ELECTRONIC SUPPLEMENTARY INFORMATION

Thermal stability and crystallochemical analysis for Co^{II}-based coordination polymers with TPP and TPPS porphyrins

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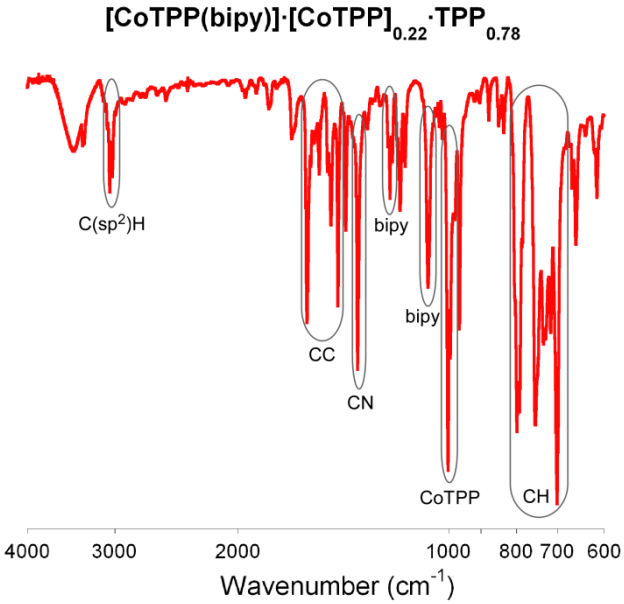

Fig. S1 IR spectra for compound **1**. The following bands (cm^{-1}) are marked: 3052 and 3028 (C(sp2)H), 1596-1441 (CC), 1349 (CN), 1210 and 1069 (bipy), 1000 (CoTPP) and 795-700 (CH).

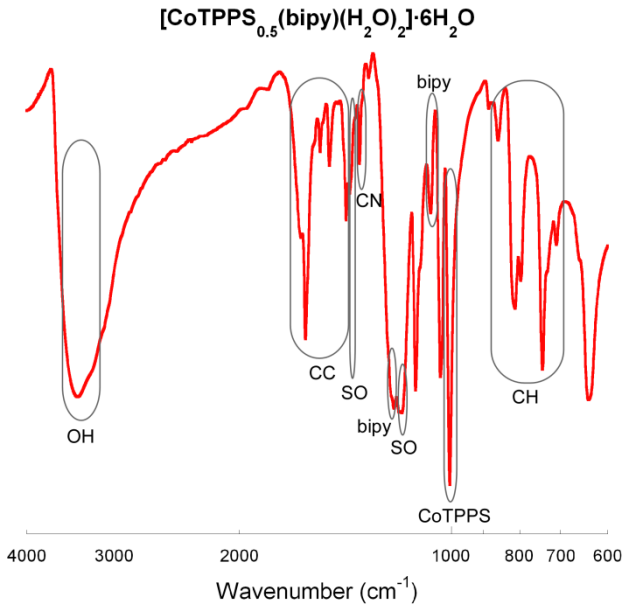

Fig. S2 IR spectra for compound **2**. The following bands (cm^{-1}) are marked: 3397 (OH), 1624-1410 (CC), 1394 and 1174 (SO), 1349 (CN), 1208 and 1076 (bipy), 1000 (CoTPPS) and 863-744 (CH).

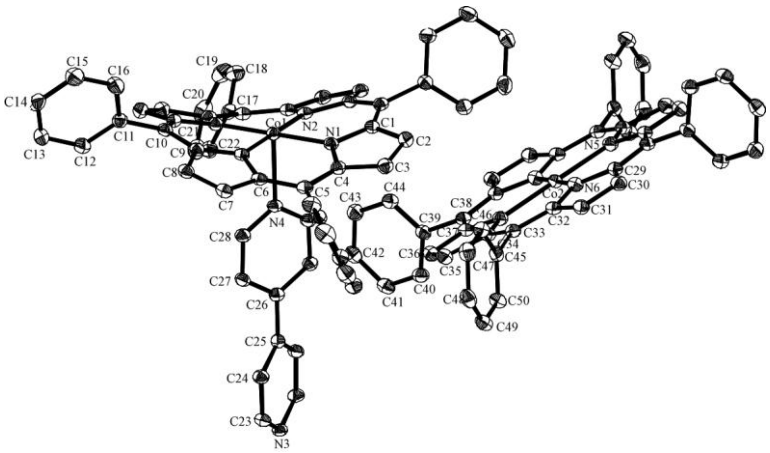

Fig. S3 Thermal ellipsoid plot (50% of probability) for compound **1**.

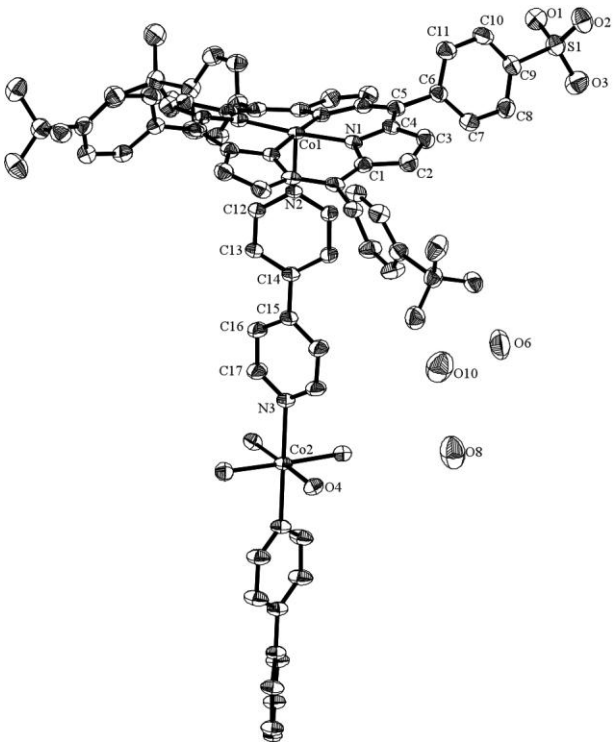

Fig. S4 Thermal ellipsoid plot (50% of probability) for compound **2**.

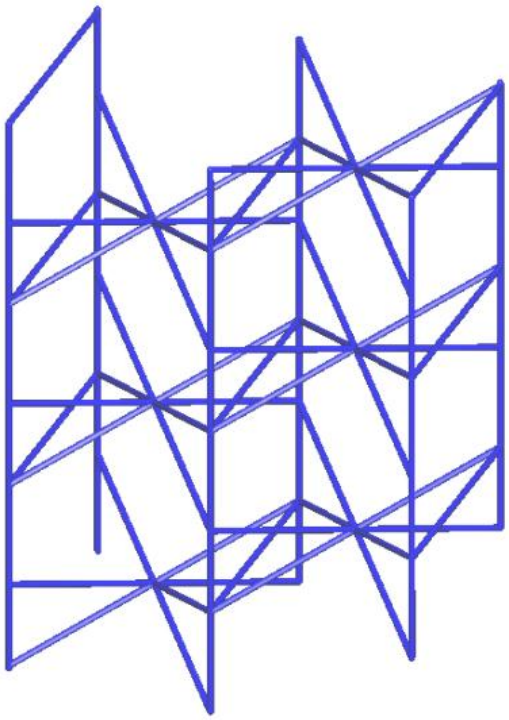

Fig. S5 Topology of the net for compound **1.**

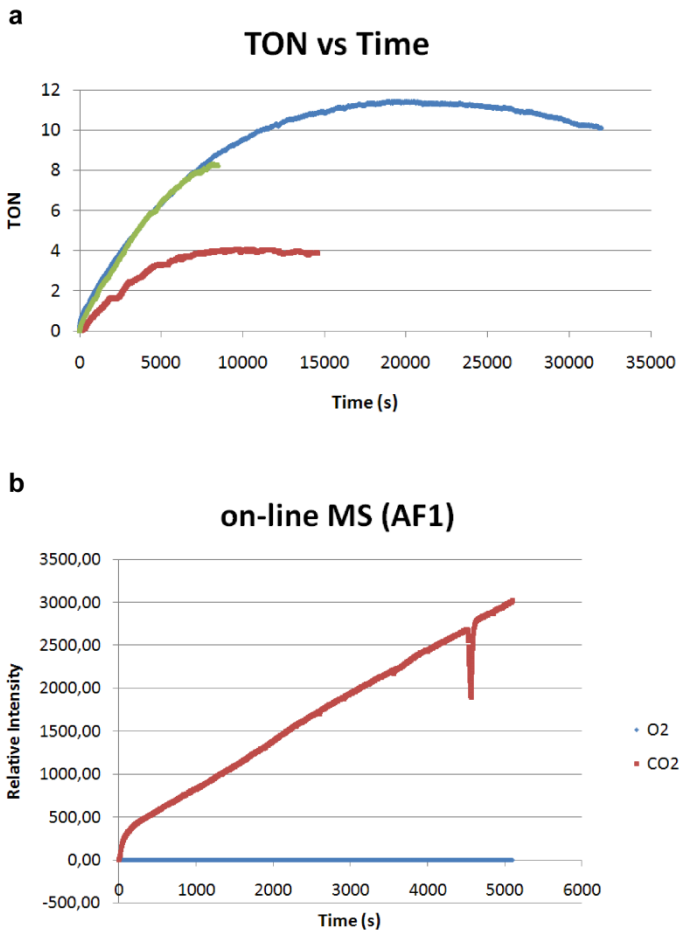

Fig. S6 _Three gas generation manometry experiments (a) and Online-MS study (b) for compound **1.**

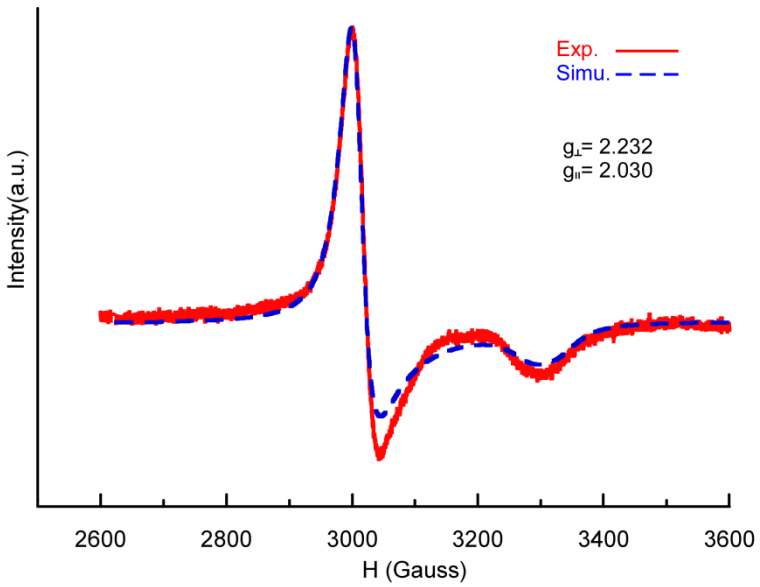

Fig. S7 X-band EPR spectrum at 5º K for compound **1**. Red line corresponds to the observed spectra and blue dashed line to the simulated one.

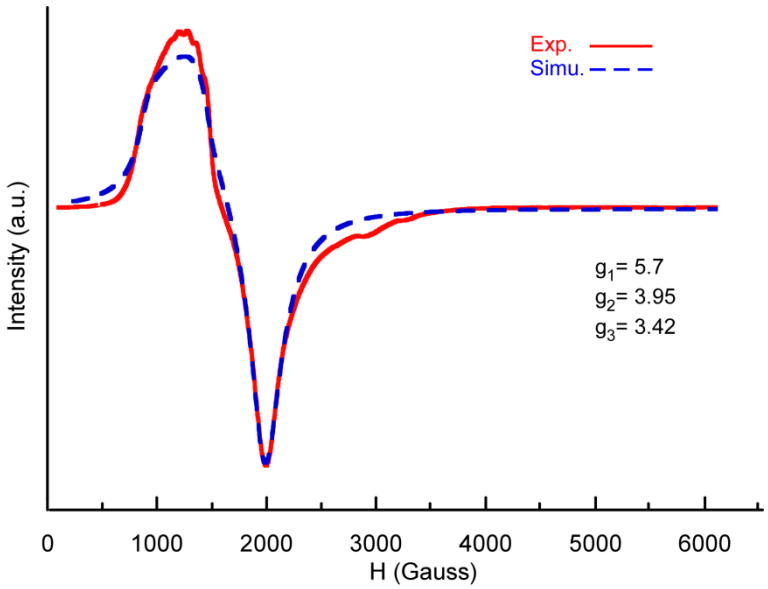

Fig. S8 X-band EPR spectrum at 5º K for compound **2**. Red line corresponds to the observed spectra and blue dashed line to the simulated one.

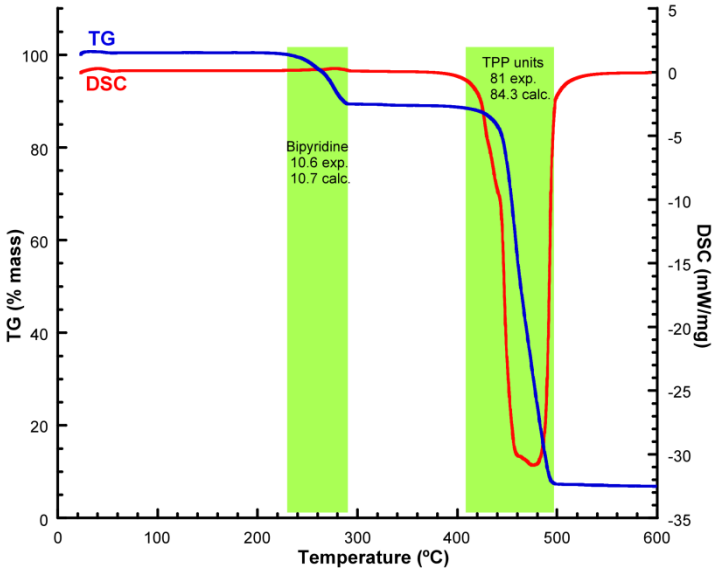

Fig. S9 Thermogravimetric analysis for compound **1**. Green ranges show the weight loss intervals.

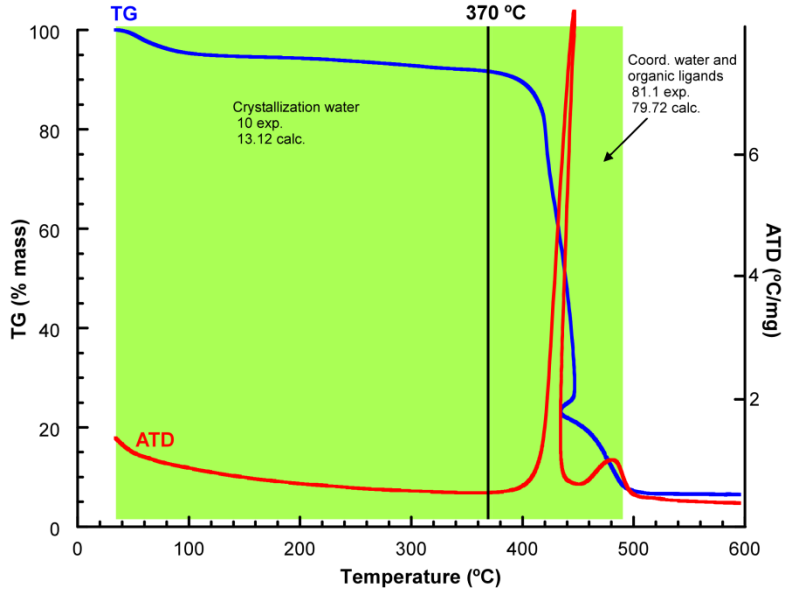

Fig. S10 Thermogravimetric analysis for compound **2**. Green ranges show the weight loss intervals.

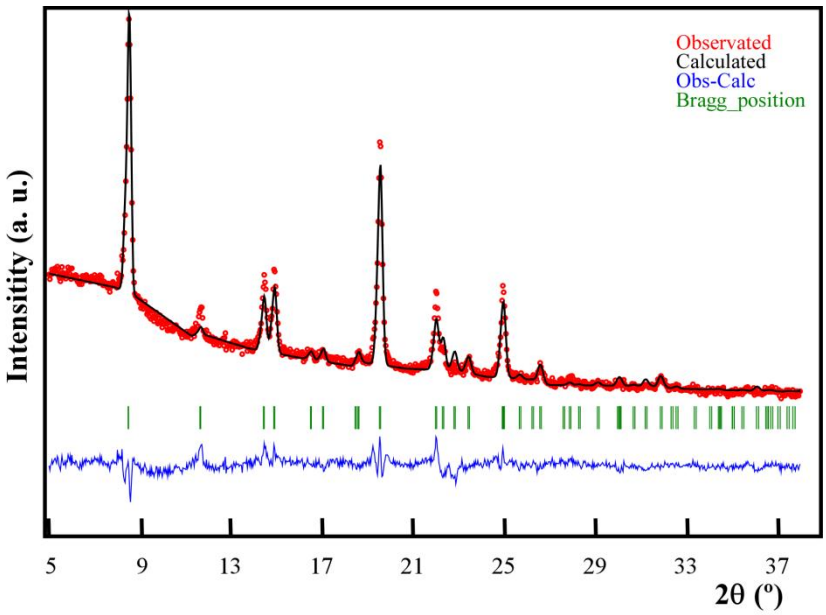

Fig. S11 Observed (red), calculated (black) and difference (blue) X-ray powder diffraction patterns for CoTPP.

Table S1 Fractional atomic coordinates ($x10^4$) and equivalent thermal factors ($x10^3$) for compound **1**.

Atoms	X	Y	Z	U_{eq}, Å^2
C(1)	4305(1)	4398(1)	1441(1)	20(1)
C(2)	4327(1)	4363(1)	840(1)	23(1)
C(3)	4826(1)	4015(1)	735(1)	23(1)
C(4)	5119(1)	3889(1)	1270(1)	20(1)
C(5)	5667(1)	3676(1)	1336(1)	20(1)
C(6)	5965(1)	3844(1)	1839(1)	19(1)
C(7)	6539(1)	3850(1)	1907(1)	22(1)
C(8)	6674(1)	4204(1)	2434(1)	21(1)
C(9)	6183(1)	4351(1)	2706(1)	18(1)
C(10)	6157(1)	4580(1)	3277(1)	20(1)
C(11)	6656(1)	4997(1)	3583(1)	21(1)
C(12)	6966(1)	4326(2)	3952(1)	28(1)
C(13)	7440(1)	4745(2)	4207(1)	30(1)
C(14)	7610(1)	5835(2)	4100(1)	28(1)
C(15)	7303(1)	6508(2)	3736(1)	32(1)
C(16)	6829(1)	6100(2)	3479(1)	28(1)
C(17)	5945(1)	3307(1)	832(1)	21(1)
C(18)	6325(1)	3981(2)	593(1)	27(1)
C(19)	6579(1)	3596(2)	127(1)	33(1)
C(20)	6455(1)	2540(2)	-101(1)	33(1)
C(21)	6075(1)	1864(2)	131(1)	31(1)
C(22)	5821(1)	2247(2)	595(1)	26(1)
C(23)	5431(1)	6731(1)	2382(1)	21(1)
C(24)	5451(1)	7913(1)	2378(1)	21(1)
C(25)	5000	8530(2)	2500	19(1)
C(26)	5000	-212(2)	2500	19(1)
C(27)	4539(1)	405(1)	2349(1)	21(1)
C(28)	4560(1)	1587(1)	2351(1)	21(1)
C(29)	7373(1)	3488(1)	6166(1)	20(1)
C(30)	6992(1)	3545(1)	6587(1)	22(1)
C(31)	6529(1)	3085(1)	6368(1)	22(1)
C(32)	6612(1)	2729(1)	5808(1)	20(1)
C(33)	6236(1)	2182(1)	5453(1)	21(1)
C(34)	6332(1)	1755(1)	4923(1)	21(1)
C(35)	5926(1)	1236(1)	4549(1)	24(1)
C(36)	6167(1)	935(1)	4082(1)	24(1)
C(37)	6721(1)	1270(1)	4169(1)	21(1)
C(38)	7097(1)	1139(1)	3769(1)	21(1)
C(39)	6941(1)	597(1)	3217(1)	20(1)
C(40)	6931(1)	-584(1)	3162(1)	24(1)
C(41)	6848(1)	-1082(2)	2639(1)	25(1)
C(42)	6765(1)	-414(2)	2165(1)	25(1)
C(43)	6755(1)	760(2)	2218(1)	26(1)
C(44)	6848(1)	1261(1)	2742(1)	24(1)
C(45)	5697(1)	2003(1)	5672(1)	21(1)
C(46)	5351(1)	2914(2)	5746(1)	24(1)
C(47)	4857(1)	2731(2)	5964(1)	28(1)
C(48)	4706(1)	1646(2)	6111(1)	27(1)
C(49)	5048(1)	740(2)	6045(1)	26(1)
C(50)	5541(1)	916(1)	5825(1)	24(1)
Co(1)	5000	4129(1)	2500	16(1)
Co(2)	7500	2500	5000	17(1)
N(1)	4794(1)	4125(1)	1695(1)	18(1)
N(2)	5756(1)	4126(1)	2338(1)	18(1)
N(3)	5000	6130(2)	2500	19(1)

N(4)	5000	2181(2)	2500	19(1)
N(5)	6813(1)	1771(1)	4683(1)	21(1)
N(6)	7129(1)	2993(1)	5700(1)	21(1)

Table S2 Anisotropic displacement parameters (A^2 x 10^3) for compound **1**.

Atoms	U11	U22	U33	U23	U13	U12
C(1)	22(1)	14(1)	22(1)	1(1)	-1(1)	0(1)
C(2)	24(1)	23(1)	23(1)	1(1)	-1(1)	1(1)
C(3)	24(1)	22(1)	23(1)	-1(1)	2(1)	1(1)
C(4)	22(1)	16(1)	21(1)	-1(1)	2(1)	0(1)
C(5)	23(1)	14(1)	23(1)	1(1)	3(1)	-1(1)
C(6)	20(1)	13(1)	24(1)	1(1)	4(1)	0(1)
C(7)	21(1)	18(1)	26(1)	2(1)	3(1)	2(1)
C(8)	20(1)	17(1)	27(1)	3(1)	1(1)	0(1)
C(9)	16(1)	13(1)	26(1)	2(1)	0(1)	-1(1)
C(10)	21(1)	14(1)	25(1)	1(1)	0(1)	1(1)
C(11)	19(1)	19(1)	23(1)	-2(1)	1(1)	0(1)
C(12)	29(1)	21(1)	32(1)	0(1)	-4(1)	1(1)
C(13)	26(1)	30(1)	34(1)	-3(1)	-8(1)	6(1)
C(14)	20(1)	30(1)	34(1)	-9(1)	-2(1)	-2(1)
C(15)	26(1)	25(1)	45(1)	1(1)	-1(1)	-7(1)
C(16)	24(1)	23(1)	36(1)	6(1)	-3(1)	-3(1)
C(17)	21(1)	21(1)	22(1)	1(1)	1(1)	4(1)
C(18)	29(1)	25(1)	29(1)	3(1)	6(1)	1(1)
C(19)	33(1)	37(1)	32(1)	8(1)	11(1)	5(1)
C(20)	36(1)	42(1)	23(1)	1(1)	7(1)	14(1)
C(21)	36(1)	30(1)	27(1)	-6(1)	-1(1)	9(1)
C(22)	26(1)	24(1)	26(1)	-1(1)	1(1)	2(1)
C(23)	20(1)	16(1)	26(1)	1(1)	4(1)	2(1)
C(24)	21(1)	16(1)	26(1)	1(1)	2(1)	-2(1)
C(25)	20(1)	18(1)	19(1)	0	0(1)	0
C(26)	22(1)	16(1)	19(1)	0	3(1)	0
C(27)	20(1)	16(1)	26(1)	-1(1)	-1(1)	-2(1)
C(28)	21(1)	15(1)	28(1)	0(1)	0(1)	1(1)
C(29)	23(1)	16(1)	22(1)	0(1)	1(1)	0(1)
C(30)	24(1)	18(1)	24(1)	-2(1)	2(1)	1(1)
C(31)	23(1)	19(1)	23(1)	-1(1)	2(1)	0(1)
C(32)	22(1)	15(1)	23(1)	0(1)	3(1)	-1(1)
C(33)	23(1)	16(1)	24(1)	2(1)	2(1)	-1(1)
C(34)	22(1)	17(1)	23(1)	2(1)	1(1)	-2(1)
C(35)	22(1)	24(1)	26(1)	0(1)	2(1)	-2(1)
C(36)	23(1)	23(1)	24(1)	-1(1)	0(1)	-3(1)
C(37)	23(1)	16(1)	23(1)	1(1)	0(1)	-2(1)
C(38)	23(1)	15(1)	24(1)	0(1)	1(1)	0(1)
C(39)	18(1)	19(1)	24(1)	-1(1)	2(1)	-2(1)
C(40)	25(1)	19(1)	27(1)	1(1)	2(1)	-1(1)
C(41)	25(1)	19(1)	32(1)	-5(1)	3(1)	-2(1)
C(42)	24(1)	28(1)	24(1)	-6(1)	3(1)	-4(1)
C(43)	26(1)	27(1)	24(1)	1(1)	1(1)	-2(1)
C(44)	25(1)	20(1)	26(1)	0(1)	0(1)	-1(1)
C(45)	21(1)	23(1)	19(1)	-2(1)	0(1)	-2(1)
C(46)	24(1)	24(1)	26(1)	1(1)	0(1)	-1(1)
C(47)	23(1)	31(1)	29(1)	-3(1)	1(1)	4(1)
C(48)	21(1)	36(1)	25(1)	-3(1)	3(1)	-6(1)
C(49)	27(1)	26(1)	26(1)	-3(1)	3(1)	-8(1)
C(50)	24(1)	21(1)	26(1)	-3(1)	3(1)	-3(1)

Co(1)	16(1)	14(1)	19(1)	0	1(1)	0
Co(2)	18(1)	16(1)	18(1)	-1(1)	2(1)	-2(1)
N(1)	19(1)	14(1)	22(1)	0(1)	1(1)	0(1)
N(2)	20(1)	13(1)	21(1)	1(1)	2(1)	0(1)
N(3)	23(1)	13(1)	20(1)	0	1(1)	0
N(4)	22(1)	13(1)	23(1)	0	1(1)	0
N(5)	22(1)	18(1)	22(1)	0(1)	2(1)	-1(1)
N(6)	21(1)	20(1)	23(1)	0(1)	1(1)	-2(1)

Table S3 Fractional atomic coordinates ($x10^4$) and isotropic thermal factors ($x10^3$) of hydrogen atoms for compound **1**.

Atoms	**X**	**Y**	**Z**	**U_{iso}, Å^2**
H(2)	4047	4547	571	28
H(3)	4957	3879	379	28
H(7)	6779	3644	1633	26
H(8)	7024	4331	2593	25
H(12)	6854	3576	4031	33
H(13)	7649	4276	4458	36
H(14)	7933	6116	4275	34
H(15)	7416	7259	3660	39
H(16)	6622	6575	3230	34
H(18)	6412	4704	748	33
H(19)	6837	4060	-35	40
H(20)	6630	2279	-416	40
H(21)	5989	1142	-26	37
H(22)	5560	1783	752	31
H(23)	5743	6327	2296	25
H(24)	5769	8294	2293	25
H(27)	4214	24	2247	25
H(28)	4245	1994	2239	25
H(30)	7052	3849	6953	26
H(31)	6207	3012	6553	26
H(35)	5562	1127	4619	29
H(36)	6005	575	3760	28
H(40)	6981	-1049	3485	28
H(41)	6849	-1886	2606	30
H(42)	6714	-757	1807	31
H(43)	6685	1222	1897	31
H(44)	6847	2064	2774	28
H(46)	5454	3660	5648	29
H(47)	4624	3352	6012	33
H(48)	4368	1523	6258	33
H(49)	4945	-3	6149	32
H(50)	5774	292	5780	28
H(1N)	7279	2860	5401	32

Table S4 Fractional atomic coordinates ($x10^4$) and equivalent thermal factors ($x10^3$) for compound **2**.

Atoms	**X**	**Y**	**Z**	**Ueq, Å2**
C(1)	8891(2)	1260(2)	1328(2)	31(1)
C(2)	8833(2)	471(2)	1244(2)	36(1)
C(3)	9508(2)	219(2)	1082(2)	37(1)
C(4)	10003(2)	844(2)	1086(1)	31(1)
C(5)	8297(2)	1728(2)	1461(1)	32(1)

C(6)	7579(2)	1366(2)	1603(2)	34(1)
C(7)	7019(2)	1305(2)	1178(2)	38(1)
C(8)	6406(2)	863(3)	1278(2)	41(1)
C(9)	6343(2)	492(2)	1815(2)	37(1)
C(10)	6863(2)	601(3)	2267(2)	45(1)
C(11)	7480(2)	1034(3)	2154(2)	43(1)
C(12)	10637(2)	2513(2)	56(2)	34(1)
C(13)	10655(2)	2486(2)	-560(2)	36(1)
C(14)	10000	2500	-886(2)	32(1)
C(15)	10000	2500	-1548(2)	32(1)
C(16)	9446(2)	2860(3)	-1869(2)	42(1)
C(17)	9469(2)	2846(2)	-2483(2)	41(1)
Co(1)	10000	2500	1250	24(1)
Co(2)	10000	2500	-3750	28(1)
N(1)	9612(2)	1480(2)	1222(1)	28(1)
N(2)	10000	2500	366(2)	27(1)
N(3)	10000	2500	-2794(2)	32(1)
S(1)	5616(1)	-156(1)	1947(1)	40(1)
O(1)	5997(2)	-842(2)	2111(1)	44(1)
O(2)	5156(2)	120(2)	2432(2)	51(1)
O(3)	5218(2)	-212(2)	1381(2)	57(1)
O(4)	9417(2)	3507(2)	-3762(1)	34(1)
O(6)	3638(5)	9557(6)	2426(5)	77(3)
O(8)	3705(5)	10413(6)	1359(6)	85(3)
O(5)	5000	10000	0	122(4)
O(7)	3565(5)	10001(7)	1957(6)	102(4)
O(9)	3637(5)	10076(5)	628(5)	84(3)
O(10)	3541(5)	10118(5)	126(5)	87(3)

Table S5 Anisotropic displacement parameters (A^2 x 10^3) for compound **2**.

Atoms	**U11**	**U22**	**U33**	**U23**	**U13**	**U12**
C(1)	37(2)	35(2)	21(1)	0(1)	-1(1)	-3(1)
C(2)	39(2)	37(2)	33(2)	-2(1)	-2(1)	-6(2)
C(3)	42(2)	35(2)	34(2)	-5(2)	-6(2)	0(2)
C(4)	41(2)	34(2)	16(1)	-3(1)	-2(1)	0(2)
C(5)	36(2)	41(2)	19(2)	-3(1)	1(1)	-3(2)
C(6)	34(2)	40(2)	27(2)	-3(1)	4(1)	-2(2)
C(7)	40(2)	46(2)	29(2)	-1(2)	4(1)	1(2)
C(8)	36(2)	49(2)	37(2)	-6(2)	1(1)	-2(2)
C(9)	34(2)	38(2)	39(2)	-3(2)	7(2)	-5(2)
C(10)	47(2)	59(3)	30(2)	7(2)	1(2)	-14(2)
C(11)	44(2)	54(2)	31(2)	0(2)	-1(2)	-11(2)
C(12)	30(2)	52(2)	21(2)	3(1)	1(1)	1(2)
C(13)	32(2)	56(2)	20(2)	4(1)	1(1)	-1(2)
C(14)	35(2)	42(3)	18(2)	0	0	-1(2)
C(15)	33(2)	45(3)	18(2)	0	0	-4(2)
C(16)	40(2)	65(3)	22(2)	-3(2)	0(2)	10(2)
C(17)	43(2)	60(2)	21(2)	2(2)	0(2)	10(2)
Co(1)	30(1)	30(1)	12(1)	0	0	0
Co(2)	35(1)	35(1)	15(1)	0	0	0
N(1)	33(1)	33(2)	16(1)	-3(1)	-1(1)	0(1)
N(2)	30(2)	36(2)	15(2)	0	0	-1(2)
N(3)	35(2)	43(2)	18(2)	0	0	0(2)
S(1)	40(1)	35(1)	45(1)	-1(1)	1(1)	-6(1)
O(1)	50(2)	38(2)	43(2)	-7(1)	0(1)	-3(1)
O(2)	46(2)	41(2)	66(2)	-3(1)	11(1)	-3(1)

O(3)	57(2)	50(2)	65(2)	9(2)	-16(2)	-17(2)
O(4)	39(1)	35(1)	29(1)	-2(1)	-7(1)	0(1)
O(6)	44(4)	97(7)	89(7)	-6(5)	6(4)	-14(4)
O(8)	57(5)	65(6)	132(10)	8(6)	-15(5)	7(4)
O(5)	110(7)	75(5)	181(10)	-9(6)	56(7)	-12(5)
O(7)	61(5)	120(9)	125(9)	-44(8)	-15(5)	22(5)
O(9)	79(6)	68(5)	105(7)	2(5)	-19(5)	1(4)
O(10)	73(5)	78(6)	110(8)	-13(5)	-10(5)	-9(4)

Table S6 Fractional atomic coordinates ($x10^4$) and isotropic thermal factors ($x10^3$) of hydrogen atoms for compound **2**.

Atoms	**X**	**Y**	**Z**	**U_{iso}, Å^2**
H(2)	8397	179	1293	44
H(3)	9633	-279	984	44
H(7)	7059	1573	812	46
H(8)	6032	814	980	49
H(10)	6793	380	2649	54
H(11)	7841	1105	2460	52
H(12)	11093	2542	269	41
H(13)	11120	2457	-763	43
H(16)	9057	3114	-1667	51
H(17)	9088	3096	-2698	50
H(20)	9660(2)	3885(2)	-3758(2)	34(1)
H(21)	9100(2)	3510(3)	-4022(2)	65(2)

Table S7 π-π interactions parameters for compound **1**.

Face-to-face

Cg^I	*Cg^{II}*	*Cg^I-Cg^{II}* (Å)	*$Cg^I\cdots Cg^{II}$* (º)
Cg(7)	Cg(17)	4.041(9)	10.77

Edge-to-face

X-H	*Cg*	*H-Cg* (Å)	*X-H···Cg* (º)
C(12)-H(12)	Cg(13)	2.51	88.10
C(13)-H(13)	Cg(12)	2.45	88.10
C(18)-H(18)	Cg(11)	2.94	87.35
C(19)-H(19)	Cg(8)	2.90	89.16
C(27)-H(27)	Cg(16)	2.68	73.96
C(47)-H(47)	Cg(1)	2.97	83.64

Table S8 Most significant bond angles (º) and distances (Å) for compound **1** and **2** (distances in bold).

Compound **1**

Co(1). CoN_6 octahedra

Co1	**N1**	**N2**	**N3**	**N4**
N4	89.84(4)	89.89(4)	180	**2.296(2)**
N3	90.16(4)	90.11(4)	**2.357(2)**	
N2	90.21(6)	**1.962(1)**		
N1	**1.966(1)**			

Co(2). CoN_4 square planar

Co2	**N5**	**N6**
N6	90.38(5)	**2.055(1)**
N5	**2.032(1)**	

Compound **2**

Co(1). CoN_6 octahedra

Co1	**N1**	**N2**
N2	88.20(7)	**1.976(4)**
N1	**1.963(3)**	

Co(2). $CoN_2(H_2O)_4$ octahedra

Co2	**O4**	**N3**
N3	90.76(6)	**2.137(4)**
O4	**2.092(3)**	

Table S9 Hydrogen bond parameters for compound **2**.

D-H	*A*	*D-H* (Å)	*H···A* (Å)	*O-H···A* (º)
O(4)-H(20)	O(3)^{i}	0.81(3)	1.93(3)	173(4)
O(4)-H(21)	O(1)^{ii}	0.82(4)	1.89(4)	178(4)

i) -1/2+x,1/2+y,1/2+z; ii) -1/4-y,-1/4+x,3/4-z

Table S10 Bond distances (Å) and angles (º) for compound **1**.

Distances

C(1)-N(1)	1.375(2)	C(29)-N(6)	1.370(2)
C(1)-C(10)^{i}	1.396(2)	C(29)-C(38)^{iv}	1.401(2)
C(1)-C(2)	1.446(2)	C(29)-C(30)	1.436(2)
C(2)-C(3)	1.357(2)	C(30)-C(31)	1.358(2)
C(2)-H(2)	0.9500	C(30)-H(30)	0.9500
C(3)-C(4)	1.445(2)	C(31)-C(32)	1.433(2)
C(3)-H(3)	0.9500	C(31)-H(31)	0.9500
C(4)-N(1)	1.374(2)	C(32)-N(6)	1.376(2)
C(4)-C(5)	1.400(2)	C(32)-C(33)	1.390(2)
C(5)-C(6)	1.395(2)	C(33)-C(34)	1.402(2)
C(5)-C(17)	1.496(2)	C(33)-C(45)	1.498(2)
C(6)-N(2)	1.376(2)	C(34)-N(5)	1.371(2)
C(6)-C(7)	1.441(2)	C(34)-C(35)	1.449(2)
C(7)-C(8)	1.353(2)	C(35)-C(36)	1.353(2)
C(7)-H(7)	0.9500	C(35)-H(35)	0.9500
C(8)-C(9)	1.442(2)	C(36)-C(37)	1.448(2)
C(8)-H(8)	0.9500	C(36)-H(36)	0.9500
C(9)-N(2)	1.372(2)	C(37)-N(5)	1.372(2)
C(9)-C(10)	1.401(2)	C(37)-C(38)	1.398(2)

C(10)-C(1)[i]	1.396(2)	C(38)-C(29)[iv]	1.401(2)
C(10)-C(11)	1.495(2)	C(38)-C(39)	1.498(2)
C(11)-C(12)	1.388(2)	C(39)-C(44)	1.390(2)
C(11)-C(16)	1.397(2)	C(39)-C(40)	1.397(2)
C(12)-C(13)	1.395(2)	C(40)-C(41)	1.388(2)
C(12)-H(12)	0.9500	C(40)-H(40)	0.9500
C(13)-C(14)	1.381(3)	C(41)-C(42)	1.388(3)
C(13)-H(13)	0.9500	C(41)-H(41)	0.9500
C(14)-C(15)	1.379(3)	C(42)-C(43)	1.390(2)
C(14)-H(14)	0.9500	C(42)-H(42)	0.9500
C(15)-C(16)	1.392(2)	C(43)-C(44)	1.393(2)
C(15)-H(15)	0.9500	C(43)-H(43)	0.9500
C(16)-H(16)	0.9500	C(44)-H(44)	0.9500
C(17)-C(18)	1.393(2)	C(45)-C(50)	1.394(2)
C(17)-C(22)	1.399(2)	C(45)-C(46)	1.399(2)
C(18)-C(19)	1.397(3)	C(46)-C(47)	1.393(2)
C(18)-H(18)	0.9500	C(46)-H(46)	0.9500
C(19)-C(20)	1.386(3)	C(47)-C(48)	1.385(3)
C(19)-H(19)	0.9500	C(47)-H(47)	0.9500
C(20)-C(21)	1.385(3)	C(48)-C(49)	1.385(3)
C(20)-H(20)	0.9500	C(48)-H(48)	0.9500
C(21)-C(22)	1.391(2)	C(49)-C(50)	1.392(2)
C(21)-H(21)	0.9500	C(49)-H(49)	0.9500
C(22)-H(22)	0.9500	C(50)-H(50)	0.9500
C(23)-N(3)	1.340(2)	Co(1)-N(2)	1.962(1)
C(23)-C(24)	1.393(2)	Co(1)-N(2)[i]	1.962(1)
C(23)-H(23)	0.9500	Co(1)-N(1)[i]	1.966(1)
C(24)-C(25)	1.394(2)	Co(1)-N(1)	1.966(1)
C(24)-H(24)	0.9500	Co(1)-N(4)	2.296(2)
C(25)-C(24)[i]	1.394(2)	Co(1)-N(3)	2.357(2)
C(25)-C(26)[ii]	1.482(3)	Co(2)-N(5)	2.032(1)
C(26)-C(27)	1.396(2)	Co(2)-N(5)[iv]	2.032(1)
C(26)-C(27)[i]	1.396(2)	Co(2)-N(6)	2.055(1)
C(26)-C(25)[iii]	1.482(3)	Co(2)-N(6)[iv]	2.055(1)
C(27)-C(28)	1.393(2)	Co(2)-H(1N)	1.22(3)
C(27)-H(27)	0.9500	N(3)-C(23)[i]	1.340(2)
C(28)-N(4)	1.338(2)	N(4)-C(28)[i]	1.338(2)
C(28)-H(28)	0.9500	N(6)-H(1N)	0.85(3)

Angles

N(1)-C(1)-C(10)[i]	124.7(1)	C(29)[iv]-C(38)-C(39)	115.3(1)
N(1)-C(1)-C(2)	110.2(1)	C(44)-C(39)-C(40)	118.8(2)
C(10)[i]-C(1)-C(2)	124.9(2)	C(44)-C(39)-C(38)	120.3(2)
C(3)-C(2)-C(1)	106.7(1)	C(40)-C(39)-C(38)	120.7(2)

C(3)-C(2)-H(2)	126.7	C(41)-C(40)-C(39)	120.5(2)
C(1)-C(2)-H(2)	126.7	C(41)-C(40)-H(40)	119.8
C(2)-C(3)-C(4)	106.9(1)	C(39)-C(40)-H(40)	119.8
C(2)-C(3)-H(3)	126.5	C(42)-C(41)-C(40)	120.4(2)
C(4)-C(3)-H(3)	126.5	C(42)-C(41)-H(41)	119.8
N(1)-C(4)-C(5)	125.4(1)	C(40)-C(41)-H(41)	119.8
N(1)-C(4)-C(3)	110.1(1)	C(41)-C(42)-C(43)	119.5(2)
C(5)-C(4)-C(3)	124.2(2)	C(41)-C(42)-H(42)	120.3
C(6)-C(5)-C(4)	122.9(1)	C(43)-C(42)-H(42)	120.3
C(6)-C(5)-C(17)	119.2(1)	C(42)-C(43)-C(44)	120.1(2)
C(4)-C(5)-C(17)	117.8(1)	C(42)-C(43)-H(43)	120.0
N(2)-C(6)-C(5)	124.9(1)	C(44)-C(43)-H(43)	120.0
N(2)-C(6)-C(7)	109.6(1)	C(39)-C(44)-C(43)	120.7(2)
C(5)-C(6)-C(7)	125.2(1)	C(39)-C(44)-H(44)	119.6
C(8)-C(7)-C(6)	107.2(1)	C(43)-C(44)-H(44)	119.6
C(8)-C(7)-H(7)	126.4	C(50)-C(45)-C(46)	118.9(2)
C(6)-C(7)-H(7)	126.4	C(50)-C(45)-C(33)	119.8(2)
C(7)-C(8)-C(9)	106.8(1)	C(46)-C(45)-C(33)	121.3(2)
C(7)-C(8)-H(8)	126.6	C(47)-C(46)-C(45)	120.3(2)
C(9)-C(8)-H(8)	126.6	C(47)-C(46)-H(46)	119.9
N(2)-C(9)-C(10)	125.8(1)	C(45)-C(46)-H(46)	119.9
N(2)-C(9)-C(8)	109.9(1)	C(48)-C(47)-C(46)	120.2(2)
C(10)-C(9)-C(8)	123.9(1)	C(48)-C(47)-H(47)	119.9
C(1)^{1}-C(10)-C(9)	122.2(1)	C(46)-C(47)-H(47)	119.9
C(1)^{1}-C(10)-C(11)	120.7(1)	C(49)-C(48)-C(47)	120.0(2)
C(9)-C(10)-C(11)	117.1(1)	C(49)-C(48)-H(48)	120.0
C(12)-C(11)-C(16)	118.4(2)	C(47)-C(48)-H(48)	120.0
C(12)-C(11)-C(10)	123.1(2)	C(48)-C(49)-C(50)	120.1(2)
C(16)-C(11)-C(10)	118.6(1)	C(48)-C(49)-H(49)	119.9
C(11)-C(12)-C(13)	120.5(2)	C(50)-C(49)-H(49)	119.9
C(11)-C(12)-H(12)	119.7	C(49)-C(50)-C(45)	120.5(2)
C(13)-C(12)-H(12)	119.7	C(49)-C(50)-H(50)	119.7
C(14)-C(13)-C(12)	120.8(2)	C(45)-C(50)-H(50)	119.7
C(14)-C(13)-H(13)	119.6	N(2)-Co(1)-N(2)^{1}	179.77(7)
C(12)-C(13)-H(13)	119.6	N(2)-Co(1)-N(1)^{1}	89.79(6)
C(15)-C(14)-C(13)	119.1(2)	N(2)^{1}-Co(1)-N(1)^{1}	90.21(6)
C(15)-C(14)-H(14)	120.5	N(2)-Co(1)-N(1)	90.21(6)
C(13)-C(14)-H(14)	120.5	N(2)^{1}-Co(1)-N(1)	89.79(6)
C(14)-C(15)-C(16)	120.7(2)	N(1)^{1}-Co(1)-N(1)	179.68(8)
C(14)-C(15)-H(15)	119.7	N(2)-Co(1)-N(4)	89.89(4)
C(16)-C(15)-H(15)	119.7	N(2)^{1}-Co(1)-N(4)	89.89(4)
C(15)-C(16)-C(11)	120.6(2)	N(1)^{1}-Co(1)-N(4)	89.84(4)
C(15)-C(16)-H(16)	119.7	N(1)-Co(1)-N(4)	89.84(4)
C(11)-C(16)-H(16)	119.7	N(2)-Co(1)-N(3)	90.11(4)

C(18)-C(17)-C(22)	118.8(2)	N(2)^{i}-Co(1)-N(3)	90.11(4)
C(18)-C(17)-C(5)	122.2(2)	N(1)^{i}-Co(1)-N(3)	90.16(4)
C(22)-C(17)-C(5)	119.0(2)	N(1)-Co(1)-N(3)	90.16(4)
C(17)-C(18)-C(19)	120.3(2)	N(4)-Co(1)-N(3)	180.0
C(17)-C(18)-H(18)	119.9	N(5)-Co(2)-N(5)^{iv}	180.00(4)
C(19)-C(18)-H(18)	119.9	N(5)-Co(2)-N(6)	90.38(5)
C(20)-C(19)-C(18)	120.3(2)	N(5)^{iv}-Co(2)-N(6)	89.62(5)
C(20)-C(19)-H(19)	119.9	N(5)-Co(2)-N(6)^{iv}	89.62(5)
C(18)-C(19)-H(19)	119.9	N(5)^{iv}-Co(2)-N(6)^{iv}	90.38(5)
C(21)-C(20)-C(19)	120.1(2)	N(6)-Co(2)-N(6)^{iv}	179.9(1)
C(21)-C(20)-H(20)	120.0	N(5)-Co(2)-H(1N)	91.4(1)
C(19)-C(20)-H(20)	120.0	N(5)^{iv}-Co(2)-H(1N)	88.6(1)
C(20)-C(21)-C(22)	119.8(2)	N(6)-Co(2)-H(1N)	4.1(1)
C(20)-C(21)-H(21)	120.1	N(6)^{iv}-Co(2)-H(1N)	176.0(1)
C(22)-C(21)-H(21)	120.1	C(4)-N(1)-C(1)	106.0(1)
C(21)-C(22)-C(17)	120.9(2)	C(4)-N(1)-Co(1)	126.6(1)
C(21)-C(22)-H(22)	119.6	C(1)-N(1)-Co(1)	127.4(1)
C(17)-C(22)-H(22)	119.6	C(9)-N(2)-C(6)	106.2(1)
N(3)-C(23)-C(24)	124.0(2)	C(9)-N(2)-Co(1)	126.8(1)
N(3)-C(23)-H(23)	118.0	C(6)-N(2)-Co(1)	126.9(1)
C(24)-C(23)-H(23)	118.0	C(23)-N(3)-C(23)^{i}	116.2(2)
C(23)-C(24)-C(25)	119.4(2)	N(2)^{i}-Co(1)-N(1)^{i}	90.21(6)
C(23)-C(24)-H(24)	120.3	N(2)-Co(1)-N(1)	90.21(6)
C(25)-C(24)-H(24)	120.3	N(2)^{i}-Co(1)-N(1)	89.79(6)
C(24)-C(25)-C(24)^{i}	117.0(2)	N(1)^{i}-Co(1)-N(1)	179.68(8)
C(24)-C(25)-C(26)^{ii}	121.5(1)	N(2)-Co(1)-N(4)	89.89(4)
C(24)^{i}-C(25)-C(26)^{ii}	121.5(1)	N(2)^{i}-Co(1)-N(4)	89.89(4)
C(27)-C(26)-C(27)^{i}	117.2(2)	N(1)^{i}-Co(1)-N(4)	89.84(4)
C(27)-C(26)-C(25)^{iii}	121.4(1)	N(1)-Co(1)-N(4)	89.84(4)
C(27)^{i}-C(26)-C(25)^{iii}	121.4(1)	N(2)-Co(1)-N(3)	90.11(4)
C(28)-C(27)-C(26)	119.3(2)	N(2)^{i}-Co(1)-N(3)	90.11(4)
C(28)-C(27)-H(27)	120.4	N(1)^{i}-Co(1)-N(3)	90.16(4)
C(26)-C(27)-H(27)	120.4	N(1)-Co(1)-N(3)	90.16(4)
N(4)-C(28)-C(27)	123.6(1)	N(4)-Co(1)-N(3)	180.0
N(4)-C(28)-H(28)	118.2	N(5)-Co(2)-N(5)^{iv}	180.00(4)
C(27)-C(28)-H(28)	118.2	N(5)-Co(2)-N(6)	90.38(5)
N(6)-C(29)-C(38)^{iv}	126.7(2)	N(5)^{iv}-Co(2)-N(6)	89.62(5)
N(6)-C(29)-C(30)	108.1(1)	N(5)-Co(2)-N(6)^{iv}	89.62(5)
C(38)^{i}v-C(29)-C(30)	125.2(2)	N(5)^{iv}-Co(2)-N(6)^{iv}	90.38(5)
C(31)-C(30)-C(29)	107.5(1)	N(6)-Co(2)-N(6)^{iv}	179.9(1)
C(31)-C(30)-H(30)	126.2	N(5)-Co(2)-H(1N)	91.4(1)
C(29)-C(30)-H(30)	126.2	N(5)^{iv}-Co(2)-H(1N)	88.6(1)
C(30)-C(31)-C(32)	107.9(1)	N(6)-Co(2)-H(1N)	4.1(1)
C(30)-C(31)-H(31)	126.0	N(6)^{iv}-Co(2)-H(1N)	175.9(1)

C(32)-C(31)-H(31)	126.0	C(4)-N(1)-C(1)	106.0(1)
N(6)-C(32)-C(33)	127.0(1)	C(4)-N(1)-Co(1)	126.6(1)
N(6)-C(32)-C(31)	107.7(1)	C(1)-N(1)-Co(1)	127.4(1)
C(33)-C(32)-C(31)	125.2(2)	C(9)-N(2)-C(6)	106.2(1)
C(32)-C(33)-C(34)	124.9(2)	C(9)-N(2)-Co(1)	126.8(1)
C(32)-C(33)-C(45)	116.5(1)	C(6)-N(2)-Co(1)	126.9(1)
C(34)-C(33)-C(45)	118.5(1)	C(23)-N(3)-C(23)^{1}	116.2(2)
N(5)-C(34)-C(33)	125.6(2)	C(23)-N(3)-Co(1)	121.91(9)
N(5)-C(34)-C(35)	110.5(1)	C(23)^{1}-N(3)-Co(1)	121.91(9)
C(33)-C(34)-C(35)	123.9(2)	C(28)-N(4)-C(28)^{1}	117.0(2)
C(36)-C(35)-C(34)	106.7(1)	C(28)-N(4)-Co(1)	121.5(2)
C(36)-C(35)-H(35)	126.6	C(28)^{1}-N(4)-Co(1)	121.5(2)
C(34)-C(35)-H(35)	126.6	C(34)-N(5)-C(37)	105.5(1)
C(35)-C(36)-C(37)	106.6(2)	C(34)-N(5)-Co(2)	126.8(1)
C(35)-C(36)-H(36)	126.7	C(37)-N(5)-Co(2)	127.5(1)
C(37)-C(36)-H(36)	126.7	C(29)-N(6)-C(32)	108.8(1)
N(5)-C(37)-C(38)	125.5(2)	C(29)-N(6)-Co(2)	125.7(1)
N(5)-C(37)-C(36)	110.7(1)	C(32)-N(6)-Co(2)	125.0(1)
C(38)-C(37)-C(36)	123.8(2)	C(29)-N(6)-H(1N)	125(2)
C(37)-C(38)-C(29)^{iv}	124.6(2)	C(32)-N(6)-H(1N)	127(2)
C(37)-C(38)-C(39)	120.2(1)		

Symmetry codes: i) -x+1,y,-z+1/2; ii) x,y+1,z; iii) x,y-1,z; iv) -x+3/2,-y+1/2,-z+1

Table S11 Bond distances (Å) and angles (º) for compound **2**.

Distances

C(1)-N(1)	1.376(5)	C(14)-C(15)	1.481(8)
C(1)-C(5)	1.391(5)	C(15)-C(16)^{iii}	1.388(5)
C(1)-C(2)	1.436(5)	C(15)-C(16)	1.388(5)
C(2)-C(3)	1.344(6)	C(16)-C(17)	1.374(5)
C(2)-H(2)	0.9500	C(16)-H(16)	0.9500
C(3)-C(4)	1.433(5)	C(17)-N(3)	1.335(5)
C(3)-H(3)	0.9500	C(17)-H(17)	0.9500
C(4)-N(1)	1.377(5)	Co(1)-N(1)^{iii}	1.963(3)
C(4)-C(5)^{i}	1.388(5)	Co(1)-N(1)	1.963(3)
C(5)-C(4)^{ii}	1.388(5)	Co(1)-N(1)^{i}	1.963(3)
C(5)-C(6)	1.481(5)	Co(1)-N(1)^{ii}	1.963(3)
C(6)-C(11)	1.381(5)	Co(1)-N(2)^{ii}	1.976(4)
C(6)-C(7)	1.388(6)	Co(1)-N(2)	1.976(4)
C(7)-C(8)	1.378(6)	Co(2)-O(4)	2.092(3)
C(7)-H(7)	0.9500	Co(2)-O(4)^{iii}	2.092(3)

C(8)-C(9)	1.377(6)	Co(2)-O(4)^{iv}	2.092(3)
C(8)-H(8)	0.9500	Co(2)-O(4)^{v}	2.092(3)
C(9)-C(10)	1.390(6)	Co(2)-N(3)^{iv}	2.137(4)
C(9)-S(1)	1.776(4)	Co(2)-N(3)	2.137(4)
C(10)-C(11)	1.378(6)	N(2)-C(12)^{iii}	1.339(4)
C(10)-H(10)	0.9500	N(3)-C(17)^{iii}	1.335(5)
C(11)-H(11)	0.9500	S(1)-O(2)	1.451(3)
C(12)-N(2)	1.339(4)	S(1)-O(3)	1.458(4)
C(12)-C(13)	1.379(5)	S(1)-O(1)	1.457(3)
C(12)-H(12)	0.9500	O(4)-H(20)	0.81(1)
C(13)-C(14)	1.384(4)	O(4)-H(21)	0.81(1)
C(13)-H(13)	0.9500	O(9)-O(10)	1.14(1)
C(14)-C(13)^{iii}	1.384(4)		

Angles

N(1)-C(1)-C(5)	125.9(3)	N(3)-C(17)-H(17)	118.3
N(1)-C(1)-C(2)	109.2(3)	C(16)-C(17)-H(17)	118.3
C(5)-C(1)-C(2)	124.8(4)	N(1)^{iii}-Co(1)-N(1)	176.4(1)
C(3)-C(2)-C(1)	107.6(3)	N(1)^{iii}-Co(1)-N(1)^{i}	90.058(5)
C(3)-C(2)-H(2)	126.2	N(1)-Co(1)-N(1)^{i}	90.057(5)
C(1)-C(2)-H(2)	126.2	N(1)^{iii}-Co(1)-N(1)^{ii}	90.054(5)
C(2)-C(3)-C(4)	107.2(3)	N(1)-Co(1)-N(1)^{ii}	90.057(5)
C(2)-C(3)-H(3)	126.4	N(1)^{i}-Co(1)-N(1)^{ii}	176.4(1)
C(4)-C(3)-H(3)	126.4	N(1)-Co(1)-N(2)^{ii}	91.80(7)
N(1)-C(4)-C(5)^{i}	125.1(3)	N(1)^{i}-Co(1)-N(2)^{ii}	88.20(7)
N(1)-C(4)-C(3)	109.6(3)	N(1)^{ii}-Co(1)-N(2)^{ii}	88.20(7)
C(5)^{i}-C(4)-C(3)	124.8(3)	N(1)^{iii}-Co(1)-N(2)	88.20(7)
C(4)^{ii}-C(5)-C(1)	122.6(3)	N(1)-Co(1)-N(2)	88.20(7)
C(4)^{ii}-C(5)-C(6)	120.4(3)	N(1)^{ii}-Co(1)-N(2)	91.80(7)
C(1)-C(5)-C(6)	116.7(3)	N(1)^{ii}-Co(1)-N(2)	91.80(7)
C(11)-C(6)-C(7)	119.0(4)	N(2)^{ii}-Co(1)-N(2)	180.0
C(11)-C(6)-C(5)	119.5(3)	O(4)-Co(2)-O(4)^{iii}	178.5(1)
C(7)-C(6)-C(5)	121.4(3)	O(4)-Co(2)-O(4)^{iv}	90.009(2)
C(8)-C(7)-C(6)	120.9(4)	O(4)^{iii}-Co(2)-O(4)^{iv}	90.014(2)
C(8)-C(7)-H(7)	119.5	O(4)-Co(2)-O(4)^{v}	90.010(2)
C(6)-C(7)-H(7)	119.5	O(4)^{iii}-Co(2)-O(4)^{v}	90.008(2)
C(7)-C(8)-C(9)	119.1(4)	O(4)^{iv}-Co(2)-O(4)^{v}	178.5(1)
C(7)-C(8)-H(8)	120.5	O(4)-Co(2)-N(3)^{iv}	89.24(6)
C(9)-C(8)-H(8)	120.5	O(4)^{iii}-Co(2)-N(3)^{iv}	89.24(6)

C(8)-C(9)-C(10)	120.7(4)	O(4)^{iv}-Co(2)-N(3)^{iv}	90.76(6)
C(8)-C(9)-S(1)	121.5(3)	O(4)^{v}-Co(2)-N(3)^{iv}	90.76(6)
C(10)-C(9)-S(1)	117.7(3)	O(4)-Co(2)-N(3)	90.76(6)
C(11)-C(10)-C(9)	119.2(4)	O(4)^{iii}-Co(2)-N(3)	90.76(6)
C(11)-C(10)-H(10)	120.4	O(4)^{iv}-Co(2)-N(3)	89.24(6)
C(9)-C(10)-H(10)	120.4	O(4)^{v}-Co(2)-N(3)	89.24(6)
C(10)-C(11)-C(6)	120.7(4)	N(3)^{iv}-Co(2)-N(3)	180.0
C(10)-C(11)-H(11)	119.7	C(1)-N(1)-C(4)	106.3(3)
C(6)-C(11)-H(11)	119.7	C(1)-N(1)-Co(1)	126.7(2)
N(2)-C(12)-C(13)	122.4(3)	C(4)-N(1)-Co(1)	127.0(2)
N(2)-C(12)-H(12)	118.8	C(12)^{iii}-N(2)-C(12)	117.7(4)
C(13)-C(12)-H(12)	118.8	C(12)^{iii}-N(2)-Co(1)	121.2(2)
C(12)-C(13)-C(14)	120.4(3)	C(12)-N(2)-Co(1)	121.2(2)
C(12)-C(13)-H(13)	119.8	C(17)^{iii}-N(3)-C(17)	117.3(5)
C(14)-C(13)-H(13)	119.8	C(17)^{iii}-N(3)-Co(2)	121.4(2)
C(13)-C(14)-C(13)^{iii}	116.5(5)	C(17)-N(3)-Co(2)	121.4(2)
C(13)-C(14)-C(15)	121.7(2)	O(2)-S(1)-O(3)	113.0(2)
C(13)^{iii}-C(14)-C(15)	121.7(2)	O(2)-S(1)-O(1)	111.7(2)
C(16)^{iii}-C(15)-C(16)	117.7(5)	O(3)-S(1)-O(1)	113.0(2)
C(16)^{iii}-C(15)-C(14)	121.1(2)	O(2)-S(1)-C(9)	108.6(2)
C(16)-C(15)-C(14)	121.2(2)	O(3)-S(1)-C(9)	105.2(2)
C(17)-C(16)-C(15)	119.1(4)	O(1)-S(1)-C(9)	104.6(2)
C(17)-C(16)-H(16)	120.4	Co(2)-O(4)-H(20)	117(3)
C(15)-C(16)-H(16)	120.4	Co(2)-O(4)-H(21)	112(4)
N(3)-C(17)-C(16)	123.4(4)	H(20)-O(4)-H(21)	112(3)

Symmetry codes: i) -y+5/4,x-3/4,-z+1/4; ii) y+3/4,-x+5/4,-z+1/4; iii) -x+2,-y+1/2,z+0; iv) y+3/4,-x+5/4,-z-3/4; v) -y+5/4,x-3/4,-z-3/4