Novel layered 2D and triply interpenetrating 3D cobalt-diazo crown ether benzene carboxylate based coordination polymers: Synthesis, structure and magnetic properties

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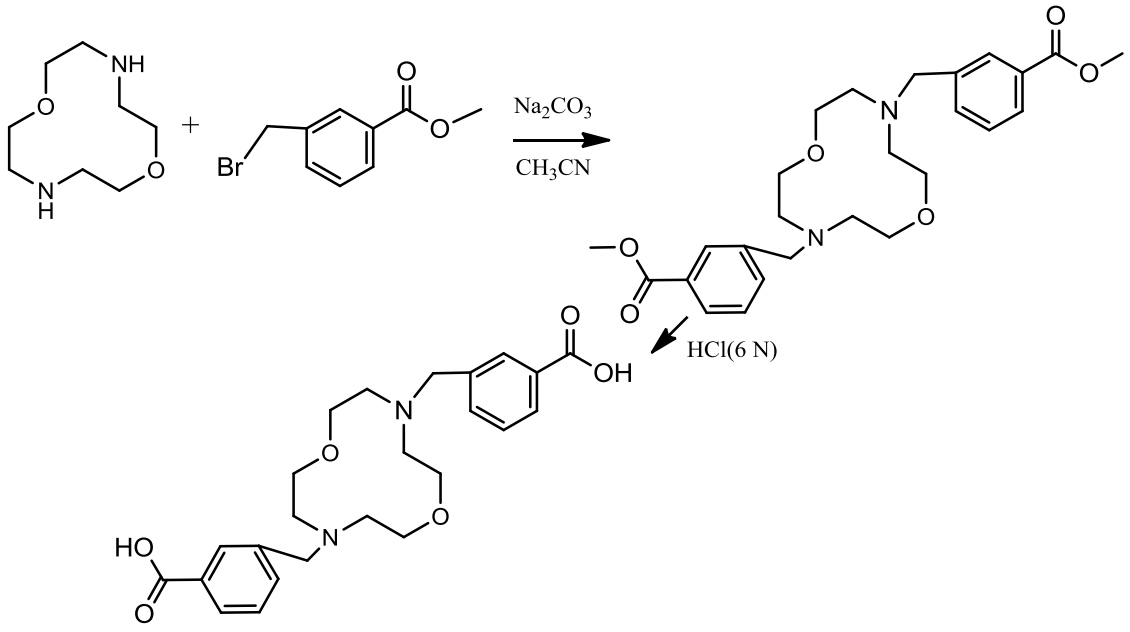
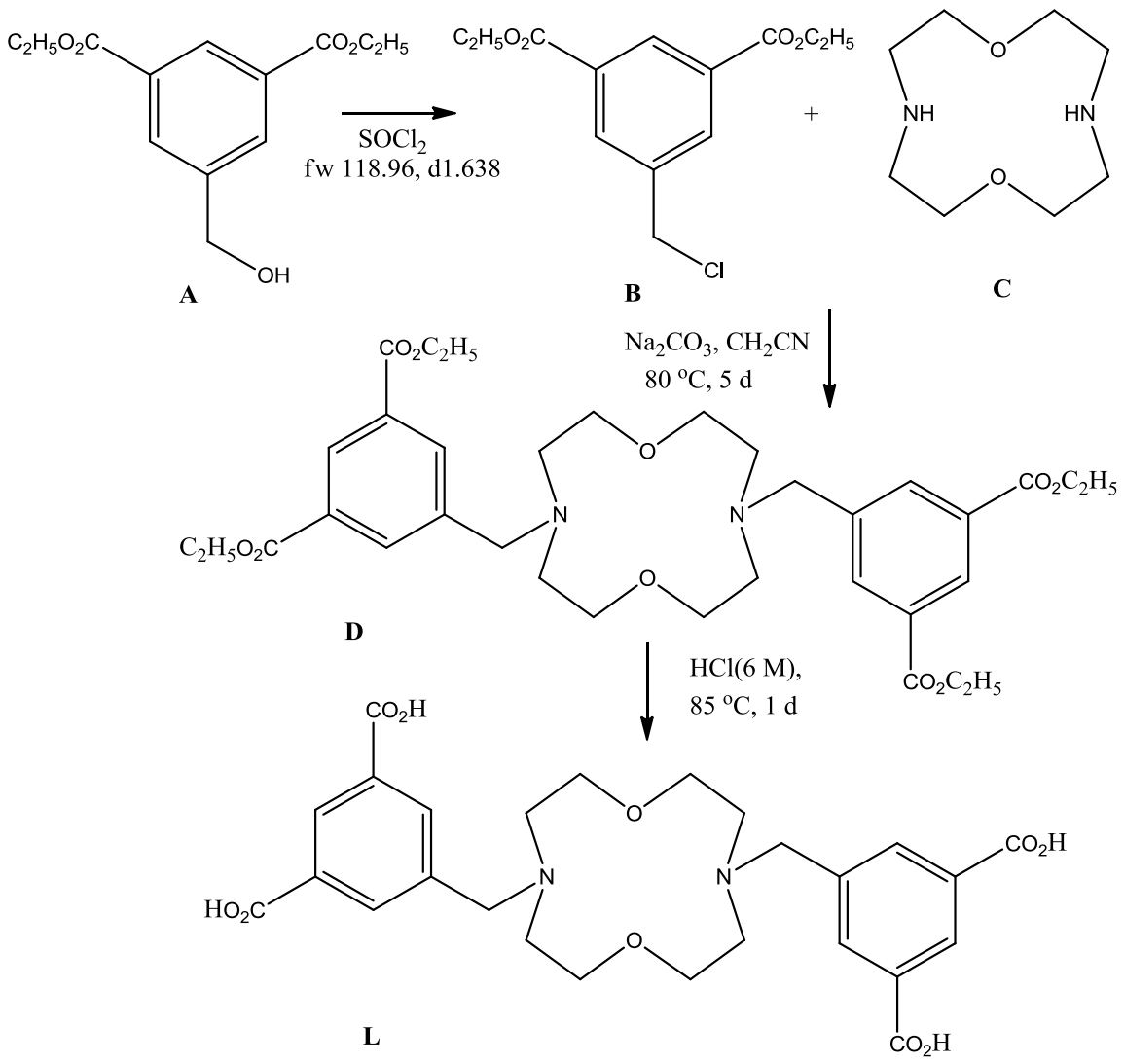
Electronic Supplemental information



Scheme S1. Synthesis of ligand **L1H$_2$**.



Scheme S2. Synthesis of ligand **L2H$_4$**

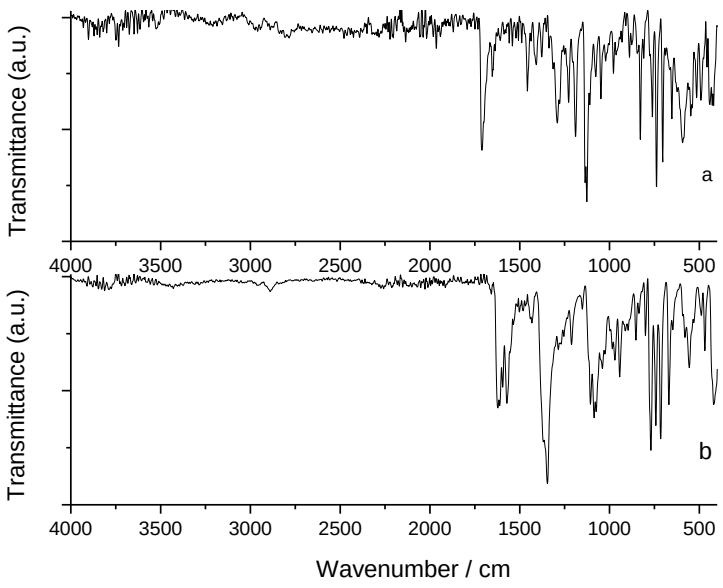


Fig. S1a . IR spectra: a) ligand **L1H$_2$**; b) compound **1**

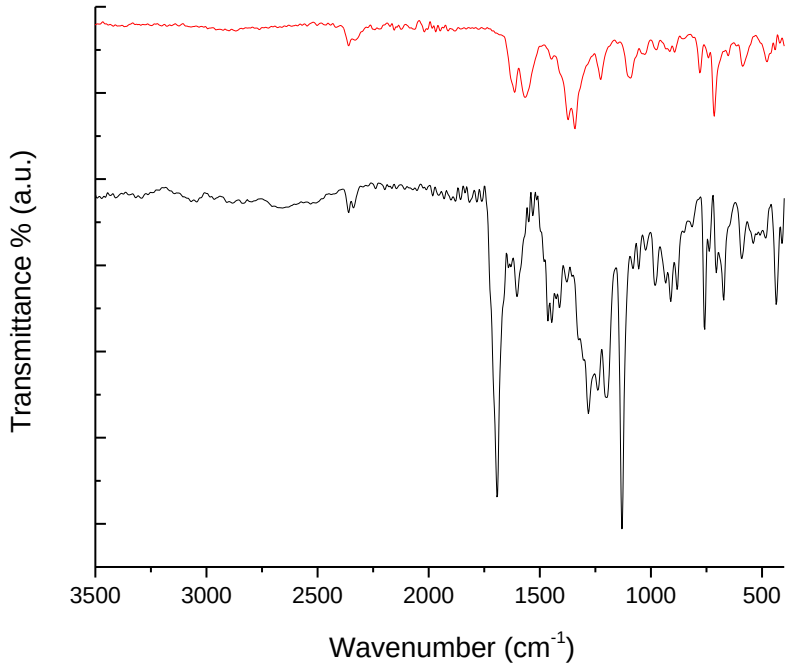


Fig. S1b. IR spectra of **L2H$_4$** (bottom) and compound **2**(top)

Compound 1

Table S1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **1**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	U(eq)
Co1	0	3657.9(3)	5000	18.76(11)
O2	4114.6(10)	343(2)	4062(2)	26.2(4)
O3	4579.5(13)	1008(3)	2090(2)	34.7(5)
O1	904.0(11)	2172(2)	6833(2)	25.7(4)
N1	809.1(12)	2449(2)	3747(2)	22.1(4)
C1	4054.1(14)	1085(3)	2823(3)	22.0(5)
C5	1411.2(12)	3712(4)	3503(2)	22.3(4)
C10	1731.9(13)	3731(4)	976(2)	24.8(4)
C2	3248.6(14)	2069(3)	2181(3)	20.7(4)
C7	-521.6(17)	1028(4)	2397(3)	30.2(6)
C3	2722.7(14)	2399(3)	3098(3)	20.4(4)
C12	3011.9(16)	2612(3)	666(3)	24.6(5)
C11	2258.1(15)	3445(4)	65(3)	27.2(5)
C6	260.8(16)	1864(3)	2227(3)	27.6(5)
C8	1596.5(15)	1559(3)	6357(3)	28.6(5)
C4	1959.6(14)	3238(3)	2497(3)	21.0(5)
C9	1265.0(16)	1060(3)	4691(3)	28.0(5)
O1W	5000	3128(4)	0	50.0(8)

Table S2 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **1**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka\times b\times U_{12}]$

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	U_{12}
Co1	14.20(18)	18.98(19)	23.4(2)	0	6.06(14)	0
O2	22.4(8)	29.9(9)	28.2(9)	7.7(8)	10.6(7)	4.4(7)
O3	29.9(10)	42.9(12)	37.5(12)	9.5(9)	19.7(9)	10.4(9)
O1	21.5(8)	28.8(9)	29.6(10)	5.7(8)	11.8(7)	6.1(7)
N1	18.3(9)	21.9(9)	25.9(10)	0.3(8)	6.5(8)	1.4(7)
C1	18.2(10)	21.5(11)	27.8(12)	0.2(9)	9.1(9)	0.5(9)
C5	17.6(8)	20.8(9)	29.2(10)	-0.7(13)	8.3(7)	0.0(12)
C10	19.3(9)	25.8(10)	27.2(10)	3.4(13)	3.9(7)	3.4(13)
C2	17.2(10)	19.1(10)	26.3(12)	0.6(9)	7.4(9)	1.2(8)
C7	25.8(13)	32.6(14)	32.4(15)	-12.7(11)	8.9(11)	-8.2(11)
C3	19.4(10)	21.9(11)	20.6(11)	1.1(9)	7.1(8)	0.3(8)
C12	27.0(12)	24.4(11)	24.8(12)	-0.5(9)	11.4(10)	0.8(9)
C11	28.8(11)	29.8(15)	21.7(11)	4.2(10)	5.3(8)	1.4(10)
C6	23.8(12)	34.8(14)	26.0(13)	-8.4(10)	10.1(10)	-5.8(10)
C8	20.2(11)	32.6(12)	33.8(14)	7.6(11)	9(1)	9.2(10)
C4	17.7(9)	21.5(11)	24.7(11)	0.7(8)	7.7(8)	-0.4(7)
C9	24.3(11)	22.3(11)	41.3(15)	3.9(10)	15.4(11)	6.1(9)

O1W	55.7(19)	48.3(18)	59(2)	0	37.8(17)	0	

Table S3. Bond Lengths for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Co1	$O2^{1}$	2.0112(17)	N1	C9	1.493(3)
Co1	$O2^{2}$	2.0112(17)	C1	C2	1.517(3)
Co1	O1	2.2443(18)	C5	C4	1.521(3)
Co1	$O1^{3}$	2.2442(18)	C10	C11	1.391(3)
Co1	N1	2.236(2)	C10	C4	1.387(3)
Co1	$N1^{3}$	2.236(2)	C2	C3	1.401(3)
O2	$Co1^{4}$	2.0112(17)	C2	C12	1.396(4)
O2	C1	1.264(3)	C7	$O1^{3}$	1.430(3)
O3	C1	1.246(3)	C7	C6	1.512(4)
O1	$C7^{3}$	1.430(3)	C3	C4	1.398(3)
O1	C8	1.431(3)	C12	C11	1.383(3)
N1	C5	1.500(3)	C8	C9	1.513(4)
N1	C6	1.493(3)			

[1]1/2-X,1/2+Y,1-Z; [2]-1/2+X,1/2+Y,+Z; [3]-X,+Y,1-Z; [4]1/2+X,-1/2+Y,+Z

Table S4. Bond Angles for **1** .

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
$O2^{1}$	Co1	$O2^{2}$	92.85(11)	C6	N1	C9	110.62(19)
$O2^{1}$	Co1	O1	79.67(7)	C9	N1	Co1	108.64(15)
$O2^{2}$	Co1	O1	158.50(6)	C9	N1	C5	111.96(18)
$O2^{2}$	Co1	$O1^{3}$	79.67(7)	O2	C1	C2	115.5(2)
$O2^{1}$	Co1	$O1^{3}$	158.50(7)	O3	C1	O2	125.1(2)
$O2^{1}$	Co1	N1	93.18(7)	O3	C1	C2	119.3(2)
$O2^{2}$	Co1	N1	123.92(7)	N1	C5	C4	116.9(2)
$O2^{1}$	Co1	$N1^{3}$	123.92(7)	C4	C10	C11	121.3(2)
$O2^{2}$	Co1	$N1^{3}$	93.18(7)	C3	C2	C1	120.0(2)
$O1^{3}$	Co1	O1	113.97(10)	C12	C2	C1	120.5(2)
$N1^{3}$	Co1	$O1^{3}$	76.93(7)	C12	C2	C3	119.4(2)
N1	Co1	$O1^{3}$	75.00(7)	$O1^{3}$	C7	C6	105.5(2)
N1	Co1	O1	76.93(7)	C4	C3	C2	120.5(2)
$N1^{3}$	Co1	O1	75.00(7)	C11	C12	C2	120.3(2)
$N1^{3}$	Co1	N1	127.16(10)	C12	C11	C10	119.7(2)
C1	O2	$Co1^{4}$	124.59(15)	N1	C6	C7	110.6(2)
$C7^{3}$	O1	Co1	115.66(15)	O1	C8	C9	108.6(2)
$C7^{3}$	O1	C8	115.3(2)	C10	C4	C5	119.9(2)
C8	O1	Co1	112.26(15)	C10	C4	C3	118.8(2)
C5	N1	Co1	106.95(15)	C3	C4	C5	121.2(2)
C6	N1	Co1	109.30(14)	N1	C9	C8	110.1(2)
C6	N1	C5	109.26(18)				

[1]1/2-X,1/2+Y,1-Z; [2]-1/2+X,1/2+Y,+Z; [3]-X,+Y,1-Z; [4]1/2+X,-1/2+Y,+Z

Table S5 Hydrogen Bonds for **1**.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1W	H	O3	0.989(7)	1.847(8)	2.822(3)	168(3)

Table S6 Torsion Angles for **1**.

A	B	C	D	Angle/°
Co1[1]	O2	C1	O3	-7.8(4)
Co1[1]	O2	C1	C2	169.17(14)
Co1	O1	C8	C9	-38.6(2)
Co1	N1	C5	C4	-172.70(15)
Co1	N1	C6	C7	-45.0(2)
Co1	N1	C9	C8	-42.7(2)
O2[2]	Co1	O1	C7[3]	70.4(3)
O2[4]	Co1	O1	C7[3]	141.42(19)
O2[2]	Co1	O1	C8	-154.46(19)
O2[4]	Co1	O1	C8	-83.40(17)
O2[2]	Co1	N1	C5	69.81(15)
O2[4]	Co1	N1	C5	-25.78(14)
O2[2]	Co1	N1	C6	-48.36(18)
O2[4]	Co1	N1	C6	-143.95(16)
O2[2]	Co1	N1	C9	-169.16(14)
O2[4]	Co1	N1	C9	95.25(15)
O2	C1	C2	C3	13.7(3)
O2	C1	C2	C12	-164.5(2)
O3	C1	C2	C3	-169.2(2)
O3	C1	C2	C12	12.7(3)
O1[3]	Co1	O1	C7[3]	-56.03(17)
O1[3]	Co1	O1	C8	79.15(16)
O1[3]	Co1	N1	C5	136.00(14)
O1	Co1	N1	C5	-104.40(14)
O1	Co1	N1	C6	137.42(16)
O1[3]	Co1	N1	C6	17.82(15)
O1[3]	Co1	N1	C9	-102.98(16)
O1	Co1	N1	C9	16.62(14)
O1[3]	C7	C6	N1	54.1(3)
O1	C8	C9	N1	54.7(3)
N1	Co1	O1	C7[3]	-122.8(2)
N1[3]	Co1	O1	C7[3]	11.93(18)
N1	Co1	O1	C8	12.35(16)
N1[3]	Co1	O1	C8	147.11(18)
N1[3]	Co1	N1	C5	-163.79(14)
N1[3]	Co1	N1	C6	78.04(15)
N1[3]	Co1	N1	C9	-42.76(13)

N1	C5	C4	C10	99.8(3)
N1	C5	C4	C3	-84.3(2)
C1	C2	C3	C4	-177.0(2)
C1	C2	C12	C11	177.1(2)
C5	N1	C6	C7	-161.7(2)
C5	N1	C9	C8	75.2(2)
C2	C3	C4	C5	-175.6(2)
C2	C3	C4	C10	0.3(4)
C2	C12	C11	C10	-0.5(4)
C7[3]	O1	C8	C9	96.7(3)
C3	C2	C12	C11	-1.1(4)
C12	C2	C3	C4	1.2(3)
C11	C10	C4	C5	174.1(3)
C11	C10	C4	C3	-1.9(4)
C6	N1	C5	C4	-54.5(3)
C6	N1	C9	C8	-162.7(2)
C4	C10	C11	C12	2.0(4)
C9	N1	C5	C4	68.4(2)
C9	N1	C6	C7	74.6(3)

[1]1/2+X,-1/2+Y,+Z; [2]-1/2+X,1/2+Y,+Z; [3]-X,+Y,1-Z; [4]1/2-X,1/2+Y,1-Z

Table S7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **1.**

Atom	*x*	*y*	*z*	U(eq)
H5A	1792	4035	4519	27
H5B	1076	4683	3046	27
H10	1206	4273	549	30
H7A	-916	747	1379	36
H7B	-366	20	3008	36
H3	2886	2049	4136	24
H12	3370	2408	44	30
H11	2100	3821	-965	33
H6A	585	1096	1784	33
H6B	90	2797	1518	33
H8A	1854	611	6994	34
H8B	2037	2408	6484	34
H9A	1744	718	4320	34
H9B	874	127	4588	34
H	4910(30)	2466(18)	840(20)	106(18)

Table S8 . Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)

for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	19(1)	6840(1)	1916(1)	31(1)
Co(2)	2484(1)	65(1)	5098(1)	40(1)
O(1)	-1019(3)	7311(4)	2663(2)	48(2)
O(1W)	932(3)	6309(4)	1145(2)	39(1)
O(2)	1127(3)	7234(4)	2596(3)	59(2)
O(2W)	-982(3)	6385(4)	1214(2)	43(1)
O(3B)	-1477(4)	13960(5)	388(3)	65(2)
O(4B)	-2279(4)	12407(7)	650(5)	107(3)
O(5A)	1645(7)	13906(6)	246(8)	55(3)
O(6A)	2519(7)	12462(14)	648(15)	106(6)
O(7)	1547(3)	595(5)	4422(3)	68(2)
O(8)	2362(3)	1561(6)	3615(3)	82(2)
O(9)	-1679(3)	491(4)	4150(3)	60(2)
O(10)	-2383(3)	1782(6)	3440(4)	87(3)
N(1)	22(3)	5366(4)	2688(2)	35(1)
N(2)	61(4)	8769(4)	1876(2)	39(1)
C(1)	-1131(6)	6541(7)	3282(5)	73(3)
C(2)	-857(5)	5406(6)	3077(4)	59(3)
C(3)	776(5)	5519(6)	3232(4)	59(3)
C(4)	1512(5)	6230(6)	2939(4)	58(2)
C(5B)	1520(7)	8303(8)	2495(7)	53(4)
C(6B)	778(7)	9200(7)	2346(6)	42(3)
C(7B)	-857(8)	9153(7)	2160(5)	45(3)
C(8B)	-1115(7)	8509(7)	2843(6)	53(3)
C(9)	127(5)	9123(5)	1078(3)	46(2)
C(10)	115(4)	10438(5)	924(3)	38(2)
C(11)	-681(4)	11046(5)	842(3)	41(2)
C(12)	-692(5)	12248(5)	688(3)	42(2)
C(13)	-1563(5)	12894(7)	583(4)	58(2)
C(14)	121(5)	12827(5)	602(3)	42(2)
C(15)	918(4)	12240(5)	669(3)	41(2)
C(16)	1791(5)	12879(6)	531(4)	52(2)
C(17)	917(4)	11038(5)	832(3)	40(2)

C(18)	94(4)	4248(5)	2256(3)	35(2)
C(19)	56(4)	3157(4)	2719(3)	33(2)
C(20)	833(4)	2650(5)	3007(3)	37(2)
C(21)	803(4)	1738(5)	3521(3)	34(2)
C(22)	1646(4)	1253(5)	3864(4)	44(2)
C(23)	-25(4)	1299(5)	3740(3)	35(2)
C(24)	-809(4)	1757(4)	3428(3)	34(2)
C(25)	-1707(4)	1320(5)	3683(4)	44(2)
C(26)	-769(4)	2671(5)	2918(3)	36(2)
O(6B)	2400(20)	12190(40)	480(50)	106(6)
C(5A)	1148(18)	8420(20)	2842(13)	53(4)
C(6A)	1110(20)	9050(20)	2093(13)	42(3)
C(7A)	-460(30)	9250(40)	2350(20)	45(3)
C(8A)	-1220(30)	8660(40)	2450(30)	53(3)
O(5B)	1830(20)	14012(7)	500(20)	55(3)
O(5WB)	-2866(12)	10871(16)	-385(9)	134(5)
O(6WA)	-2472(10)	9209(14)	813(8)	148(5)
O(3W)	-4848(7)	11060(10)	-219(6)	143(3)
O(4W)	690(5)	8003(7)	4522(4)	103(2)
O(6WB)	-3210(30)	9290(40)	280(20)	148(5)
O(5WA)	-3280(30)	10370(40)	-140(20)	134(5)

Table S9. Bond lengths [Å] and angles [°] for **2.**

Co(1)-O(1)	2.130(4)	C(1)-H(1B)	0.9900

Co(1)-O(1W)	2.047(4)	C(2)-H(2A)	0.9900
Co(1)-O(2)	2.089(5)	C(2)-H(2B)	0.9900
Co(1)-O(2W)	2.008(4)	C(3)-H(3A)	0.9900
Co(1)-N(1)	2.175(4)	C(3)-H(3B)	0.9900
Co(1)-N(2)	2.195(5)	C(4)-H(4A)	0.9900
Co(2)-O(7)	1.934(5)	C(4)-H(4B)	0.9900
Co(2)-O(5A)#1	1.955(10)	C(5A)-H(5AA)	0.9900
Co(2)-O(5B)#1	1.91(3)	C(5A)-H(5AB)	0.9900
Co(2)-O(9)#2	1.926(5)	C(5B)-H(5BA)	0.9900
Co(2)-O(3B)#3	1.969(6)	C(5B)-H(5BB)	0.9900
O(1)-C(1)	1.427(9)	C(6A)-H(6AA)	0.9900
O(1)-C(8B)	1.408(9)	C(6A)-H(6AB)	0.9900
O(1)-C(8A)	1.61(5)	C(6B)-H(6BA)	0.9900
O(2)-C(4)	1.415(8)	C(6B)-H(6BB)	0.9900
O(2)-C(5B)	1.362(10)	C(7A)-H(7AA)	0.9900
O(2)-C(5A)	1.42(2)	C(7A)-H(7AB)	0.9900
O(3B)-C(13)	1.269(10)	C(7B)-H(7BA)	0.9900
O(4B)-C(13)	1.209(10)	C(7B)-H(7BB)	0.9900
O(5A)-C(16)	1.292(11)	C(8A)-H(8AA)	0.9800
O(5B)-C(16)	1.291(11)	C(8A)-H(8AB)	1.0000
O(6A)-C(16)	1.200(14)	C(8B)-H(8BA)	0.9900
O(6B)-C(16)	1.20(4)	C(8B)-H(8BB)	0.9900
O(7)-C(22)	1.261(9)	C(9)-H(9A)	0.9900
O(8)-C(22)	1.214(8)	C(9)-H(9B)	0.9900
O(9)-C(25)	1.262(8)	C(11)-H(11)	0.9500
O(10)-C(25)	1.212(8)	C(14)-H(14)	0.9500
O(1W)-H(1WB)	1.01(3)	C(17)-H(17)	0.9500
O(1W)-H(1WA)	1.00(6)	C(18)-H(18A)	0.9900
O(2W)-H(2WA)	0.98(3)	C(18)-H(18B)	0.9900
O(2W)-H(2WB)	0.97(3)	C(20)-H(20)	0.9500
N(1)-C(2)	1.494(9)	C(23)-H(23)	0.9500
C(26)-H(26)	0.9500	O(1)-Co(1)-O(2W)	85.50(16)
N(1)-C(18)	1.494(7)	O(1)-Co(1)-N(1)	77.72(16)
N(1)-C(3)	1.489(8)	O(1W)-Co(1)-N(1)	102.05(17)
N(2)-C(6A)	1.64(3)	O(1W)-Co(1)-N(2)	104.64(18)

N(2)-C(6B)	1.439(12)	O(2)-Co(1)-O(2W)	175.51(18)
N(2)-C(9)	1.494(7)	O(2)-Co(1)-N(1)	78.32(18)
N(2)-C(7B)	1.530(13)	O(2)-Co(1)-N(2)	77.43(19)
N(2)-C(7A)	1.28(4)	O(2W)-Co(1)-N(1)	101.38(17)
C(1)-C(2)	1.404(11)	O(2W)-Co(1)-N(2)	104.95(19)
C(3)-C(4)	1.466(10)	N(1)-Co(1)-N(2)	142.27(15)
C(7A)-C(8A)	1.33(6)	O(5A)#1-Co(2)-O(7)	119.2(4)
C(7B)-C(8B)	1.484(14)	O(5B)#1-Co(2)-O(7)	103.3(10)
C(9)-C(10)	1.521(8)	O(7)-Co(2)-O(9)#2	95.3(2)
C(10)-C(11)	1.379(8)	O(3B)#3-Co(2)-O(7)	123.3(2)
C(10)-C(17)	1.388(8)	O(5A)#1-Co(2)-O(9)#2	115.0(3)
C(11)-C(12)	1.394(8)	O(3B)#3-Co(2)-O(5A)#1	86.6(3)
C(12)-C(14)	1.389(10)	O(5B)#1-Co(2)-O(9)#2	122.1(7)
C(12)-C(13)	1.501(10)	O(3B)#3-Co(2)-O(5B)#1	94.4(8)
C(14)-C(15)	1.366(9)	O(3B)#3-Co(2)-O(9)#2	119.6(2)
C(15)-C(17)	1.398(8)	Co(1)-O(1)-C(1)	115.5(4)
C(15)-C(16)	1.513(9)	Co(1)-O(1)-C(8B)	117.7(5)
C(18)-C(19)	1.495(7)	Co(1)-O(1)-C(8A)	103.0(18)
C(19)-C(20)	1.387(8)	C(1)-O(1)-C(8B)	113.7(6)
C(19)-C(26)	1.399(8)	C(1)-O(1)-C(8A)	138.4(19)
C(20)-C(21)	1.390(8)	Co(1)-O(2)-C(4)	113.2(4)
C(21)-C(22)	1.497(8)	Co(1)-O(2)-C(5B)	116.8(6)
C(21)-C(23)	1.393(8)	Co(1)-O(2)-C(5A)	113.6(11)
C(23)-C(24)	1.390(8)	C(4)-O(2)-C(5B)	127.3(6)
C(24)-C(25)	1.505(8)	C(4)-O(2)-C(5A)	128.6(11)
C(24)-C(26)	1.387(7)	Co(2)#4-O(3B)-C(13)	122.0(5)
C(1)-H(1A)	0.9900	Co(2)#5-O(5A)-C(16)	128.7(8)
O(1)-Co(1)-O(1W)	174.94(17)	Co(2)#5-O(5B)-C(16)	132(2)
O(1)-Co(1)-O(2)	98.78(18)	Co(2)-O(7)-C(22)	126.4(4)
O(1)-Co(1)-N(2)	77.94(18)	Co(2)#2-O(9)-C(25)	134.1(4)
O(1W)-Co(1)-O(2)	86.09(18)	H(1WA)-O(1W)-H(1WB)	110(7)
O(1W)-Co(1)-O(2W)	89.61(17)	Co(1)-O(1W)-H(1WA)	123(4)

Co(1)-O(1W)-H(1WB)	127(6)	C(11)-C(12)-C(13)	120.8(6)

H(2WA)-O(2W)-H(2WB)	103(4)	C(13)-C(12)-C(14)	120.5(6)
Co(1)-O(2W)-H(2WA)	129(3)	O(3B)-C(13)-C(12)	114.3(6)
Co(1)-O(2W)-H(2WB)	127(3)	O(3B)-C(13)-O(4B)	123.9(8)
Co(1)-N(1)-C(3)	108.9(4)	O(4B)-C(13)-C(12)	121.7(7)
C(3)-N(1)-C(18)	112.4(5)	C(12)-C(14)-C(15)	121.1(5)
Co(1)-N(1)-C(2)	106.3(4)	C(14)-C(15)-C(16)	119.9(5)
C(2)-N(1)-C(3)	110.3(5)	C(14)-C(15)-C(17)	119.5(6)
C(2)-N(1)-C(18)	109.8(4)	C(16)-C(15)-C(17)	120.5(5)
Co(1)-N(1)-C(18)	108.9(3)	O(5A)-C(16)-O(6A)	125.0(11)
Co(1)-N(2)-C(7A)	113(2)	O(5A)-C(16)-C(15)	111.0(7)
C(6B)-N(2)-C(9)	114.4(6)	O(6B)-C(16)-C(15)	111(2)
Co(1)-N(2)-C(9)	107.6(3)	O(5B)-C(16)-O(6B)	128(2)
Co(1)-N(2)-C(6A)	102.4(8)	O(5B)-C(16)-C(15)	121.7(14)
Co(1)-N(2)-C(7B)	104.4(4)	O(6A)-C(16)-C(15)	124.0(10)
C(7A)-N(2)-C(9)	124.8(19)	C(10)-C(17)-C(15)	120.6(5)
C(7B)-N(2)-C(9)	108.3(5)	N(1)-C(18)-C(19)	114.4(4)
C(6A)-N(2)-C(9)	95.8(9)	C(20)-C(19)-C(26)	118.2(5)
Co(1)-N(2)-C(6B)	110.0(4)	C(18)-C(19)-C(20)	121.0(5)
O(1)-C(1)-C(2)	108.8(7)	C(18)-C(19)-C(26)	120.7(5)
N(1)-C(2)-C(1)	114.3(6)	C(19)-C(20)-C(21)	121.6(5)
N(1)-C(3)-C(4)	113.0(6)	C(20)-C(21)-C(23)	119.5(5)
O(2)-C(4)-C(3)	107.5(6)	C(22)-C(21)-C(23)	119.6(5)
N(2)-C(7A)-C(8A)	114(4)	C(20)-C(21)-C(22)	120.9(5)
N(2)-C(7B)-C(8B)	112.2(7)	O(7)-C(22)-C(21)	116.1(5)
O(1)-C(8A)-C(7A)	111(4)	O(8)-C(22)-C(21)	118.6(6)
O(1)-C(8B)-C(7B)	105.0(7)	O(7)-C(22)-O(8)	125.2(6)
N(2)-C(9)-C(10)	116.0(4)	C(21)-C(23)-C(24)	119.6(5)
C(9)-C(10)-C(11)	121.4(5)	C(25)-C(24)-C(26)	119.7(5)
C(11)-C(10)-C(17)	118.8(5)	C(23)-C(24)-C(26)	120.2(5)
C(9)-C(10)-C(17)	119.8(5)	C(23)-C(24)-C(25)	120.0(5)
C(10)-C(11)-C(12)	121.4(6)	O(9)-C(25)-O(10)	125.7(6)
C(11)-C(12)-C(14)	118.6(6)	O(9)-C(25)-C(24)	115.3(5)
O(10)-C(25)-C(24)	119.0(6)	C(8A)-C(7A)-H(7AB)	110.00
C(19)-C(26)-C(24)	120.7(5)	N(2)-C(7A)-H(7AB)	108.00
O(1)-C(1)-H(1A)	110.00	C(8A)-C(7A)-H(7AA)	109.00

O(1)-C(1)-H(1B)	110.00	H(7AA)-C(7A)-H(7AB)	108.00
C(2)-C(1)-H(1A)	110.00	N(2)-C(7B)-H(7BA)	109.00
C(2)-C(1)-H(1B)	110.00	C(8B)-C(7B)-H(7BB)	109.00
H(1A)-C(1)-H(1B)	108.00	H(7BA)-C(7B)-H(7BB)	108.00
N(1)-C(2)-H(2A)	109.00	N(2)-C(7B)-H(7BB)	109.00
N(1)-C(2)-H(2B)	109.00	C(8B)-C(7B)-H(7BA)	109.00
C(1)-C(2)-H(2A)	109.00	H(8AA)-C(8A)-H(8AB)	108.00
C(1)-C(2)-H(2B)	109.00	C(7A)-C(8A)-H(8AA)	110.00
H(2A)-C(2)-H(2B)	108.00	C(7A)-C(8A)-H(8AB)	109.00
N(1)-C(3)-H(3A)	109.00	O(1)-C(8A)-H(8AA)	109.00
N(1)-C(3)-H(3B)	109.00	O(1)-C(8A)-H(8AB)	109.00
C(4)-C(3)-H(3A)	109.00	O(1)-C(8B)-H(8BA)	111.00
C(4)-C(3)-H(3B)	109.00	O(1)-C(8B)-H(8BB)	111.00
H(3A)-C(3)-H(3B)	108.00	C(7B)-C(8B)-H(8BA)	111.00
O(2)-C(4)-H(4A)	110.00	C(7B)-C(8B)-H(8BB)	111.00
O(2)-C(4)-H(4B)	110.00	H(8BA)-C(8B)-H(8BB)	109.00
C(3)-C(4)-H(4A)	110.00	N(2)-C(9)-H(9A)	108.00
C(3)-C(4)-H(4B)	110.00	N(2)-C(9)-H(9B)	108.00
H(4A)-C(4)-H(4B)	109.00	C(10)-C(9)-H(9A)	108.00
O(2)-C(5A)-H(5AA)	112.00	C(10)-C(9)-H(9B)	108.00
O(2)-C(5A)-H(5AB)	112.00	H(9A)-C(9)-H(9B)	107.00
H(5AA)-C(5A)-H(5AB)	110.00	C(10)-C(11)-H(11)	119.00
H(5BA)-C(5B)-H(5BB)	108.00	C(12)-C(11)-H(11)	119.00
O(2)-C(5B)-H(5BA)	110.00	C(15)-C(14)-H(14)	119.00
O(2)-C(5B)-H(5BB)	110.00	C(12)-C(14)-H(14)	119.00
N(2)-C(6A)-H(6AA)	112.00	C(15)-C(17)-H(17)	120.00
N(2)-C(6A)-H(6AB)	112.00	C(10)-C(17)-H(17)	120.00
H(6AA)-C(6A)-H(6AB)	110.00	N(1)-C(18)-H(18A)	109.00
H(6BA)-C(6B)-H(6BB)	108.00	C(19)-C(18)-H(18A)	109.00
N(2)-C(6B)-H(6BA)	109.00	C(19)-C(18)-H(18B)	109.00
N(2)-C(6B)-H(6BB)	109.00	N(1)-C(18)-H(18B)	109.00
N(2)-C(7A)-H(7AA)	108.00	H(18A)-C(18)-H(18B)	108.00
C(21)-C(20)-H(20)	119.00		
C(19)-C(20)-H(20)	119.00		
C(21)-C(23)-H(23)	120.00		

C(24)-C(23)-H(23)	120.00	
C(19)-C(26)-H(26)	120.00	
C(24)-C(26)-H(26)	120.00	

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1/2, y-3/2, -z+1/2$

#2 $-x, -y, -z+1$

#3 $x+1/2, -y+3/2, z+1/2$

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

#5 $-x+1/2, y+3/2, -z+1/2$

Table S10. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	35(1)	25(1)	32(1)	0(1)	-2(1)	1(1)
Co(2)	35(1)	30(1)	55(1)	11(1)	3(1)	-1(1)
O(1)	52(3)	37(2)	54(3)	1(2)	15(2)	8(2)
O(1W)	33(2)	43(2)	42(2)	0(2)	4(2)	1(2)
O(2)	64(3)	37(2)	75(3)	11(2)	-34(3)	-13(2)
O(2W)	36(2)	49(2)	43(2)	-4(2)	-7(2)	3(2)
O(3B)	72(3)	57(3)	65(3)	1(2)	-4(3)	32(3)
O(4B)	56(4)	122(6)	145(6)	81(5)	40(4)	28(4)
O(5A)	70(5)	39(3)	56(6)	-1(3)	-11(4)	-33(3)
O(6A)	54(5)	110(9)	152(14)	86(8)	-44(6)	-35(6)
O(7)	47(3)	57(3)	98(4)	39(3)	-16(3)	-2(2)
O(8)	33(3)	121(5)	92(4)	34(4)	13(3)	19(3)
O(9)	48(3)	48(3)	84(3)	29(2)	25(2)	2(2)
O(10)	33(3)	113(5)	114(5)	56(4)	-5(3)	-12(3)
N(1)	51(3)	26(2)	27(2)	-3(2)	1(2)	-2(2)
N(2)	64(3)	25(2)	29(2)	1(2)	-1(2)	3(2)
C(1)	77(5)	67(5)	75(5)	14(4)	42(4)	7(4)
C(2)	75(5)	46(4)	57(4)	5(3)	29(4)	-6(3)
C(3)	81(5)	44(4)	51(4)	8(3)	-25(4)	-12(3)
C(4)	56(4)	49(4)	67(4)	11(3)	-20(3)	1(3)
C(5B)	41(6)	41(4)	78(8)	-17(5)	-4(4)	-4(4)
C(6B)	60(7)	27(4)	40(5)	-7(4)	0(4)	-2(4)
C(7B)	61(7)	33(3)	42(5)	7(3)	3(4)	16(4)
C(8B)	76(6)	41(4)	42(6)	12(4)	23(5)	25(4)
C(9)	74(4)	27(3)	36(3)	-1(2)	2(3)	-6(3)
C(10)	59(4)	28(3)	27(2)	1(2)	1(2)	-1(2)
C(11)	53(4)	36(3)	35(3)	10(2)	3(2)	-4(3)
C(12)	59(4)	40(3)	28(3)	8(2)	2(2)	7(3)
C(13)	69(5)	61(4)	43(3)	18(3)	17(3)	23(4)
C(14)	72(4)	26(3)	27(3)	2(2)	1(3)	-5(3)
C(15)	60(4)	32(3)	30(3)	5(2)	-6(2)	-6(3)

C(16)	62(4)	51(4)	41(3)	13(3)	-14(3)	-16(3)
C(17)	54(4)	33(3)	34(3)	8(2)	-4(2)	1(2)
C(18)	49(3)	29(3)	28(2)	-1(2)	1(2)	-3(2)
C(19)	43(3)	27(2)	30(3)	3(2)	-1(2)	-2(2)
C(20)	37(3)	32(3)	43(3)	-1(2)	7(2)	-3(2)
C(21)	35(3)	30(3)	38(3)	-1(2)	-1(2)	4(2)
C(22)	38(3)	34(3)	61(4)	2(3)	-4(3)	5(2)
C(23)	44(3)	25(2)	36(3)	3(2)	2(2)	1(2)
C(24)	36(3)	26(2)	40(3)	1(2)	1(2)	-5(2)
C(25)	43(3)	37(3)	51(3)	4(3)	3(3)	-9(3)
C(26)	39(3)	32(3)	38(3)	4(2)	-8(2)	-4(2)
O(6B)	54(5)	110(9)	152(14)	86(8)	-44(6)	-35(6)
C(5A)	41(6)	41(4)	78(8)	-17(5)	-4(4)	-4(4)
C(6A)	60(7)	27(4)	40(5)	-7(4)	0(4)	-2(4)
C(7A)	61(7)	33(3)	42(5)	7(3)	3(4)	16(4)
C(8A)	76(6)	41(4)	42(6)	12(4)	23(5)	25(4)
O(5B)	70(5)	39(3)	56(6)	-1(3)	-11(4)	-33(3)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2**.

	x	y	z	U(eq)
H(2WA)	-950(30)	6070(60)	705(15)	64
H(3A)	546	5899	3687	71
H(2B)	-814	4913	3531	71
H(2WB)	-1611(16)	6580(60)	1260(30)	64
H(4A)	1925	6469	3348	69
H(4B)	1855	5771	2572	69
H(6BA)	525	9448	2828	51
H(6BB)	1044	9904	2111	51
H(5BA)	1932	8271	2068	64
H(3B)	1012	4735	3374	71
H(9B)	690	8794	878	55
H(5BB)	1871	8527	2944	64
H(11)	-1233	10637	890	50
H(7BA)	-843	10007	2267	54
H(7BB)	-1316	9015	1766	54
H(14)	123	13645	494	50
H(17)	1471	10628	881	48
H(8BA)	-716	8724	3266	63
H(8BB)	-1743	8688	2976	63
H(18A)	668	4253	1984	42
H(18B)	-399	4222	1882	42
H(20)	1399	2933	2848	45
H(23)	-53	689	4100	42
H(26)	-1307	2969	2701	43
H(9A)	-378	8757	798	55
H(1WA)	750(50)	5980(80)	650(30)	100(30)
H(1A)	-766	6821	3710	87
H(1B)	-1768	6529	3430	87
H(1WB)	1606(15)	6380(110)	1180(50)	147
H(2A)	-1323	5057	2748	71

H(8AA)	-1598	8691	1997	63
H(8AB)	-1561	9031	2862	63
H(5AA)	1708	8601	3122	64
H(5AB)	624	8611	3152	64
H(6AA)	1529	8705	1731	51
H(6AB)	1223	9904	2143	51
H(7AA)	-605	10055	2174	54
H(7AB)	-131	9321	2829	54

Table S12. Hydrogen bonds for **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1W)-H(1WA)...O(3B)#6	1.00(6)	2.17(6)	2.899(7)	128(6)
O(1W)-H(1WB)...O(8)#7	1.01(3)	1.59(3)	2.588(6)	170(7)
O(2W)-H(2WA)...O(3B)#8	0.98(3)	2.59(7)	3.212(7)	122(4)
O(2W)-H(2WA)...O(5A)#6	0.98(3)	1.99(4)	2.810(14)	140(4)
O(2W)-H(2WB)...O(10)#9	0.97(3)	1.62(3)	2.562(7)	165(6)
C(1)-H(1B)...O(4B)#10	0.9900	2.4100	3.223(12)	139.00
C(4)-H(4A)...O(6A)#11	0.9900	2.2700	3.22(2)	160.00
C(5B)-H(5BA)...O(8)#7	0.9900	2.5400	3.281(12)	132.00
C(11)-H(11)...O(6WA)	0.9500	2.4600	3.388(16)	165.00

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1/2, y-3/2, -z+1/2$

#2 $-x, -y, -z+1$

#3 $x+1/2, -y+3/2, z+1/2$

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

#5 $-x+1/2, y+3/2, -z+1/2$

#6 $-x, -y+2, -z$

#7 $-x+1/2, y+1/2, -z+1/2$

#8 $x, y-1, z$

#9 $-x-1/2, y+1/2, -z+1/2$

#10 $-x-1/2, y-1/2, -z+1/2$

#11 $-x+1/2, y-1/2, -z+1/2$