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Supplementary Information :

Recurrent H-bond graph motifs between metal tris-ethylenediamine cations and uncoordinated oxalate anions: Fitting a three pin plug into a two pin socket

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Crystallographic data for 1

Table 1. Crystal data and structure refinement for **1**.

Identification code	**1**
Empirical formula	$C_6H_{20}CuN_4O_6$
Formula weight	307.80
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a=6.4347(6) Å alpha = 90.268(4)° b=6.9170(7) Å beta = 107.581(4)° c=7.7596(6) Å gamma = 108.201(3)°
Volume	310.89(5) $Å^3$
Crystal size	0.06 x 0.06 x 0.06 mm
Theta range for data collection	3.12 to 27.58°
Limiting indices	-8<=h<=8, -9<=k<=8, -10<=l<=10
Reflections collected / unique	3144 / 1407 [R(int) = 0.0811]
Completeness to theta = 27.58	98.1 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1407 / 3 / 85
Goodness-of-fit on F^2	1.081
Final R indices [I>2sigma(I)]	R1 = 0.0414, wR2 = 0.0951
R indices (all data)	R1 = 0.0460, wR2 = 0.0982
Largest diff. peak and hole	0.531 and -0.562 e. $Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **1**.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	5000	0	0	17(1)
O(1W)	7361(4)	164(3)	-2217(3)	25(1)
N(1)	7697(4)	-101(4)	2150(3)	20(1)
N(2)	6420(4)	3037(3)	558(3)	19(1)
C(1)	8806(5)	1973(5)	3160(4)	23(1)
C(2)	8823(5)	3515(5)	1786(4)	25(1)
O(1)	4177(4)	4652(3)	2629(3)	25(1)
O(2)	5011(4)	7459(3)	4465(3)	27(1)
C(3)	4764(5)	5602(4)	4157(4)	17(1)

Table 3. Anisotropic displacement parameters (Å^2 x 10^3) for **1**.
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}
Cu(1)	17(1)	17(1)	17(1)	2(1)	4(1)	6(1)
O(1W)	28(1)	22(1)	24(1)	-2(1)	7(1)	9(1)
N(1)	17(1)	23(1)	21(1)	6(1)	6(1)	9(1)
N(2)	20(1)	18(1)	19(1)	1(1)	6(1)	6(1)
C(1)	16(1)	29(2)	19(1)	-2(1)	2(1)	5(1)
C(2)	19(2)	24(2)	26(2)	1(1)	4(1)	4(1)
O(1)	31(1)	29(1)	16(1)	-1(1)	7(1)	13(1)
O(2)	38(1)	17(1)	25(1)	4(1)	8(1)	9(1)
C(3)	15(1)	18(1)	19(1)	2(1)	7(1)	5(1)

Table 4. Bond lengths [Å] and angles [°] for **1**.

Cu(1)-N(2)#1	1.997(2)
Cu(1)-N(2)	1.997(2)
Cu(1)-N(1)#1	2.031(2)
Cu(1)-N(1)	2.031(2)
O(1W)-H(1W)	0.875(10)
O(1W)-H(2W)	0.878(10)
N(1)-C(1)	1.481(4)
N(1)-H(1A)	0.9000
N(1)-H(1B)	0.9000
N(2)-C(2)	1.482(4)
N(2)-H(2A)	0.9000
N(2)-H(2B)	0.9000
C(1)-C(2)	1.511(4)
C(1)-H(1C)	0.9700
C(1)-H(1D)	0.9700
C(2)-H(2C)	0.9700
C(2)-H(2D)	0.9700
O(1)-C(3)	1.244(3)
O(2)-C(3)	1.256(3)
C(3)-C(3)#2	1.557(5)
N(2)#1-Cu(1)-N(2)	180.0
N(2)#1-Cu(1)-N(1)#1	85.21(10)
N(2)-Cu(1)-N(1)#1	94.79(10)
N(2)#1-Cu(1)-N(1)	94.79(10)
N(2)-Cu(1)-N(1)	85.21(10)
N(1)#1-Cu(1)-N(1)	180.00(14)
H(1W)-O(1W)-H(2W)	105.7(15)
C(1)-N(1)-Cu(1)	107.45(17)
C(1)-N(1)-H(1A)	110.2
Cu(1)-N(1)-H(1A)	110.2
C(1)-N(1)-H(1B)	110.2
Cu(1)-N(1)-H(1B)	110.2
H(1A)-N(1)-H(1B)	108.5
C(2)-N(2)-Cu(1)	108.42(17)
C(2)-N(2)-H(2A)	110.0
Cu(1)-N(2)-H(2A)	110.0
C(2)-N(2)-H(2B)	110.0
Cu(1)-N(2)-H(2B)	110.0
H(2A)-N(2)-H(2B)	108.4
N(1)-C(1)-C(2)	108.0(2)
N(1)-C(1)-H(1C)	110.1
C(2)-C(1)-H(1C)	110.1
N(1)-C(1)-H(1D)	110.1
C(2)-C(1)-H(1D)	110.1
H(1C)-C(1)-H(1D)	108.4
N(2)-C(2)-C(1)	107.4(2)
N(2)-C(2)-H(2C)	110.2
C(1)-C(2)-H(2C)	110.2
N(2)-C(2)-H(2D)	110.2
C(1)-C(2)-H(2D)	110.2
H(2C)-C(2)-H(2D)	108.5
O(1)-C(3)-O(2)	125.7(3)
O(1)-C(3)-C(3)#2	117.6(3)
O(2)-C(3)-C(3)#2	116.8(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z #2 -x+1,-y+1,-z+1

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **1**.

	x	y	z	U(eq)
H(1W)	6830(60)	-980(30)	-2930(30)	30
H(2W)	6900(60)	1060(30)	-2900(30)	30
H(1A)	7194	-1020	2875	24
H(1B)	8714	-471	1759	24
H(2A)	6414	3623	-476	23
H(2B)	5606	3531	1098	23
H(1C)	10373	2138	3910	28
H(1D)	7952	2175	3943	28
H(2C)	9383	4892	2398	30
H(2D)	9826	3423	1096	30

Table 6. Hydrogen bonds for **1** [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1W)···O(1)#1	0.875(10)	2.45(2)	3.149(3)	138(3)
O(1W)-H(1W)···O(2)#3	0.875(10)	2.092(19)	2.872(3)	148(2)
O(1W)-H(2W)···O(2)#4	0.878(10)	1.986(15)	2.839(3)	164(3)
N(1)-H(1A)···O(2)#5	0.90	2.18	3.024(3)	156.6
N(1)-H(1B)···O(1W)#6	0.90	2.38	3.179(3)	147.7
N(2)-H(2A)···O(1)#4	0.90	2.07	2.944(3)	163.9
N(2)-H(2B)···O(1)	0.90	1.99	2.881(3)	171.6

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z #2 -x+1,-y+1,-z+1 #3 x,y-1,z-1
#4 -x+1,-y+1,-z #5 x,y-1,z #6 -x+2,-y,-z

Crystallographic data for 2

Table 7. Crystal data and structure refinement for **2**.

Identification code	**2**
Empirical formula	$C_8H_{24}CuN_6O_4$
Formula weight	331.87
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P $2_1/c$
Unit cell dimensions	a = 9.8795(9)Å alpha = 90° b = 9.6336(9)Å beta = 91.718(5)° c = 14.4612(15)Å gamma = 90°
Volume	1375.7(2) $Å^3$
Crystal size	0.12 x 0.10 x 0.08 mm
Theta range for data collection	2.95 to 27.51°
Limiting indices	-12<=h<=12, -12<=k<=12, -18<=l<=18
Reflections collected / unique	12548 / 3153 [R(int) = 0.1087]
Completeness to theta = 27.51	99.4 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3153 / 0 / 172
Goodness-of-fit on F^2	1.038
Final R indices [I>2σ(I)]	R1 = 0.0628, wR2 = 0.1265
R indices (all data)	R1 = 0.1153, wR2 = 0.1430
Largest diff. peak and hole	0.621 and -0.431 $e.Å^{-3}$

Table 8. 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)
Cu(1)	7502(1)	292(1)	3307(1)	24(1)
O(4)	6380(3)	-1271(4)	7124(3)	41(1)
O(2)	6398(3)	1080(3)	6046(2)	33(1)
O(1)	8531(3)	1377(3)	6544(3)	33(1)
O(3)	8580(3)	-1434(4)	6876(3)	46(1)
N(5)	6380(4)	833(4)	1823(3)	30(1)
N(4)	8895(4)	-1048(4)	4515(3)	34(1)
N(6)	8849(4)	-545(4)	2413(3)	24(1)
N(2)	6121(4)	1380(4)	4027(3)	27(1)
N(1)	8581(4)	2094(4)	3369(3)	26(1)
N(3)	6384(4)	-1466(4)	3441(3)	27(1)
C(2)	6430(5)	2867(5)	3924(4)	33(1)
C(6)	8626(5)	3(5)	1470(3)	28(1)
C(4)	8266(5)	-2410(5)	4381(4)	35(1)
C(1)	7951(5)	3037(5)	4029(4)	34(1)
C(5)	7131(5)	-77(5)	1213(3)	29(1)
C(3)	6745(5)	-2254(5)	4279(4)	37(1)
C(7)	7470(5)	676(5)	6442(3)	24(1)
C(8)	7486(5)	-820(5)	6851(3)	27(1)

Table 9. 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}
Cu(1)	21(1)	21(1)	29(1)	-2(1)	4(1)	-1(1)
O(4)	21(2)	39(2)	62(3)	20(2)	4(2)	-2(2)
O(2)	29(2)	33(2)	38(2)	5(2)	0(2)	4(2)
O(1)	28(2)	22(2)	50(2)	-2(2)	3(2)	-4(2)
O(3)	25(2)	32(2)	82(3)	18(2)	15(2)	9(2)
N(5)	22(2)	26(2)	41(3)	0(2)	0(2)	0(2)
N(4)	26(2)	46(3)	29(2)	-4(2)	0(2)	0(2)
N(6)	23(2)	20(2)	31(2)	-1(2)	5(2)	-1(2)
N(2)	22(2)	26(2)	33(2)	-5(2)	0(2)	-1(2)
N(1)	25(2)	23(2)	30(2)	-2(2)	1(2)	-1(2)
N(3)	22(2)	23(2)	36(2)	-3(2)	2(2)	-2(2)
C(2)	32(3)	29(3)	37(3)	-6(2)	5(2)	1(2)
C(6)	32(3)	28(3)	25(3)	-5(2)	5(2)	2(2)
C(4)	36(3)	31(3)	39(3)	13(2)	-7(2)	-1(2)
C(1)	32(3)	23(3)	45(3)	-11(2)	1(2)	-4(2)
C(5)	33(3)	25(3)	27(3)	-2(2)	-3(2)	2(2)
C(3)	33(3)	38(3)	38(3)	5(3)	1(2)	-10(2)
C(7)	26(3)	22(2)	24(3)	-4(2)	7(2)	2(2)
C(8)	22(2)	29(2)	31(3)	1(2)	-4(2)	1(2)

Table 10. Bond lengths [Å] and angles [°] for **2**.

Cu(1)-N(2)	2.032(4)
Cu(1)-N(3)	2.034(3)
Cu(1)-N(1)	2.038(4)
Cu(1)-N(6)	2.048(3)
Cu(1)-N(5)	2.442(4)
Cu(1)-N(4)	2.544(4)
O(4)-C(8)	1.250(5)
O(2)-C(7)	1.251(6)
O(1)-C(7)	1.251(5)
O(3)-C(8)	1.232(5)
N(5)-C(5)	1.462(6)
N(5)-H(5A)	0.9000
N(5)-H(5B)	0.9000
N(4)-C(4)	1.462(6)
N(4)-H(4A)	0.9000
N(4)-H(4B)	0.9000
N(6)-C(6)	1.473(6)
N(6)-H(6A)	0.9000
N(6)-H(6B)	0.9000
N(2)-C(2)	1.473(6)
N(2)-H(2A)	0.9000
N(2)-H(2B)	0.9000
N(1)-C(1)	1.469(6)
N(1)-H(1A)	0.9000
N(1)-H(1B)	0.9000
N(3)-C(3)	1.465(6)
N(3)-H(3A)	0.9000
N(3)-H(3B)	0.9000
C(2)-C(1)	1.515(7)
C(2)-H(2C)	0.9700
C(2)-H(2D)	0.9700
C(6)-C(5)	1.514(7)
C(6)-H(6C)	0.9700
C(6)-H(6D)	0.9700
C(4)-C(3)	1.514(7)
C(4)-H(4C)	0.9700
C(4)-H(4D)	0.9700
C(1)-H(1C)	0.9700
C(1)-H(1D)	0.9700
C(5)-H(5C)	0.9700
C(5)-H(5D)	0.9700
C(3)-H(3D)	0.9700
C(3)-H(3C)	0.9700
C(7)-C(8)	1.558(7)
N(2)-Cu(1)-N(3)	90.35(15)
N(2)-Cu(1)-N(1)	84.07(14)
N(3)-Cu(1)-N(1)	171.83(16)
N(2)-Cu(1)-N(6)	170.17(15)
N(3)-Cu(1)-N(6)	95.58(15)
N(1)-Cu(1)-N(6)	90.79(14)
N(2)-Cu(1)-N(5)	92.66(15)
N(3)-Cu(1)-N(5)	91.62(15)
N(1)-Cu(1)-N(5)	94.59(15)
N(6)-Cu(1)-N(5)	79.38(14)
N(2)-Cu(1)-N(4)	105.54(15)
N(3)-Cu(1)-N(4)	78.24(14)
N(1)-Cu(1)-N(4)	97.48(15)
N(6)-Cu(1)-N(4)	83.40(14)
N(5)-Cu(1)-N(4)	159.06(13)
C(5)-N(5)-Cu(1)	100.2(3)

C(5)-N(5)-H(5A)	111.7
Cu(1)-N(5)-H(5A)	111.7
C(5)-N(5)-H(5B)	111.7
Cu(1)-N(5)-H(5B)	111.7
H(5A)-N(5)-H(5B)	109.5
C(4)-N(4)-Cu(1)	98.3(3)
C(4)-N(4)-H(4A)	112.1
Cu(1)-N(4)-H(4A)	112.1
C(4)-N(4)-H(4B)	112.1
Cu(1)-N(4)-H(4B)	112.1
H(4A)-N(4)-H(4B)	109.7
C(6)-N(6)-Cu(1)	111.2(3)
C(6)-N(6)-H(6A)	109.4
Cu(1)-N(6)-H(6A)	109.4
C(6)-N(6)-H(6B)	109.4
Cu(1)-N(6)-H(6B)	109.4
H(6A)-N(6)-H(6B)	108.0
C(2)-N(2)-Cu(1)	107.8(3)
C(2)-N(2)-H(2A)	110.2
Cu(1)-N(2)-H(2A)	110.2
C(2)-N(2)-H(2B)	110.2
Cu(1)-N(2)-H(2B)	110.2
H(2A)-N(2)-H(2B)	108.5
C(1)-N(1)-Cu(1)	108.9(3)
C(1)-N(1)-H(1A)	109.9
Cu(1)-N(1)-H(1A)	109.9
C(1)-N(1)-H(1B)	109.9
Cu(1)-N(1)-H(1B)	109.9
H(1A)-N(1)-H(1B)	108.3
C(3)-N(3)-Cu(1)	113.0(3)
C(3)-N(3)-H(3A)	109.0
Cu(1)-N(3)-H(3A)	109.0
C(3)-N(3)-H(3B)	109.0
Cu(1)-N(3)-H(3B)	109.0
H(3A)-N(3)-H(3B)	107.8
N(2)-C(2)-C(1)	107.7(4)
N(2)-C(2)-H(2C)	110.2
C(1)-C(2)-H(2C)	110.2
N(2)-C(2)-H(2D)	110.2
C(1)-C(2)-H(2D)	110.2
H(2C)-C(2)-H(2D)	108.5
N(6)-C(6)-C(5)	109.1(4)
N(6)-C(6)-H(6C)	109.9
C(5)-C(6)-H(6C)	109.9
N(6)-C(6)-H(6D)	109.9
C(5)-C(6)-H(6D)	109.9
H(6C)-C(6)-H(6D)	108.3
N(4)-C(4)-C(3)	109.9(4)
N(4)-C(4)-H(4C)	109.7
C(3)-C(4)-H(4C)	109.7
N(4)-C(4)-H(4D)	109.7
C(3)-C(4)-H(4D)	109.7
H(4C)-C(4)-H(4D)	108.2
N(1)-C(1)-C(2)	107.9(4)
N(1)-C(1)-H(1C)	110.1
C(2)-C(1)-H(1C)	110.1
N(1)-C(1)-H(1D)	110.1
C(2)-C(1)-H(1D)	110.1
H(1C)-C(1)-H(1D)	108.4
N(5)-C(5)-C(6)	109.3(4)
N(5)-C(5)-H(5C)	109.8
C(6)-C(5)-H(5C)	109.8
N(5)-C(5)-H(5D)	109.8
C(6)-C(5)-H(5D)	109.8

H(5C)-C(5)-H(5D)	108.3
N(3)-C(3)-C(4)	110.4(4)
N(3)-C(3)-H(3D)	109.6
C(4)-C(3)-H(3D)	109.6
N(3)-C(3)-H(3C)	109.6
C(4)-C(3)-H(3C)	109.6
H(3D)-C(3)-H(3C)	108.1
O(1)-C(7)-O(2)	125.5(4)
O(1)-C(7)-C(8)	117.1(4)
O(2)-C(7)-C(8)	117.4(4)
O(3)-C(8)-O(4)	126.7(5)
O(3)-C(8)-C(7)	117.0(4)
O(4)-C(8)-C(7)	116.3(4)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **2**.

	x	y	z	U(eq)
H(5A)	5494	617	1821	36
H(5B)	6478	1733	1672	36
H(4A)	9782	-1058	4389	41
H(4B)	8784	-718	5090	41
H(6A)	9698	-346	2612	29
H(6B)	8756	-1474	2405	29
H(2A)	5279	1199	3805	32
H(2B)	6169	1138	4629	32
H(1A)	9442	1917	3553	31
H(1B)	8589	2491	2806	31
H(3A)	5502	-1236	3452	32
H(3B)	6502	-2010	2944	32
H(2C)	5982	3401	4394	39
H(2D)	6115	3194	3321	39
H(6C)	9140	-537	1036	33
H(6D)	8931	959	1442	33
H(4C)	8490	-3001	4907	42
H(4D)	8612	-2844	3831	42
H(1C)	8205	3989	3901	40
H(1D)	8252	2811	4656	40
H(5C)	6981	208	575	34
H(5D)	6816	-1025	1274	34
H(3D)	6326	-3164	4247	44
H(3C)	6406	-1777	4816	44

Table 12. Hydrogen bonds for **2** [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1A) ··O(3)#1	0.90	2.12	2.907(5)	145.7
N(1)-H(1B) ··O(1)#2	0.90	2.13	3.022(5)	173.9
N(2)-H(2A) ··O(4)#3	0.90	2.09	2.939(5)	157.3
N(2)-H(2A) ··O(2)#3	0.90	2.76	3.436(5)	132.6
N(2)-H(2B) ··O(2)	0.90	2.06	2.938(5)	166.2
N(3)-H(3A)···O(2)#3	0.90	2.04	2.892(5)	157.9
N(3)-H(3B)···O(4)#4	0.90	2.04	2.895(5)	158.6
N(4)-H(4A)···O(1)#1	0.90	2.20	3.024(5)	152.4
N(4)-H(4B)···O(3)	0.90	2.69	3.458(5)	144.3
N(5)-H(5A)···O(4)#3	0.90	2.51	3.191(5)	132.3
N(5)-H(5B)···O(2)#2	0.90	2.29	3.179(5)	168.0
N(6)-H(6A)···O(1)#1	0.90	2.33	3.063(5)	139.2
N(6)-H(6A)···O(3)#1	0.90	2.51	3.314(5)	148.9
N(6)-H(6B)···O(3)#4	0.90	2.16	3.022(5)	159.9

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z+1 #2 x,-y+1/2,z-1/2 #3 -x+1,-y,-z+1
#4 x,-y-1/2,z-1/2

Crystallographic data for 3

Table 13. Crystal data and structure refinement for **3**.

Identification code	**3**
Empirical formula	$C_9H_{27.61}CoN_6O_{7.805}$
Formula weight	403.78
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 7.4525(19) Å alpha = 71.49(2) ° b = 8.971(2) Å beta = 89.61(2) ° c = 13.349(4) Å gamma = 82.827(18) °
Volume	839.2(4) $Å^3$
Z, Calculated density	2, 1.598 Mg/m^3
Crystal size	0.14 x 0.13 x 0.09 mm
Theta range for data collection	3.14 to 27.56 °
Limiting indices	-9<=h<=9, -11<=k<=11, -17<=l<=17
Reflections collected / unique	10682 / 3799 [R(int) = 0.1896]
Completeness to theta = 27.56	98.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3799 / 0 / 216
Goodness-of-fit on F^2	1.071
Final R indices [I>2sigma(I)]	R1 = 0.0789, wR2 = 0.2028
R indices (all data)	R1 = 0.0896, wR2 = 0.2147
Largest diff. peak and hole	1.725 and -1.215 $e.Å^{-3}$

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **3**.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co(1)	9219(1)	1281(1)	2244(1)	17(1)
O(1)	5910(5)	5234(5)	1750(3)	34(1)
O(3)	8060(5)	6416(4)	106(2)	27(1)
O(2)	6473(6)	7148(5)	2390(3)	43(1)
O(4)	7881(6)	8675(4)	499(3)	33(1)
O(5)	2716(5)	-275(6)	4946(3)	45(1)
C(7)	6548(7)	6489(6)	1697(3)	26(1)
C(8)	7588(6)	7258(6)	676(3)	22(1)
C(9)	4154(7)	206(10)	4601(4)	48(2)
N(3)	11360(5)	2353(5)	2260(3)	26(1)
N(6)	6936(5)	444(5)	2152(3)	25(1)
N(5)	8403(5)	2925(5)	907(3)	22(1)
N(2)	9979(6)	-514(5)	3540(3)	24(1)
N(1)	10511(6)	-75(5)	1492(3)	25(1)
N(4)	8109(6)	2528(5)	3106(3)	26(1)
C(5)	6972(6)	2386(6)	388(3)	24(1)
C(4)	9510(8)	3272(7)	3489(4)	34(1)
C(6)	5764(6)	1594(7)	1268(3)	28(1)
O(6)	4433(5)	1028(8)	3657(3)	66(2)
C(1)	11777(8)	-1331(7)	2254(4)	35(1)
C(2)	10759(9)	-1929(6)	3256(4)	37(1)
C(3)	10801(8)	3780(6)	2599(4)	34(1)
O(1W)	3272(14)	2423(12)	5623(7)	53(2)
O(2W)	4511(12)	4478(13)	3962(7)	53(2)
O(3W)	2270(30)	3130(20)	5566(14)	53(2)
O(4W)	4374(18)	5181(19)	4064(9)	53(2)

Table 15. Bond lengths [Å] and angles [°] for **3**.

Co(1)-N(4)	1.959(4)
Co(1)-N(5)	1.962(4)
Co(1)-N(6)	1.963(4)
Co(1)-N(3)	1.966(4)
Co(1)-N(1)	1.970(4)
Co(1)-N(2)	1.981(4)
O(1)-C(7)	1.257(7)
O(3)-C(8)	1.253(6)
O(2)-C(7)	1.244(6)
O(4)-C(8)	1.264(6)
O(5)-C(9)	1.236(7)
C(7)-C(8)	1.567(6)
C(9)-O(6)	1.273(6)
C(9)-C(9)#1	1.585(10)
N(3)-C(3)	1.501(7)
N(3)-H(3A)	0.9200
N(3)-H(3B)	0.9200
N(6)-C(6)	1.496(6)
N(6)-H(6A)	0.9200
N(6)-H(6B)	0.9200
N(5)-C(5)	1.484(6)
N(5)-H(5A)	0.9200
N(5)-H(5B)	0.9200
N(2)-C(2)	1.487(6)
N(2)-H(2A)	0.9200
N(2)-H(2B)	0.9200
N(1)-C(1)	1.488(6)
N(1)-H(1A)	0.9200
N(1)-H(1B)	0.9200
N(4)-C(4)	1.481(7)
N(4)-H(4A)	0.9200
N(4)-H(4B)	0.9200
C(5)-C(6)	1.519(6)
C(5)-H(5C)	0.9900
C(5)-H(5D)	0.9900
C(4)-C(3)	1.514(8)
C(4)-H(4C)	0.9900
C(4)-H(4D)	0.9900
C(6)-H(6C)	0.9900
C(6)-H(6D)	0.9900
C(1)-C(2)	1.512(7)
C(1)-H(1C)	0.9900
C(1)-H(1D)	0.9900
C(2)-H(2C)	0.9900
C(2)-H(2D)	0.9900
C(3)-H(3C)	0.9900
C(3)-H(3D)	0.9900
O(1W)-O(3W)	0.899(19)
O(2W)-O(4W)	0.682(13)
N(4)-Co(1)-N(5)	93.42(16)
N(4)-Co(1)-N(6)	90.94(18)
N(5)-Co(1)-N(6)	85.85(17)
N(4)-Co(1)-N(3)	85.89(18)
N(5)-Co(1)-N(3)	88.88(17)
N(6)-Co(1)-N(3)	173.68(17)
N(4)-Co(1)-N(1)	174.36(15)
N(5)-Co(1)-N(1)	91.59(16)
N(6)-Co(1)-N(1)	92.02(18)
N(3)-Co(1)-N(1)	91.60(18)
N(4)-Co(1)-N(2)	90.16(16)

N(5)-Co(1)-N(2)	175.07(16)
N(6)-Co(1)-N(2)	90.70(17)
N(3)-Co(1)-N(2)	94.78(17)
N(1)-Co(1)-N(2)	85.01(15)
O(2)-C(7)-O(1)	126.1(5)
O(2)-C(7)-C(8)	117.2(5)
O(1)-C(7)-C(8)	116.7(4)
O(3)-C(8)-O(4)	125.6(4)
O(3)-C(8)-C(7)	117.3(4)
O(4)-C(8)-C(7)	117.2(4)
O(5)-C(9)-O(6)	126.7(5)
O(5)-C(9)-C(9)#1	118.2(5)
O(6)-C(9)-C(9)#1	115.1(6)
C(3)-N(3)-Co(1)	108.5(3)
C(3)-N(3)-H(3A)	110.0
Co(1)-N(3)-H(3A)	110.0
C(3)-N(3)-H(3B)	110.0
Co(1)-N(3)-H(3B)	110.0
H(3A)-N(3)-H(3B)	108.4
C(6)-N(6)-Co(1)	109.4(3)
C(6)-N(6)-H(6A)	109.8
Co(1)-N(6)-H(6A)	109.8
C(6)-N(6)-H(6B)	109.8
Co(1)-N(6)-H(6B)	109.8
H(6A)-N(6)-H(6B)	108.2
C(5)-N(5)-Co(1)	109.6(3)
C(5)-N(5)-H(5A)	109.7
Co(1)-N(5)-H(5A)	109.7
C(5)-N(5)-H(5B)	109.7
Co(1)-N(5)-H(5B)	109.7
H(5A)-N(5)-H(5B)	108.2
C(2)-N(2)-Co(1)	110.1(3)
C(2)-N(2)-H(2A)	109.6
Co(1)-N(2)-H(2A)	109.6
C(2)-N(2)-H(2B)	109.6
Co(1)-N(2)-H(2B)	109.6
H(2A)-N(2)-H(2B)	108.2
C(1)-N(1)-Co(1)	108.8(3)
C(1)-N(1)-H(1A)	109.9
Co(1)-N(1)-H(1A)	109.9
C(1)-N(1)-H(1B)	109.9
Co(1)-N(1)-H(1B)	109.9
H(1A)-N(1)-H(1B)	108.3
C(4)-N(4)-Co(1)	109.7(3)
C(4)-N(4)-H(4A)	109.7
Co(1)-N(4)-H(4A)	109.7
C(4)-N(4)-H(4B)	109.7
Co(1)-N(4)-H(4B)	109.7
H(4A)-N(4)-H(4B)	108.2
N(5)-C(5)-C(6)	105.7(3)
N(5)-C(5)-H(5C)	110.6
C(6)-C(5)-H(5C)	110.6
N(5)-C(5)-H(5D)	110.6
C(6)-C(5)-H(5D)	110.6
H(5C)-C(5)-H(5D)	108.7
N(4)-C(4)-C(3)	107.1(4)
N(4)-C(4)-H(4C)	110.3
C(3)-C(4)-H(4C)	110.3
N(4)-C(4)-H(4D)	110.3
C(3)-C(4)-H(4D)	110.3
H(4C)-C(4)-H(4D)	108.5
N(6)-C(6)-C(5)	108.5(4)
N(6)-C(6)-H(6C)	110.0
C(5)-C(6)-H(6C)	110.0

N(6)-C(6)-H(6D)	110.0
C(5)-C(6)-H(6D)	110.0
H(6C)-C(6)-H(6D)	108.4
N(1)-C(1)-C(2)	106.6(4)
N(1)-C(1)-H(1C)	110.4
C(2)-C(1)-H(1C)	110.4
N(1)-C(1)-H(1D)	110.4
C(2)-C(1)-H(1D)	110.4
H(1C)-C(1)-H(1D)	108.6
N(2)-C(2)-C(1)	106.9(4)
N(2)-C(2)-H(2C)	110.3
C(1)-C(2)-H(2C)	110.3
N(2)-C(2)-H(2D)	110.3
C(1)-C(2)-H(2D)	110.3
H(2C)-C(2)-H(2D)	108.6
N(3)-C(3)-C(4)	106.2(4)
N(3)-C(3)-H(3C)	110.5
C(4)-C(3)-H(3C)	110.5
N(3)-C(3)-H(3D)	110.5
C(4)-C(3)-H(3D)	110.5
H(3C)-C(3)-H(3D)	108.7

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1

Table 16. Anisotropic displacement parameters ($Å^2$ x 10^3) for **3**.
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)	12(1)	28(1)	10(1)	-5(1)	2(1)	-1(1)
O(1)	21(2)	38(2)	32(2)	4(2)	3(1)	-4(2)
O(3)	30(2)	31(2)	22(1)	-10(1)	7(1)	-2(2)
O(2)	60(3)	52(2)	21(2)	-16(2)	15(2)	-5(2)
O(4)	44(2)	34(2)	25(2)	-11(1)	9(2)	-16(2)
O(5)	16(2)	91(3)	16(2)	-1(2)	1(1)	-2(2)
C(7)	20(2)	36(3)	17(2)	0(2)	2(2)	0(2)
C(8)	15(2)	35(2)	15(2)	-5(2)	2(2)	-3(2)
C(9)	16(2)	106(5)	10(2)	-4(2)	4(2)	-3(3)
N(3)	18(2)	41(2)	16(2)	-4(2)	0(1)	-7(2)
N(6)	17(2)	43(2)	14(2)	-7(2)	4(1)	-6(2)
N(5)	19(2)	30(2)	16(2)	-6(1)	5(1)	-3(2)
N(2)	23(2)	31(2)	14(2)	-4(1)	2(1)	1(2)
N(1)	27(2)	30(2)	17(2)	-7(2)	1(2)	0(2)
N(4)	28(2)	32(2)	15(2)	-7(2)	3(2)	8(2)
C(5)	20(2)	36(3)	15(2)	-7(2)	-1(2)	-2(2)
C(4)	47(3)	37(3)	21(2)	-15(2)	-2(2)	0(2)
C(6)	13(2)	47(3)	23(2)	-9(2)	-2(2)	-5(2)
O(6)	13(2)	148(5)	11(2)	8(2)	2(1)	-3(2)
C(1)	35(3)	41(3)	20(2)	-6(2)	0(2)	13(2)
C(2)	51(4)	32(3)	19(2)	-2(2)	5(2)	9(2)
C(3)	46(3)	33(3)	24(2)	-8(2)	-5(2)	-10(2)

Table 17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **3**.

	x	y	z	U(eq)
H(3A)	12237	1674	2722	31
H(3B)	11828	2657	1596	31
H(6A)	7168	-516	2034	30
H(6B)	6350	290	2779	30
H(5A)	7957	3848	1034	27
H(5B)	9364	3124	468	27
H(2A)	10828	-234	3921	29
H(2B)	8997	-750	3955	29
H(1A)	9695	-531	1206	30
H(1B)	11145	524	951	30
H(4A)	7232	3301	2710	32
H(4B)	7569	1882	3673	32
H(5C)	7510	1625	36	29
H(5D)	6270	3298	-147	29
H(4C)	10166	2505	4122	41
H(4D)	8946	4201	3677	41
H(6C)	5050	2402	1521	34
H(6D)	4913	1031	1001	34
H(1C)	12865	-890	2397	41
H(1D)	12164	-2204	1965	41
H(2C)	9785	-2518	3139	44
H(2D)	11589	-2647	3831	44
H(3C)	10194	4663	2003	41
H(3D)	11869	4136	2848	41

Table 18. Hydrogen bonds for **3** [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1A)···O(4)#2	0.92	1.98	2.895(6)	175.0
N(1)-H(1B)···O(4)#3	0.92	2.01	2.880(5)	158.3
N(2)-H(2A)···O(5)#4	0.92	1.96	2.854(6)	164.0
N(2)-H(2B)···O(5)#1	0.92	2.27	3.019(5)	138.0
N(2)-H(2B)···O(1W)#1	0.92	2.35	3.136(11)	143.6
N(2)-H(2B)···O(3W)#1	0.92	2.34	2.99(2)	127.0
N(3)-H(3B)···O(3)#3	0.92	2.16	3.044(5)	160.1
N(3)-H(3A)···O(6)#4	0.92	1.98	2.848(5)	157.5
N(4)-H(4A)···O(1)	0.92	1.95	2.848(5)	165.1
N(4)-H(4B)···O(5)#1	0.92	1.98	2.860(6)	160.4
N(4)-H(4B)···O(6)	0.92	2.55	3.182(7)	126.2
N(5)-H(5A)···O(1)	0.92	2.25	3.083(6)	150.9
N(5)-H(5A)···O(3)	0.92	2.25	2.949(5)	131.9
N(5)-H(5B)···O(3)#3	0.92	2.10	2.992(5)	162.5
N(6)-H(6A)···O(2)#2	0.92	2.13	2.936(6)	146.3
N(6)-H(6A)···O(4)#2	0.92	2.42	3.132(5)	134.6
N(6)-H(6B)···O(6)	0.92	2.02	2.856(6)	150.2
N(6)-H(6B)···O(1W)#1	0.92	2.66	3.272(10)	124.3

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1 #2 x,y-1,z #3 -x+2,-y+1,-z
#4 x+1,y,z

Crystallographic data for 4

Table 19. Crystal data and structure refinement for **4**.

Identification code	**4**
Empirical formula	$C_{18}H_{62}Co_2N_{12}O_{19}$
Formula weight	868.66
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 28.964(2) Å alpha = 90 ° b = 10.3615(5) Å beta = 114.446(2) ° c = 12.7579(8) Å gamma = 90 °
Volume	3485.6(4) $Å^3$
Z, Calculated density	4, 1.655 Mg/m^3
Crystal size	0.23 x 0.17 x 0.12 mm
Theta range for data collection	2.94 to 27.49 °
Limiting indices	-37<=h<=37, -12<=k<=13, -16<=l<=15
Reflections collected / unique	12762 / 3970 [R(int) = 0.1440]
Completeness to theta = 27.49	98.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3970 / 3 / 241
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0641, wR2 = 0.1532
R indices (all data)	R1 = 0.1132, wR2 = 0.1759
Largest diff. peak and hole	0.758 and -0.724 $e.Å^{-3}$

Table 20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **4**.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co(1)	1302(1)	1552(1)	1175(1)	16(1)
O(4)	3315(1)	1340(3)	5743(3)	34(1)
O(3)	2786(1)	1498(3)	3860(3)	34(1)
O(1)	2029(1)	514(3)	4330(3)	29(1)
O(2)	2572(1)	128(4)	6124(3)	34(1)
C(4)	1572(2)	-1037(5)	1810(4)	26(1)
N(3)	1813(1)	2893(4)	1886(3)	23(1)
C(7)	2456(2)	573(4)	5134(4)	21(1)
N(5)	849(1)	90(4)	459(3)	20(1)
C(5)	1803(2)	2817(5)	-14(4)	25(1)
N(6)	1811(1)	253(3)	1968(3)	20(1)
C(3)	1168(2)	-1081(5)	611(4)	26(1)
N(4)	1504(1)	1641(3)	-126(3)	20(1)
C(6)	2141(2)	2996(5)	1251(4)	24(1)
C(8)	2896(2)	1220(4)	4897(4)	25(1)
O(5)	123(1)	-1204(4)	1292(3)	36(1)
O(6)	640(1)	-495(4)	3058(3)	36(1)
C(9)	216(2)	-853(5)	2311(4)	23(1)
N(1)	752(1)	2803(4)	391(3)	25(1)
C(1A)	570(3)	3345(6)	1236(6)	30(2)
C(2A)	581(2)	2285(7)	2026(6)	31(2)
C(1B)	407(7)	2750(30)	994(16)	30(2)
C(2B)	753(8)	2825(18)	2236(18)	31(2)
N(2)	1096(1)	1665(4)	2453(3)	23(1)
O(1W)	1583(1)	5635(3)	2154(3)	31(1)
O(2W)	829(2)	4542(4)	4543(4)	53(1)
O(3W)	0	5186(7)	2500	59(2)
O(4WA)	776(2)	6637(5)	2449(6)	51(2)
O(4WB)	614(8)	6317(18)	1520(20)	51(2)

Table 21. Bond lengths [Å] and angles [°] for **4**.

Co(1)-N(6)	1.943(4)
Co(1)-N(2)	1.957(4)
Co(1)-N(3)	1.958(4)
Co(1)-N(5)	1.964(4)
Co(1)-N(1)	1.975(4)
Co(1)-N(4)	1.977(3)
O(4)-C(8)	1.252(6)
O(3)-C(8)	1.259(6)
O(1)-C(7)	1.239(5)
O(2)-C(7)	1.252(5)
C(4)-N(6)	1.481(6)
C(4)-C(3)	1.494(7)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700
N(3)-C(6)	1.485(5)
N(3)-H(3A)	0.9000
N(3)-H(3B)	0.9000
C(7)-C(8)	1.577(6)
N(5)-C(3)	1.488(6)
N(5)-H(5A)	0.9000
N(5)-H(5B)	0.9000
C(5)-N(4)	1.469(5)
C(5)-C(6)	1.513(6)
C(5)-H(5C)	0.9700
C(5)-H(5D)	0.9700
N(6)-H(6A)	0.9000
N(6)-H(6B)	0.9000
C(3)-H(3C)	0.9700
C(3)-H(3D)	0.9700
N(4)-H(4C)	0.9000
N(4)-H(4D)	0.9000
C(6)-H(6C)	0.9700
C(6)-H(6D)	0.9700
O(5)-C(9)	1.267(5)
O(6)-C(9)	1.258(5)
C(9)-C(9)#1	1.518(8)
N(1)-C(1A)	1.491(6)
N(1)-C(1B)	1.492(10)
N(1)-H(1B)	0.9000
N(1)-H(1A)	0.9000
N(1)-H(1C)	0.9000
N(1)-H(1D)	0.9000
C(1A)-C(2A)	1.482(8)
C(1A)-H(1E)	0.9700
C(1A)-H(1F)	0.9700
C(2A)-N(2)	1.502(6)
C(2A)-H(2E)	0.9700
C(2A)-H(2F)	0.9700
C(1B)-C(2B)	1.485(12)
C(1B)-H(1G)	0.9700
C(1B)-H(1H)	0.9700
C(2B)-N(2)	1.510(10)
C(2B)-H(2G)	0.9700
C(2B)-H(2H)	0.9700
N(2)-H(2B)	0.9000
N(2)-H(2A)	0.9000
N(2)-H(2C)	0.9000
N(2)-H(2D)	0.9000
O(4WA)-O(4WB)	1.13(2)
N(6)-Co(1)-N(2)	92.00(15)

N(6)-Co(1)-N(3)	89.13(16)
N(2)-Co(1)-N(3)	90.26(15)
N(6)-Co(1)-N(5)	85.71(16)
N(2)-Co(1)-N(5)	93.36(15)
N(3)-Co(1)-N(5)	173.80(15)
N(6)-Co(1)-N(1)	176.18(15)
N(2)-Co(1)-N(1)	85.52(15)
N(3)-Co(1)-N(1)	93.78(17)
N(5)-Co(1)-N(1)	91.52(16)
N(6)-Co(1)-N(4)	92.60(15)
N(2)-Co(1)-N(4)	173.87(16)
N(3)-Co(1)-N(4)	85.77(15)
N(5)-Co(1)-N(4)	91.02(14)
N(1)-Co(1)-N(4)	90.08(15)
N(6)-C(4)-C(3)	106.9(4)
N(6)-C(4)-H(4A)	110.3
C(3)-C(4)-H(4A)	110.3
N(6)-C(4)-H(4B)	110.3
C(3)-C(4)-H(4B)	110.3
H(4A)-C(4)-H(4B)	108.6
C(6)-N(3)-Co(1)	109.3(3)
C(6)-N(3)-H(3A)	109.8
Co(1)-N(3)-H(3A)	109.8
C(6)-N(3)-H(3B)	109.8
Co(1)-N(3)-H(3B)	109.8
H(3A)-N(3)-H(3B)	108.3
O(1)-C(7)-O(2)	125.2(4)
O(1)-C(7)-C(8)	118.1(4)
O(2)-C(7)-C(8)	116.7(4)
C(3)-N(5)-Co(1)	108.0(3)
C(3)-N(5)-H(5A)	110.1
Co(1)-N(5)-H(5A)	110.1
C(3)-N(5)-H(5B)	110.1
Co(1)-N(5)-H(5B)	110.1
H(5A)-N(5)-H(5B)	108.4
N(4)-C(5)-C(6)	107.5(4)
N(4)-C(5)-H(5C)	110.2
C(6)-C(5)-H(5C)	110.2
N(4)-C(5)-H(5D)	110.2
C(6)-C(5)-H(5D)	110.2
H(5C)-C(5)-H(5D)	108.5
C(4)-N(6)-Co(1)	110.1(3)
C(4)-N(6)-H(6A)	109.6
Co(1)-N(6)-H(6A)	109.6
C(4)-N(6)-H(6B)	109.6
Co(1)-N(6)-H(6B)	109.6
H(6A)-N(6)-H(6B)	108.2
N(5)-C(3)-C(4)	106.9(4)
N(5)-C(3)-H(3C)	110.3
C(4)-C(3)-H(3C)	110.3
N(5)-C(3)-H(3D)	110.3
C(4)-C(3)-H(3D)	110.3
H(3C)-C(3)-H(3D)	108.6
C(5)-N(4)-Co(1)	109.0(3)
C(5)-N(4)-H(4C)	109.9
Co(1)-N(4)-H(4C)	109.9
C(5)-N(4)-H(4D)	109.9
Co(1)-N(4)-H(4D)	109.9
H(4C)-N(4)-H(4D)	108.3
N(3)-C(6)-C(5)	107.2(3)
N(3)-C(6)-H(6C)	110.3
C(5)-C(6)-H(6C)	110.3
N(3)-C(6)-H(6D)	110.3
C(5)-C(6)-H(6D)	110.3

H(6C)-C(6)-H(6D)	108.5
O(4)-C(8)-O(3)	128.0(4)
O(4)-C(8)-C(7)	116.7(4)
O(3)-C(8)-C(7)	115.2(4)
O(6)-C(9)-O(5)	126.1(4)
O(6)-C(9)-C(9)#1	115.7(5)
O(5)-C(9)-C(9)#1	118.3(5)
C(1A)-N(1)-C(1B)	29.6(9)
C(1A)-N(1)-Co(1)	109.5(3)
C(1B)-N(1)-Co(1)	106.5(10)
C(1A)-N(1)-H(1B)	109.8
C(1B)-N(1)-H(1B)	134.2
Co(1)-N(1)-H(1B)	109.8
C(1A)-N(1)-H(1A)	109.8
C(1B)-N(1)-H(1A)	84.0
Co(1)-N(1)-H(1A)	109.8
H(1B)-N(1)-H(1A)	108.2
C(1A)-N(1)-H(1C)	82.3
C(1B)-N(1)-H(1C)	110.4
Co(1)-N(1)-H(1C)	110.4
H(1B)-N(1)-H(1C)	29.7
H(1A)-N(1)-H(1C)	130.5
C(1A)-N(1)-H(1D)	131.0
C(1B)-N(1)-H(1D)	110.4
Co(1)-N(1)-H(1D)	110.4
H(1B)-N(1)-H(1D)	81.8
H(1A)-N(1)-H(1D)	28.5
H(1C)-N(1)-H(1D)	108.6
C(2A)-C(1A)-N(1)	107.3(5)
C(2A)-C(1A)-H(1E)	110.3
N(1)-C(1A)-H(1E)	110.3
C(2A)-C(1A)-H(1F)	110.3
N(1)-C(1A)-H(1F)	110.3
H(1E)-C(1A)-H(1F)	108.5
C(1A)-C(2A)-N(2)	107.6(5)
C(1A)-C(2A)-H(2E)	110.2
N(2)-C(2A)-H(2E)	110.2
C(1A)-C(2A)-H(2F)	110.2
N(2)-C(2A)-H(2F)	110.2
H(2E)-C(2A)-H(2F)	108.5
C(2B)-C(1B)-N(1)	104.3(15)
C(2B)-C(1B)-H(1G)	110.9
N(1)-C(1B)-H(1G)	110.9
C(2B)-C(1B)-H(1H)	110.9
N(1)-C(1B)-H(1H)	110.9
H(1G)-C(1B)-H(1H)	108.9
C(1B)-C(2B)-N(2)	104.7(15)
C(1B)-C(2B)-H(2G)	110.8
N(2)-C(2B)-H(2G)	110.8
C(1B)-C(2B)-H(2H)	110.8
N(2)-C(2B)-H(2H)	110.8
H(2G)-C(2B)-H(2H)	108.9
C(2A)-N(2)-C(2B)	27.8(9)
C(2A)-N(2)-Co(1)	108.8(3)
C(2B)-N(2)-Co(1)	107.4(10)
C(2A)-N(2)-H(2B)	109.9
C(2B)-N(2)-H(2B)	132.2
Co(1)-N(2)-H(2B)	109.9
C(2A)-N(2)-H(2A)	109.9
C(2B)-N(2)-H(2A)	85.3
Co(1)-N(2)-H(2A)	109.9
H(2B)-N(2)-H(2A)	108.3
C(2A)-N(2)-H(2C)	84.4
C(2B)-N(2)-H(2C)	110.2
Co(1)-N(2)-H(2C)	110.2

H(2B)-N(2)-H(2C)	27.7
H(2A)-N(2)-H(2C)	129.5
C(2A)-N(2)-H(2D)	130.7
C(2B)-N(2)-H(2D)	110.2
Co(1)-N(2)-H(2D)	110.2
H(2B)-N(2)-H(2D)	83.5
H(2A)-N(2)-H(2D)	27.1
H(2C)-N(2)-H(2D)	108.5

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table 22. Anisotropic displacement parameters ($Å^2$ x 10^3) for **4**.
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)	16(1)	15(1)	16(1)	-1(1)	6(1)	-1(1)
O(4)	22(2)	37(2)	39(2)	-1(2)	9(2)	-6(2)
O(3)	40(2)	37(2)	29(2)	5(2)	19(2)	-7(2)
O(1)	20(2)	39(2)	25(2)	0(2)	7(2)	-2(2)
O(2)	22(2)	50(2)	28(2)	14(2)	9(2)	2(2)
C(4)	26(3)	17(2)	35(3)	2(2)	13(2)	-1(2)
N(3)	23(2)	19(2)	27(2)	-4(2)	10(2)	-5(2)
C(7)	19(2)	23(3)	19(2)	-2(2)	7(2)	5(2)
N(5)	18(2)	21(2)	20(2)	1(2)	6(2)	1(2)
C(5)	25(3)	22(3)	30(3)	4(2)	12(2)	-4(2)
N(6)	22(2)	19(2)	19(2)	2(2)	9(2)	3(2)
C(3)	26(3)	18(2)	35(3)	-4(2)	14(2)	-2(2)
N(4)	20(2)	19(2)	20(2)	1(2)	7(2)	-1(2)
C(6)	19(2)	25(3)	29(3)	-1(2)	12(2)	-4(2)
C(8)	31(3)	15(2)	32(3)	-3(2)	17(2)	-3(2)
O(5)	27(2)	58(3)	27(2)	-1(2)	14(2)	-1(2)
O(6)	23(2)	54(2)	25(2)	7(2)	4(2)	-14(2)
C(9)	15(2)	29(3)	20(2)	1(2)	2(2)	-8(2)
N(1)	23(2)	27(2)	25(2)	-1(2)	10(2)	3(2)
C(1A)	26(4)	27(4)	37(4)	2(3)	13(3)	10(3)
C(2A)	31(4)	30(4)	39(4)	5(3)	22(4)	11(3)
C(1B)	26(4)	27(4)	37(4)	2(3)	13(3)	10(3)
C(2B)	31(4)	30(4)	39(4)	5(3)	22(4)	11(3)
N(2)	21(2)	22(2)	26(2)	-2(2)	9(2)	1(2)
O(1W)	27(2)	28(2)	34(2)	-2(2)	10(2)	7(2)
O(2W)	46(3)	44(3)	68(3)	-14(2)	23(2)	0(2)
O(3W)	40(4)	78(5)	57(4)	0	17(3)	0
O(4WA)	48(3)	43(3)	74(4)	10(3)	40(3)	7(2)
O(4WB)	48(3)	43(3)	74(4)	10(3)	40(3)	7(2)

Table 23. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **4**.

	x	y	z	U(eq)
H(4A)	1426	-1168	2363	31
H(4B)	1822	-1707	1920	31
H(3A)	1660	3655	1864	28
H(3B)	2003	2693	2627	28
H(5A)	633	-26	794	24
H(5B)	666	245	-296	24
H(5C)	1581	3556	-305	30
H(5D)	2007	2733	-451	30
H(6A)	2049	251	1687	24
H(6B)	1963	442	2724	24
H(3C)	1318	-1084	58	31
H(3D)	964	-1854	499	31
H(4C)	1689	942	-122	24
H(4D)	1226	1654	-797	24
H(6C)	2402	2336	1511	28
H(6D)	2304	3835	1381	28
H(1B)	866	3444	86	30
H(1A)	494	2408	-184	30
H(1C)	879	3603	435	30
H(1D)	582	2592	-356	30
H(1E)	788	4046	1664	36
H(1F)	227	3674	839	36
H(2E)	320	1655	1624	37
H(2F)	522	2623	2669	37
H(1G)	170	3462	768	36
H(1H)	217	1943	824	36
H(2G)	563	2790	2709	37
H(2H)	948	3618	2402	37
H(2B)	1084	871	2726	28
H(2A)	1322	2139	3027	28
H(2C)	930	944	2489	28
H(2D)	1370	1756	3124	28

Table 24. Hydrogen bonds for **4** [Å and °].

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
N(1)-H(1A)···O(5)#2	0.90	2.16	3.045(5)	168.4
N(1)-H(1B)···O(2W)#3	0.90	2.19	2.999(5)	149.6
N(2)-H(2A)···O(4)#4	0.90	2.17	3.039(5)	163.5
N(2)-H(2C)···O(6)	0.90	1.99	2.863(5)	162.9
N(3)-H(3A)···O(1W)	0.90	2.11	2.970(5)	158.8
N(3)-H(3B)···O(3)	0.90	2.49	3.240(5)	141.2
N(4)-H(4C)···O(1)#5	0.90	2.08	2.942(5)	161.5
N(4)-H(4D)···O(6)#5	0.90	2.10	2.870(5)	143.2
N(5)-H(5B)···O(5)#2	0.90	2.33	3.007(5)	132.0
N(5)-H(5B)···O(6)#5	0.90	2.09	2.896(5)	149.2
N(6)-H(6B)···O(1)	0.90	1.98	2.824(5)	155.8
N(6)-H(6B)···O(3)	0.90	2.47	3.134(5)	130.5
N(6)-H(6A)···O(2)#5	0.90	1.96	2.852(5)	168.5

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2 #2 -x,-y,-z #3 x,-y+1,z-1/2
#4 -x+1/2,-y+1/2,-z+1 #5 x,-y,z-1/2