(37)	120.6(8)
C(4)-N(4)	1.327(6)	C(38)-C(39)-C(40)	120.4(8)
C(5)-N(7)	1.335(6)	C(35)-C(40)-C(39)	119.4(8)
C(7)-C(8)	1.384(6)	C(42)-C(41)-O(11)	109.2(11)
C(12)-N(6)	1.328(5)	O(9)-N(9)-O(10)	122.5(6)
C(27)-N(6)	1.462(6)	O(9)-N(9)-O(8)	119.0(5)
N(1)-Co(1)	1.846(3)	O(6)-N(10)-O(5)	118.0(8)
N(2)-Ag(3)#4	2.384(4)	O(7)-N(10)-O(5)	119.0(7)
N(3)-Co(1)	1.850(3)	C(6)-O(2)-Ag(1)#1	127.1(3)
N(4)-Ag(1)#5	2.385(4)	N(10)-O(5)-Ag(3)	107.5(5)
N(5)-Co(1)	1.955(4)	N(10)-O(5)-Ag(2)#2	101.5(5)
N(6)-Co(1)	1.958(4)	Ag(3)-O(5)-Ag(2)#2	151.0(3)
N(7)-Co(1)	1.967(4)	N(9)-O(8)-Ag(1)	100.2(4)
N(8)-Co(1)	1.958(4)	N(9)-O(9)-Ag(2)#3	105.8(4)
Ag(1)-O(2)#6	2.316(4)	N(3)-C(1)-C(2)	118.1(4)
Ag(1)-O(1)	2.346(4)	N(3)-C(1)-C(5)	113.3(4)
Ag(1)-N(4)#5	2.385(4)	C(2)-C(1)-C(5)	128.5(4)
Ag(2)-O(3)	2.247(4)	N(4)-C(2)-C(1)	121.4(4)
Ag(3)-O(4)	2.322(3)	N(3)-C(3)-C(4)	118.1(4)
Ag(3)-N(2)#4	2.384(4)	N(3)-C(3)-C(6)	111.8(4)
Bond angles		N(4)-C(4)-C(3)	121.6(4)
C(6)-N(8)-C(34)	117.2(4)	O(1)-C(5)-N(7)	129.6(4)
C(6)-N(8)-Co(1)	116.6(3)	O(1)-C(5)-C(1)	119.5(4)
C(34)-N(8)-Co(1)	126.1(3)	N(7)-C(5)-C(1)	110.9(4)
N(1)-Co(1)-N(3)	179.28(17)	O(2)-C(6)-N(8)	128.3(4)
N(1)-Co(1)-N(5)	81.32(16)	O(2)-C(6)-C(3)	120.6(4)
N(3)-Co(1)-N(5)	98.12(16)	N(8)-C(6)-C(3)	111.2(4)
N(1)-Co(1)-N(8)	98.49(16)	N(1)-C(7)-C(8)	118.4(4)
N(3)-Co(1)-N(8)	81.05(15)	N(1)-C(7)-C(11)	112.2(4)
N(5)-Co(1)-N(8)	92.36(16)	C(8)-C(7)-C(11)	129.3(4)
N(1)-Co(1)-N(6)	81.57(15)	N(2)-C(8)-C(7)	121.1(5)
N(8)-Co(1)-N(6)	90.97(16)	N(1)-C(9)-C(10)	117.3(4)
N(1)-Co(1)-N(7)	98.97(16)	N(1)-C(9)-C(12)	113.0(4)
N(3)-Co(1)-N(7)	81.50(15)	C(10)-C(9)-C(12)	129.7(4)
N(5)-Co(1)-N(7)	90.87(16)	N(2)-C(10)-C(9)	122.2(4)
O(2)#6-Ag(1)-O(1)	103.53(13)	O(3)-C(11)-N(5)	127.7(4)
O(2)#6-Ag(1)-N(4)#5	132.37(14)	O(3)-C(11)-C(7)	121.0(4)
O(1)-Ag(1)-N(4)#5	87.58(13)	N(5)-C(11)-C(7)	111.3(4)
O(2)#6-Ag(1)-O(8)	102.85(16)	O(4)-C(12)-N(6)	130.0(4)
O(1)-Ag(1)-O(8)	130.77(17)	O(4)-C(12)-C(9)	118.9(4)
N(4)#5-Ag(1)-O(8)	103.84(17)	N(6)-C(12)-C(9)	111.1(4)

O(3)-Ag(2)-O(9)#7	119.73(16)	N(6)-C(27)-C(28)	113.1(4)
C(5)-O(1)-Ag(1)	144.0(3)	C(7)-N(1)-C(9)	122.4(4)
C(11)-O(3)-Ag(2)	131.9(3)	C(7)-N(1)-Co(1)	119.4(3)
C(12)-O(4)-Ag(3)	140.4(3)	C(9)-N(1)-Co(1)	118.2(3)
C(12)-N(6)-C(27)	118.7(4)	C(10)-N(2)-C(8)	118.6(4)
C(12)-N(6)-Co(1)	116.0(3)	C(10)-N(2)-Ag(3)#4	116.6(3)
C(27)-N(6)-Co(1)	125.3(3)	C(8)-N(2)-Ag(3)#4	124.8(3)
C(5)-N(7)-C(20)	118.4(4)	C(1)-N(3)-C(3)	122.2(4)
C(5)-N(7)-Co(1)	115.6(3)	C(1)-N(3)-Co(1)	118.5(3)
C(11)-N(5)-C(13)	117.1(4)	C(3)-N(3)-Co(1)	119.2(3)
C(11)-N(5)-Co(1)	115.7(3)	C(4)-N(4)-C(2)	118.6(4)
C(13)-N(5)-Co(1)	126.6(3)	C(4)-N(4)-Ag(1)#5	126.1(3)
		C(2)-N(4)-Ag(1)#5	115.1(3)

Symmetry transformations used to generate equivalent atoms:

#1: x+1,y,z #2: x+1,y-1,z #3: x,y-1,z #4: -x+1,-y+1,-z+1 #5: -x+1,-y+1,-z

#6: x-1,y,z #7: x,y+1,z #8: x-1,y+1,z

Table S5. Bond lengths and Bond angles of 6

Bond lengths		Bond angles	
C(1)-N(1)	1.324(8)	N(1)-C(1)-C(2)	122.0(5)
C(2)-N(2)	1.322(7)	N(2)-C(2)-C(1)	118.0(5)
C(2)-C(9)	1.499(8)	N(2)-C(2)-C(9)	113.0(4)
C(3)-N(2)	1.328(7)	C(1)-C(2)-C(9)	128.7(5)
C(3)-C(4)	1.398(8)	N(2)-C(3)-C(4)	116.6(5)
C(3)-C(10)	1.497(8)	N(2)-C(3)-C(10)	113.0(5)
C(4)-N(1)	1.329(8)	C(4)-C(3)-C(10)	130.3(5)
C(5)-C(11)	1.499(8)	N(3)-C(5)-C(6)	118.2(5)
C(6)-N(4)	1.330(8)	N(3)-C(5)-C(11)	111.7(5)
C(7)-N(3)	1.330(7)	N(4)-C(6)-C(5)	121.9(6)
C(8)-N(4)	1.329(8)	N(3)-C(7)-C(8)	117.6(5)
C(9)-O(1)	1.247(7)	C(8)-C(7)-C(12)	130.0(5)
C(9)-N(7)	1.332(7)	N(4)-C(8)-C(7)	122.6(6)
C(11)-O(4)	1.253(7)	O(1)-C(9)-N(7)	128.0(5)
C(11)-N(8)	1.320(7)	O(1)-C(9)-C(2)	120.8(5)
C(12)-O(3)	1.251(6)	N(7)-C(9)-C(2)	111.1(4)
C(12)-N(6)	1.330(7)	O(2)-C(10)-N(5)	128.1(5)
C(13)-N(6)	1.456(7)	O(2)-C(10)-C(3)	121.0(5)
C(13)-C(17)	1.505(8)	N(5)-C(10)-C(3)	110.9(4)
C(14)-N(8)	1.468(7)	N(8)-C(11)-C(5)	111.9(5)
C(14)-C(23)	1.505(8)	O(3)-C(12)-N(6)	127.6(5)
C(15)-N(5)	1.460(7)	N(6)-C(13)-C(17)	114.4(4)
C(19)-C(20)	1.357(10)	N(5)-C(15)-C(29)	114.5(4)
C(26)-C(27)	1.389(11)	C(22)-C(17)-C(13)	122.0(5)
C(27)-C(28)	1.367(10)	C(19)-C(18)-C(17)	120.4(6)
C(29)-C(30)	1.377(8)	C(20)-C(19)-C(18)	120.1(6)
C(32)-C(33)	1.359(11)	C(20)-C(21)-C(22)	119.9(6)

C(35)-C(40)	1.381(8)	C(24)-C(23)-C(28)	117.7(6)
C(36)-C(37)	1.397(9)	C(24)-C(23)-C(14)	119.6(5)
C(37)-C(38)	1.378(10)	C(25)-C(24)-C(23)	120.9(7)
N(2)-Co	1.849(4)	C(27)-C(28)-C(23)	121.0(7)
N(6)-Co	1.977(4)	C(30)-C(29)-C(34)	118.7(6)
N(7)-Co	1.962(4)	C(30)-C(29)-C(15)	122.1(5)
N(8)-Co	1.963(4)	C(34)-C(29)-C(15)	119.2(5)
N(9)-Ag(2)	2.086(7)	C(31)-C(30)-C(29)	120.7(6)
N(3)-Co-N(2)	178.95(19)	C(33)-C(34)-C(29)	120.2(6)
N(3)-Co-N(7)	97.34(18)	C(36)-C(35)-C(40)	119.5(6)
N(2)-Co-N(7)	81.71(18)	C(36)-C(35)-C(16)	121.9(5)
N(5)-Co-N(7)	163.65(18)	C(40)-C(35)-C(16)	118.5(5)
N(3)-Co-N(8)	81.55(18)	C(35)-C(36)-C(37)	120.2(6)
N(7)-Co-N(8)	91.49(18)	C(38)-C(37)-C(36)	120.2(6)
N(5)-Co-N(6)	90.09(18)	C(39)-C(38)-C(37)	119.1(7)
N(9)-Ag(2)-O(8)	176.2(3)	C(38)-C(39)-C(40)	121.0(7)
C(12)-N(6)-Co	114.7(4)	N(9)-C(42)-C(41)	178.1(7)
C(13)-N(6)-Co	126.2(4)	C(1)-N(1)-C(4)	117.7(5)
C(9)-N(7)-C(16)	116.8(4)	C(2)-N(2)-C(3)	123.0(5)
C(9)-N(7)-Co	115.4(4)	C(2)-N(2)-Co	118.7(4)
C(16)-N(7)-Co	126.5(4)	C(3)-N(2)-Co	118.2(4)
C(11)-N(8)-C(14)	117.7(4)	C(7)-N(3)-C(5)	121.7(5)
C(11)-N(8)-Co	115.7(4)	C(7)-N(3)-Co	119.1(4)
C(14)-N(8)-Co	125.6(4)	C(5)-N(3)-Co	119.2(4)
C(42)-N(9)-Ag(2)	175.5(7)	C(8)-N(4)-C(6)	117.8(5)