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Explosive Werner-type cobalt(III) complexes†

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Supplementary Information

Fig. S1 ORTEP diagram of **2** with thermal displacement parameters drawn at 50% probability.

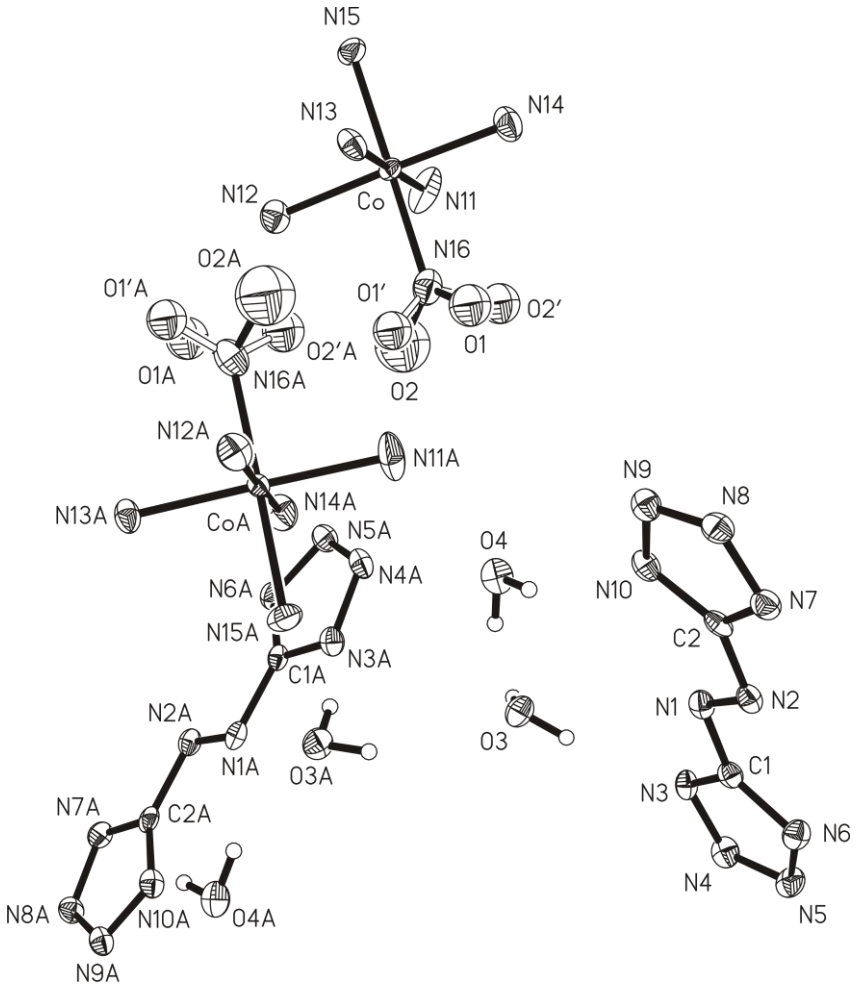

Fig. S2 Packing diagram of **2**. View along the *b* axis.

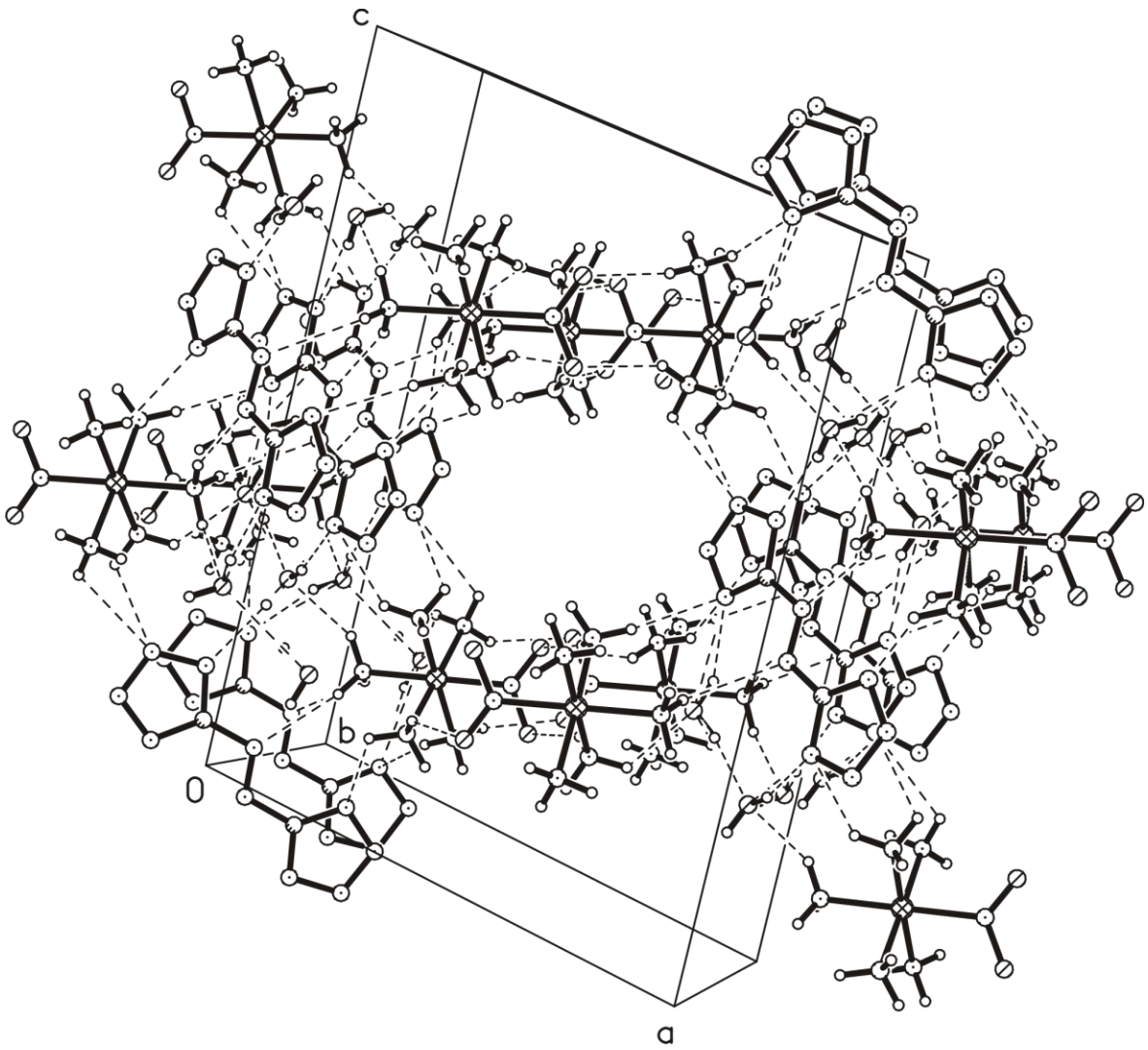

Table S1. Crystal data and structure refinement of **2**.

Identification code	ip103	
Empirical formula	$C_2 H_{19} Co N_{16} O_4$	
Formula weight	390.21	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 12.510(3) Å	α= 90°
	b = 7.4092(15) Å	β= 100.07(3)°
	c = 17.702(4) Å	γ = 90°
Volume	1615.5(6) $Å^3$	
Z	4	
Density (calculated)	1.605 Mg/m^3	
Absorption coefficient	1.111 mm^{-1}	
F(000)	808	
Crystal size	0.45 x 0.31 x 0.12 mm^3	
Theta range for data collection	2.34 to 28.28°	
Index ranges	-14<=h<=16, -9<=k<=9, -23<=l<=23	
Reflections collected	10430	
Independent reflections	3973 [R(int) = 0.0601]	
Completeness to theta = 28.00°	99.1 %	
Absorption correction	Sphere	
Max. and min. transmission	0.4912 and 0.4819	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3973 / 35 / 243	
Goodness-of-fit on F^2	1.096	
Final R indices [I>2sigma(I)]	R1 = 0.0577, wR2 = 0.1246	
R indices (all data)	R1 = 0.0817, wR2 = 0.1341	
Largest diff. peak and hole	0.565 and -0.731 $e.Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] of **2**.

Co-N(13)	1.941(3)	N(6)-C(1)	1.325(5)
Co-N(16)	1.946(4)	N(7)-N(8)	1.330(4)
Co-N(14)	1.949(3)	N(7)-C(2)	1.335(4)
Co-N(11)	1.956(3)	N(8)-N(9)	1.325(4)
Co-N(12)	1.965(3)	N(9)-N(10)	1.338(4)
Co-N(15)	1.969(3)	N(10)-C(2)	1.338(5)
N(1)-N(2)	1.252(4)	N(16)-O(1')	1.164(9)
N(1)-C(1)	1.410(5)	N(16)-O(1)	1.176(5)
N(2)-C(2)	1.407(5)	N(16)-O(2')	1.251(8)
N(3)-C(1)	1.333(4)	N(16)-O(2)	1.279(6)
N(3)-N(4)	1.338(4)	O(1')-O(2')#1	1.702(13)
N(4)-N(5)	1.317(4)	O(2')-O(1')#2	1.702(13)
N(5)-N(6)	1.344(4)		
N(13)-Co-N(16)	89.65(15)	N(8)-N(9)-N(10)	109.4(3)
N(13)-Co-N(14)	90.36(14)	C(2)-N(10)-N(9)	104.1(3)
N(16)-Co-N(14)	89.91(15)	N(6)-C(1)-N(3)	112.5(3)
N(13)-Co-N(11)	179.14(16)	N(6)-C(1)-N(1)	129.9(3)
N(16)-Co-N(11)	91.21(16)	N(3)-C(1)-N(1)	117.6(3)
N(14)-Co-N(11)	89.57(16)	N(7)-C(2)-N(10)	112.4(3)
N(13)-Co-N(12)	90.47(14)	N(7)-C(2)-N(2)	119.0(3)
N(16)-Co-N(12)	88.87(15)	N(10)-C(2)-N(2)	128.6(3)
N(14)-Co-N(12)	178.52(16)	O(1')-N(16)-O(1)	75.7(5)
N(11)-Co-N(12)	89.63(16)	O(1')-N(16)-O(2')	123.5(7)
N(13)-Co-N(15)	89.78(15)	O(1)-N(16)-O(2')	63.8(5)
N(16)-Co-N(15)	179.28(14)	O(1')-N(16)-O(2)	72.3(6)
N(14)-Co-N(15)	90.53(15)	O(1)-N(16)-O(2)	121.0(5)
N(11)-Co-N(15)	89.36(16)	O(2')-N(16)-O(2)	96.0(6)
N(12)-Co-N(15)	90.70(14)	O(1')-N(16)-Co	121.7(5)
N(2)-N(1)-C(1)	112.6(3)	O(1)-N(16)-Co	123.6(4)
N(1)-N(2)-C(2)	111.7(3)	O(2')-N(16)-Co	113.4(5)
C(1)-N(3)-N(4)	104.7(3)	O(2)-N(16)-Co	115.3(4)
N(5)-N(4)-N(3)	108.8(3)	N(16)-O(1')-O(2')#1	136.5(7)
N(4)-N(5)-N(6)	110.1(3)	N(16)-O(2')-O(1')#2	137.6(8)
C(1)-N(6)-N(5)	103.8(3)		
N(8)-N(7)-C(2)	104.3(3)		
N(9)-N(8)-N(7)	109.8(3)		

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

Table S3. Hydrogen bonds [Å and °] of **2**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(11)-H(11A)...N(6)#3	0.91	2.55	3.047(4)	115.3
N(11)-H(11C)...O(1)#2	0.91	2.43	3.213(6)	143.9
N(12)-H(12A)...N(10)#1	0.91	2.51	3.353(5)	155.1
N(12)-H(12A)...N(6)#3	0.91	2.66	3.151(4)	114.9
N(12)-H(12B)...O(1)#1	0.91	2.28	3.167(6)	165.4
N(13)-H(13A)...O(4)#1	0.91	2.45	3.011(4)	119.7
N(13)-H(13B)...N(8)#4	0.91	2.59	3.118(4)	117.5
N(13)-H(13C)...O(2)#1	0.91	2.21	3.004(7)	145.9
N(14)-H(14A)...N(3)#5	0.91	2.57	3.179(5)	125.1
N(14)-H(14A)...O(3)#5	0.91	2.59	3.487(5)	167.2
N(14)-H(14C)...N(8)#4	0.91	2.59	3.115(5)	117.6
N(15)-H(15A)...N(2)#3	0.91	2.41	3.273(4)	157.7
N(15)-H(15B)...O(3)#5	0.91	2.22	3.017(4)	145.5
N(15)-H(15C)...N(1)#1	0.91	2.52	3.176(4)	129.2
O(3)-HW1...N(3)	0.83(2)	2.01(3)	2.825(4)	166(7)
O(3)-HW2...N(7)#6	0.83(2)	2.06(2)	2.887(4)	174(6)
O(4)-HW3...N(10)	0.84(2)	2.11(3)	2.899(4)	157(6)
O(4)-HW4...O(3)	0.85(2)	2.07(3)	2.891(4)	162(6)

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

Fig. S3 ORTEP diagram of **3** with thermal displacement parameters drawn at 50% probability.

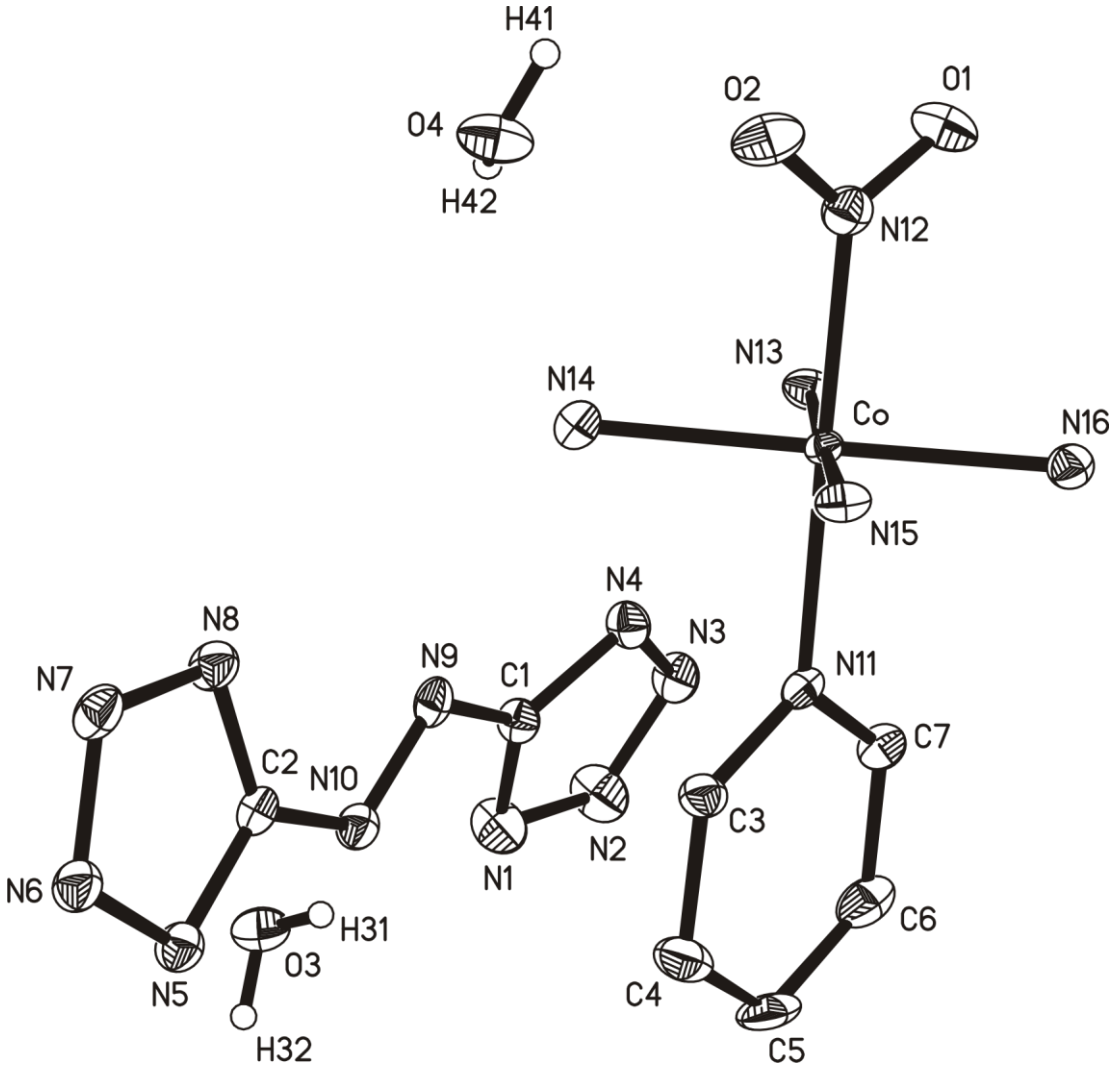

Fig. S4 Packing diagram of **3**. View along the *b* axis.

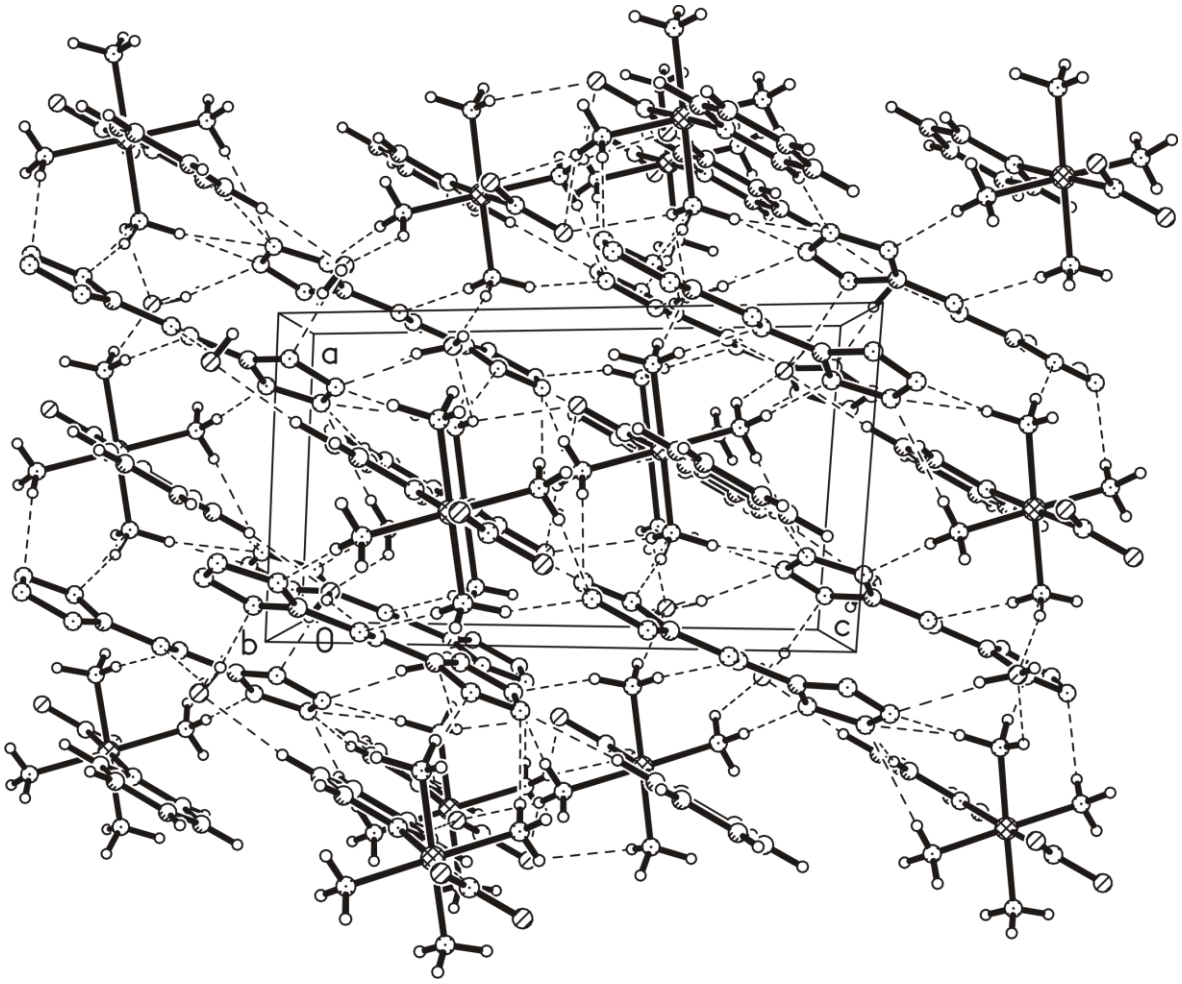

Table S4. Crystal data and structure refinement of **3**.

Identification code	ip123	
Empirical formula	$C_7H_{21}CoN_{16}O_4$	
Formula weight	452.28	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.3460(15) Å	α= 71.60(3)°
	b = 9.907(2) Å	β= 83.33(3)°
	c = 13.308(3) Å	γ = 78.54(3)°
Volume	899.2(3) $Å^3$	
Z	2	
Density (calculated)	1.671 Mg/m^3	
Absorption coefficient	1.011 mm^{-1}	
F(000)	468	
Crystal size	0.45 x 0.19 x 0.03 mm^3	
Theta range for data collection	2.30 to 28.28°	
Index ranges	-9<=h<=9, -13<=k<=13, -17<=l<=17	
Reflections collected	9386	
Independent reflections	4440 [R(int) = 0.0721]	
Completeness to theta = 28.28°	99.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4440 / 4 / 305	
Goodness-of-fit on F^2	1.193	
Final R indices [I>2sigma(I)]	R1 = 0.0611, wR2 = 0.1225	
R indices (all data)	R1 = 0.0795, wR2 = 0.1282	
Largest diff. peak and hole	0.682 and -0.873 $e.Å^{-3}$	

Table S5. Bond lengths [Å] and angles [°] of **3**.

Co-N(12)	1.899(3)	N(5)-N(6)	1.340(4)
Co-N(16)	1.956(3)	N(6)-N(7)	1.327(5)
Co-N(15)	1.961(3)	N(7)-N(8)	1.334(4)
Co-N(14)	1.961(3)	N(8)-C(2)	1.345(5)
Co-N(13)	1.961(3)	N(9)-N(10)	1.261(5)
Co-N(11)	1.996(3)	N(9)-C(1)	1.408(5)
O(1)-N(12)	1.234(4)	N(10)-C(2)	1.399(5)
O(2)-N(12)	1.238(4)	N(11)-C(3)	1.346(5)
N(1)-N(2)	1.334(5)	N(11)-C(7)	1.348(5)
N(1)-C(1)	1.336(5)	C(3)-C(4)	1.366(5)
N(2)-N(3)	1.331(5)	C(4)-C(5)	1.384(6)
N(3)-N(4)	1.338(4)	C(5)-C(6)	1.387(6)
N(4)-C(1)	1.334(5)	C(6)-C(7)	1.378(5)
N(5)-C(2)	1.333(5)		
N(12)-Co-N(16)	89.65(15)	N(7)-N(8)-C(2)	104.0(3)
N(12)-Co-N(15)	88.18(14)	N(10)-N(9)-C(1)	112.8(3)
N(16)-Co-N(15)	87.72(15)	N(9)-N(10)-C(2)	113.4(3)
N(12)-Co-N(14)	89.57(15)	C(3)-N(11)-C(7)	117.6(3)
N(16)-Co-N(14)	179.17(16)	C(3)-N(11)-Co	120.5(2)
N(15)-Co-N(14)	91.97(15)	C(7)-N(11)-Co	121.9(3)
N(12)-Co-N(13)	89.38(14)	O(1)-N(12)-O(2)	120.2(3)
N(16)-Co-N(13)	91.90(15)	O(1)-N(12)-Co	119.2(3)
N(15)-Co-N(13)	177.53(15)	O(2)-N(12)-Co	120.5(3)
N(14)-Co-N(13)	88.38(15)	N(4)-C(1)-N(1)	113.0(3)
N(12)-Co-N(11)	178.98(15)	N(4)-C(1)-N(9)	119.9(3)
N(16)-Co-N(11)	89.78(14)	N(1)-C(1)-N(9)	127.1(4)
N(15)-Co-N(11)	90.96(13)	N(5)-C(2)-N(8)	112.7(3)
N(14)-Co-N(11)	91.00(14)	N(5)-C(2)-N(10)	120.3(3)
N(13)-Co-N(11)	91.48(14)	N(8)-C(2)-N(10)	127.0(3)
N(2)-N(1)-C(1)	103.9(3)	N(11)-C(3)-C(4)	123.1(4)
N(3)-N(2)-N(1)	109.7(3)	C(3)-C(4)-C(5)	119.5(4)
N(2)-N(3)-N(4)	109.5(3)	C(4)-C(5)-C(6)	117.9(4)
C(1)-N(4)-N(3)	103.9(3)	C(7)-C(6)-C(5)	119.6(4)
C(2)-N(5)-N(6)	103.9(3)	N(11)-C(7)-C(6)	122.2(4)
N(7)-N(6)-N(5)	109.9(3)		
N(6)-N(7)-N(8)	109.5(3)		

Table S6. Hydrogen bonds [Å and °] of **3**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(32)...N(10)#1	0.83(2)	2.31(5)	3.039(5)	147(7)
O(4)-H(41)...N(5)#2	0.82(2)	2.06(3)	2.858(5)	164(6)
O(4)-H(42)...N(2)#3	0.83(2)	2.11(3)	2.905(5)	162(6)
N(14)-H(14A)...O(4)	0.81(5)	2.06(5)	2.861(5)	169(5)
N(16)-H(16B)...N(8)#4	0.90(5)	2.11(5)	2.985(5)	165(4)
N(16)-H(16C)...O(1)	0.80(5)	2.47(5)	2.875(5)	112(4)

Symmetry transformations used to generate equivalent atoms:

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

#4 x+1,y,z

Fig. S5 ORTEPdiagram of **4** with thermal displacement parameters drawn at 50% probability.

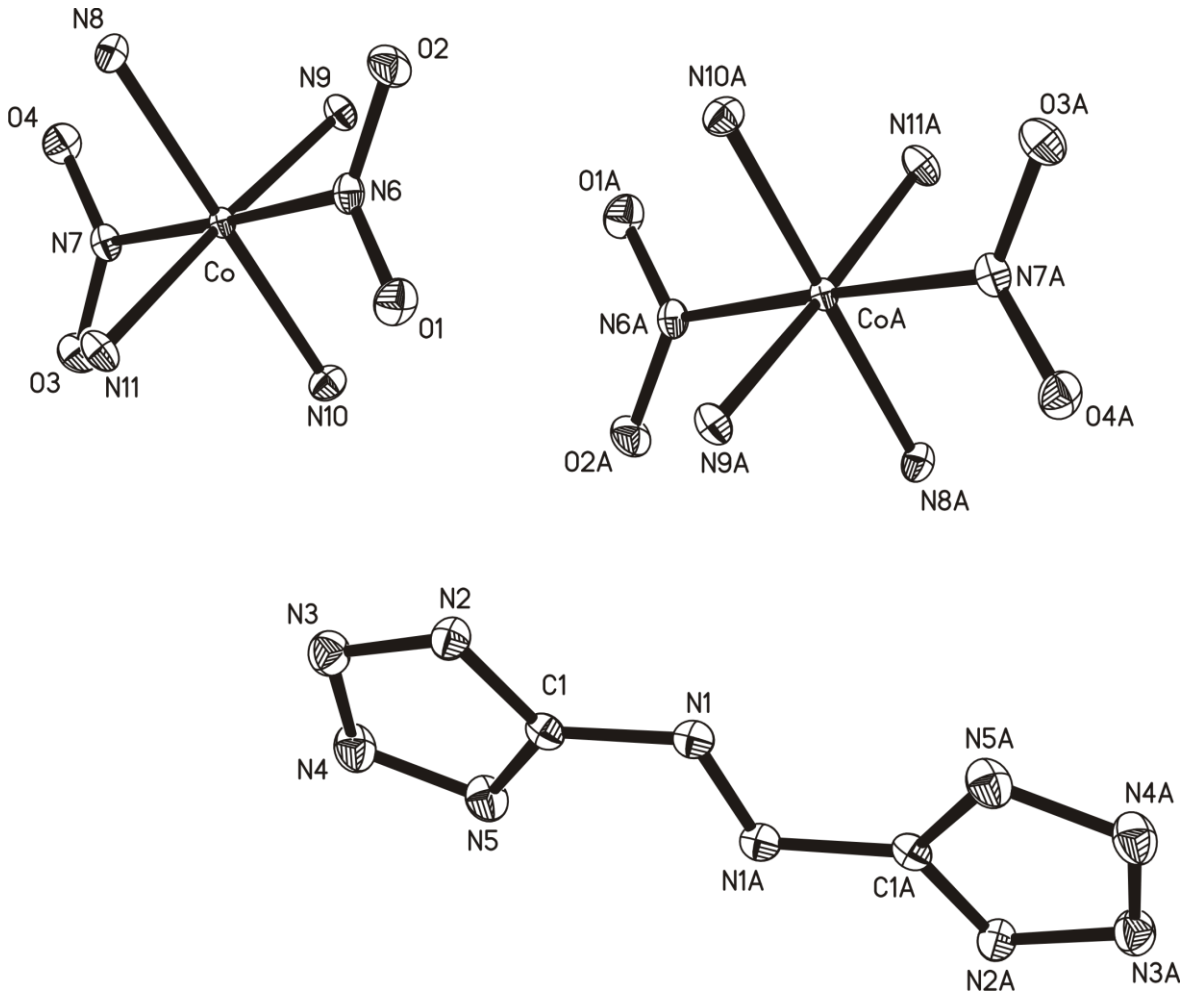

Fig. S6 Packing diagram of **4**. View along the *a* axis.

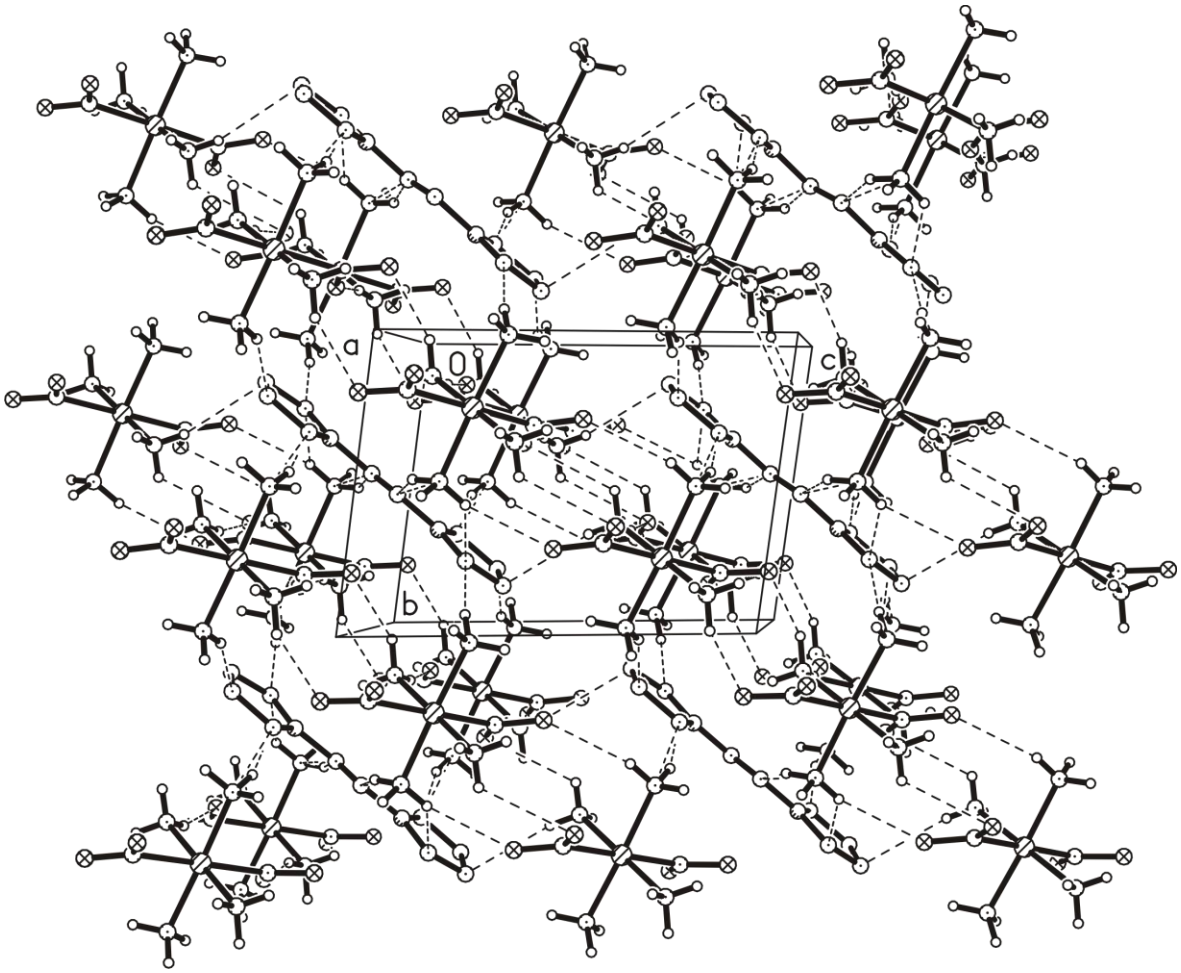

Table S7. Crystal data and structure refinement of **4**.

Identification code	ip99	
Empirical formula	$C_2H_{24}Co_2N_{22}O_8$	
Formula weight	602.22	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.1228(14) Å	α= 96.49(3)°
	b = 7.3402(15) Å	β= 105.79(3)°
	c = 10.138(2) Å	γ = 95.10(3)°
Volume	502.79(17) $Å^3$	
Z	1	
Density (calculated)	1.989 Mg/m^3	
Absorption coefficient	1.740 mm^{-1}	
F(000)	308	
Crystal size	0.60 x 0.30 x 0.05 mm^3	
Theta range for data collection	2.11 to 28.28°	
Index ranges	-9<=h<=8, -9<=k<=9, -13<=l<=13	
Reflections collected	5276	
Independent reflections	2457 [R(int) = 0.0567]	
Completeness to theta = 28.00°	98.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2457 / 0 / 202	
Goodness-of-fit on F^2	1.099	
Final R indices [I>2sigma(I)]	R1 = 0.0325, wR2 = 0.0861	
R indices (all data)	R1 = 0.0348, wR2 = 0.0876	
Largest diff. peak and hole	1.132 and -0.821 $e.Å^{-3}$	

Table S8. Bond lengths [Å] and angles [°]of **4**.

C(1)-N(2)	1.331(2)	N(3)-N(4)	1.326(2)
C(1)-N(5)	1.336(2)	N(4)-N(5)	1.342(2)
C(1)-N(1)	1.405(2)	N(8)-H(8A)	0.80(3)
Co-N(7)	1.9319(15)	N(8)-H(8B)	0.86(3)
Co-N(6)	1.9360(15)	N(8)-H(8C)	0.87(3)
Co-N(9)	1.9453(16)	N(9)-H(9A)	0.89(3)
Co-N(8)	1.9514(17)	N(9)-H(9B)	0.88(3)
Co-N(11)	1.9532(16)	N(9)-H(9C)	0.88(3)
Co-N(10)	1.9555(18)	N(10)-H(10A)	0.82(3)
O(1)-N(6)	1.239(2)	N(10)-H(10B)	0.79(4)
O(2)-N(6)	1.238(2)	N(10)-H(10C)	0.82(4)
O(3)-N(7)	1.241(2)	N(11)-H(11A)	0.86(3)
O(4)-N(7)	1.238(2)	N(11)-H(11B)	0.87(3)
N(1)-N(1)#1	1.251(3)	N(11)-H(11C)	0.90(4)
N(2)-N(3)	1.339(2)		
N(2)-C(1)-N(5)	112.51(16)	N(3)-N(4)-N(5)	109.80(16)
N(2)-C(1)-N(1)	120.23(15)	C(1)-N(5)-N(4)	103.95(15)
N(5)-C(1)-N(1)	127.13(16)	O(2)-N(6)-O(1)	120.22(15)
N(7)-Co-N(6)	177.95(6)	O(2)-N(6)-Co	119.98(12)
N(7)-Co-N(9)	89.24(7)	O(1)-N(6)-Co	119.79(12)
N(6)-Co-N(9)	90.04(7)	O(4)-N(7)-O(3)	119.89(15)
N(7)-Co-N(8)	89.28(7)	O(4)-N(7)-Co	119.64(12)
N(6)-Co-N(8)	88.80(7)	O(3)-N(7)-Co	120.47(12)
N(9)-Co-N(8)	90.63(7)	Co-N(8)-H(8A)	110(2)
N(7)-Co-N(11)	90.78(7)	Co-N(8)-H(8B)	116(2)
N(6)-Co-N(11)	90.03(7)	H(8A)-N(8)-H(8B)	104(3)
N(9)-Co-N(11)	177.01(6)	Co-N(8)-H(8C)	113(2)
N(8)-Co-N(11)	92.35(8)	H(8A)-N(8)-H(8C)	108(3)
N(7)-Co-N(10)	90.81(7)	H(8B)-N(8)-H(8C)	104(3)
N(6)-Co-N(10)	91.10(7)	Co-N(9)-H(9A)	112.7(18)
N(9)-Co-N(10)	89.16(7)	Co-N(9)-H(9B)	111.6(17)
N(8)-Co-N(10)	179.77(6)	H(9A)-N(9)-H(9B)	104(2)
N(11)-Co-N(10)	87.86(8)	Co-N(9)-H(9C)	110.3(19)
N(1)#1-N(1)-C(1)	113.37(18)	H(9A)-N(9)-H(9C)	108(3)
C(1)-N(2)-N(3)	104.68(15)	H(9B)-N(9)-H(9C)	110(3)
N(4)-N(3)-N(2)	109.05(16)	Co-N(10)-H(10A)	112(2)

Co-N(10)-H(10B)	107(3)	Co-N(11)-H(11B)	111(2)
H(10A)-N(10)-H(10B)	111(3)	H(11A)-N(11)-H(11B)	111(3)
Co-N(10)-H(10C)	112(3)	Co-N(11)-H(11C)	113(2)
H(10A)-N(10)-H(10C)	112(3)	H(11A)-N(11)-H(11C)	109(3)
H(10B)-N(10)-H(10C)	102(3)	H(11B)-N(11)-H(11C)	107(3)
Co-N(11)-H(11A)	106.8(19)		

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

Table S9. Hydrogen bonds [Å and °] of **4**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(8)-H(8A)...O(4)	0.80(3)	2.39(3)	2.801(2)	113(3)
N(8)-H(8A)...N(5)#2	0.80(3)	2.65(3)	3.410(3)	159(3)
N(8)-H(8B)...O(4)#3	0.86(3)	2.33(3)	3.028(2)	138(3)
N(8)-H(8B)...O(3)#3	0.86(3)	2.61(3)	3.173(2)	124(2)
N(8)-H(8B)...N(2)#4	0.86(3)	2.64(3)	3.276(2)	131(2)
N(8)-H(8C)...O(2)	0.87(3)	2.32(3)	2.849(2)	119(3)
N(8)-H(8C)...O(3)#5	0.87(3)	2.46(3)	3.300(2)	161(3)
N(9)-H(9A)...N(1)#6	0.89(3)	2.22(3)	2.984(2)	143(2)
N(9)-H(9B)...N(5)#7	0.88(3)	2.12(3)	2.973(2)	162(2)
N(9)-H(9C)...O(1)#6	0.88(3)	2.34(3)	3.142(2)	152(3)
N(9)-H(9C)...N(2)#6	0.88(3)	2.49(3)	3.117(2)	129(2)
N(10)-H(10A)...O(3)	0.82(3)	2.37(3)	2.874(2)	120(3)
N(10)-H(10A)...O(2)#8	0.82(3)	2.53(3)	3.310(2)	160(3)
N(10)-H(10B)...O(1)	0.79(4)	2.48(4)	2.909(2)	116(3)
N(10)-H(10B)...N(3)	0.79(4)	2.55(4)	3.289(2)	158(3)
N(10)-H(10C)...O(2)#6	0.82(4)	2.56(4)	3.104(2)	125(3)
N(11)-H(11A)...O(1)	0.86(3)	2.47(3)	2.945(2)	116(2)
N(11)-H(11B)...N(4)#9	0.87(3)	2.28(3)	3.095(2)	157(3)
N(11)-H(11B)...O(3)	0.87(3)	2.51(3)	3.019(2)	118(3)
N(11)-H(11C)...N(2)#4	0.90(4)	2.17(4)	3.057(2)	168(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+2 #2 x-1,y,z-1 #3 -x,-y,-z
#4 -x,-y,-z+1 #5 x-1,y,z #6 -x,-y+1,-z+1
#7 -x+1,-y+1,-z+1 #8 x+1,y,z #9 -x+1,-y,-z+1

Fig. S7 ORTEP diagram of **5** with thermal displacement parameters drawn at 50% probability.

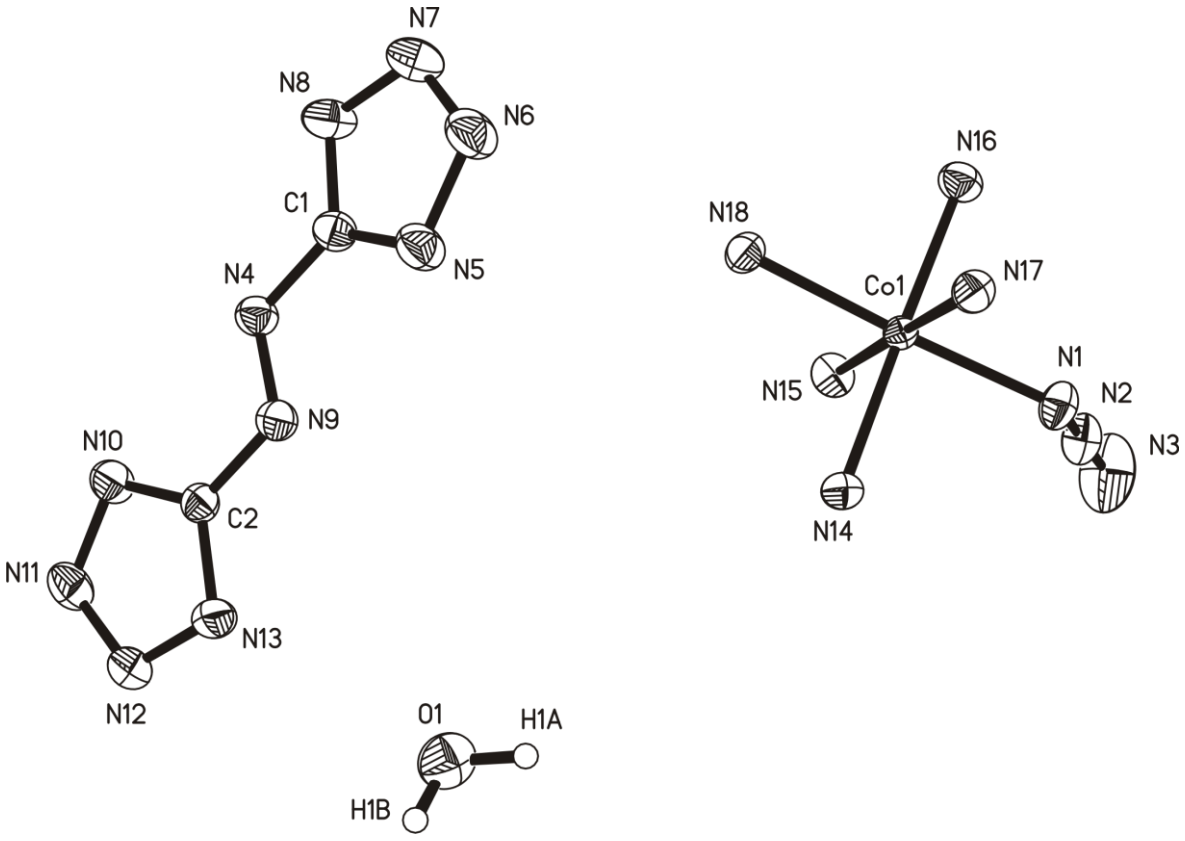

Fig. S8 Packing diagram of **5**. View along the *b* axis.

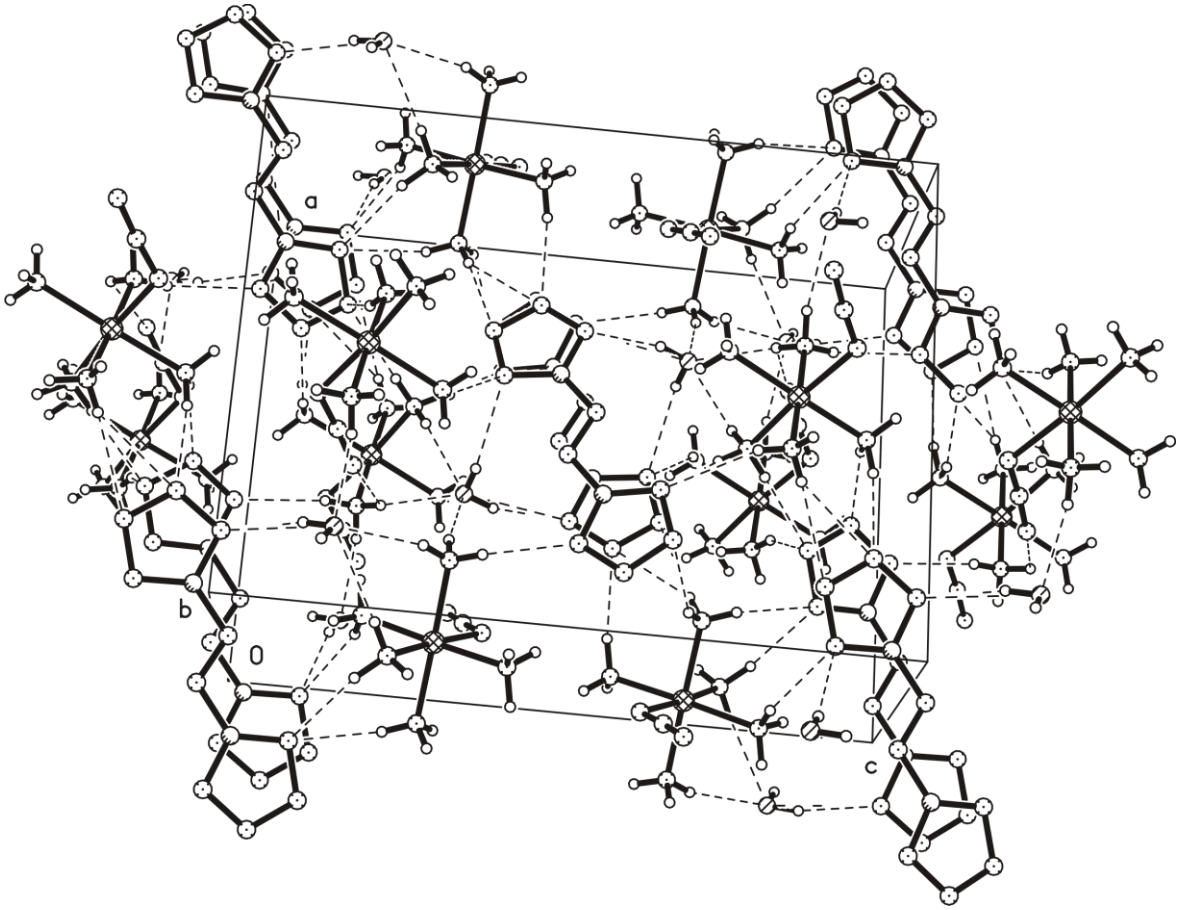

Table S10. Crystal data and structure refinement of **5**.

Identification code	bl154a	
Empirical formula	$C_2 H_{17} Co N_{18} O$	
Formula weight	368.21	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 12.067(2) Å	α= 90°
	b = 7.4493(15) Å	β= 90.94(3)°
	c = 15.764(3) Å	γ = 90°
Volume	1416.8(5) $Å^3$	
Z	4	
Density (calculated)	1.726 Mg/m^3	
Absorption coefficient	1.250 mm^{-1}	
F(000)	760	
Crystal size	0.50 x 0.40 x 0.30 mm^3	
Theta range for data collection	2.58 to 26.37°	
Index ranges	-15<=h<=15, -8<=k<=8, -19<=l<=19	
Reflections collected	12494	
Independent reflections	2764 [R(int) = 0.0244]	
Completeness to theta = 26.37°	95.4 %	
Absorption correction	Sphere	
Max. and min. transmission	0.4295 and 0.4186	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2764 / 0 / 267	
Goodness-of-fit on F^2	0.974	
Final R indices [I>2sigma(I)]	R1 = 0.0226, wR2 = 0.0563	
R indices (all data)	R1 = 0.0266, wR2 = 0.0573	
Largest diff. peak and hole	0.375 and -0.195 $e.Å^{-3}$	

Table S11. Bond lengths [Å] and angles [°]of **5**.

Co(1)-N(14)	1.9496(13)	N(12)-N(13)	1.335(2)
Co(1)-N(1)	1.9550(14)	N(13)-C(2)	1.332(2)
Co(1)-N(17)	1.9566(13)	N(14)-H(14A)	0.86(2)
Co(1)-N(18)	1.9637(14)	N(14)-H(14B)	0.85(3)
Co(1)-N(16)	1.9758(14)	N(14)-H(14C)	0.84(2)
Co(1)-N(15)	1.9804(14)	N(15)-H(15A)	0.81(3)
N(1)-N(2)	1.189(2)	N(15)-H(15B)	0.88(3)
N(2)-N(3)	1.157(2)	N(15)-H(15C)	0.84(3)
N(4)-N(9)	1.2553(18)	N(16)-H(16A)	0.84(4)
N(4)-C(1)	1.411(2)	N(16)-H(16B)	0.78(3)
N(5)-C(1)	1.330(2)	N(16)-H(16C)	0.80(4)
N(5)-N(6)	1.3458(19)	N(17)-H(17A)	0.83(2)
N(6)-N(7)	1.317(2)	N(17)-H(17B)	0.89(3)
N(7)-N(8)	1.336(2)	N(17)-H(17C)	0.90(3)
N(8)-C(1)	1.330(2)	N(18)-H(18A)	0.90(2)
N(9)-C(2)	1.407(2)	N(18)-H(18B)	0.83(2)
N(10)-C(2)	1.330(2)	N(18)-H(18C)	0.85(3)
N(10)-N(11)	1.3411(19)	O(1)-H(1A)	0.84(3)
N(11)-N(12)	1.318(2)	O(1)-H(1B)	0.73(3)
N(14)-Co(1)-N(1)	89.27(7)	N(9)-N(4)-C(1)	112.34(13)
N(14)-Co(1)-N(17)	90.01(6)	C(1)-N(5)-N(6)	103.87(13)
N(1)-Co(1)-N(17)	84.93(6)	N(7)-N(6)-N(5)	109.40(13)
N(14)-Co(1)-N(18)	91.66(7)	N(6)-N(7)-N(8)	109.80(13)
N(1)-Co(1)-N(18)	175.72(6)	C(1)-N(8)-N(7)	104.10(13)
N(17)-Co(1)-N(18)	90.89(6)	N(4)-N(9)-C(2)	113.09(12)
N(14)-Co(1)-N(16)	177.41(7)	C(2)-N(10)-N(11)	103.85(13)
N(1)-Co(1)-N(16)	89.09(7)	N(12)-N(11)-N(10)	109.89(13)
N(17)-Co(1)-N(16)	91.84(7)	N(11)-N(12)-N(13)	109.21(12)
N(18)-Co(1)-N(16)	90.12(7)	C(2)-N(13)-N(12)	104.50(13)
N(14)-Co(1)-N(15)	88.04(7)	Co(1)-N(14)-H(14A)	109.4(15)
N(1)-Co(1)-N(15)	95.13(7)	Co(1)-N(14)-H(14B)	112.7(15)
N(17)-Co(1)-N(15)	178.05(6)	H(14A)-N(14)-H(14B)	106(2)
N(18)-Co(1)-N(15)	89.09(7)	Co(1)-N(14)-H(14C)	113.9(14)
N(16)-Co(1)-N(15)	90.10(7)	H(14A)-N(14)-H(14C)	107(2)
N(2)-N(1)-Co(1)	123.02(11)	H(14B)-N(14)-H(14C)	107(2)
N(3)-N(2)-N(1)	176.35(18)	Co(1)-N(15)-H(15A)	109(2)

Co(1)-N(15)-H(15B)	113.4(15)	H(17A)-N(17)-H(17C)	111(2)
H(15A)-N(15)-H(15B)	107(3)	H(17B)-N(17)-H(17C)	105(2)
Co(1)-N(15)-H(15C)	115.5(19)	Co(1)-N(18)-H(18A)	109.8(15)
H(15A)-N(15)-H(15C)	103(3)	Co(1)-N(18)-H(18B)	111.4(15)
H(15B)-N(15)-H(15C)	108(3)	H(18A)-N(18)-H(18B)	108.9(19)
Co(1)-N(16)-H(16A)	117(2)	Co(1)-N(18)-H(18C)	110.7(16)
Co(1)-N(16)-H(16B)	114(2)	H(18A)-N(18)-H(18C)	107(2)
H(16A)-N(16)-H(16B)	106(3)	H(18B)-N(18)-H(18C)	109(2)
Co(1)-N(16)-H(16C)	112(2)	H(1A)-O(1)-H(1B)	101(2)
H(16A)-N(16)-H(16C)	101(3)	N(5)-C(1)-N(8)	112.82(14)
H(16B)-N(16)-H(16C)	105(3)	N(5)-C(1)-N(4)	127.92(13)
Co(1)-N(17)-H(17A)	108.8(16)	N(8)-C(1)-N(4)	119.26(14)
Co(1)-N(17)-H(17B)	111.5(14)	N(10)-C(2)-N(13)	112.54(14)
H(17A)-N(17)-H(17B)	109(2)	N(10)-C(2)-N(9)	128.14(13)
Co(1)-N(17)-H(17C)	112.2(15)	N(13)-C(2)-N(9)	119.31(13)

Table S12. Hydrogen bonds [Å and °] of **5**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...N(8)#1	0.84(3)	2.01(3)	2.832(2)	166(2)
O(1)-H(1B)...N(5)#2	0.73(3)	2.34(3)	3.044(2)	162(3)
N(14)-H(14A)...O(1)#3	0.86(2)	2.24(2)	3.090(2)	170.1(19)
N(14)-H(14B)...O(1)#4	0.85(3)	2.26(3)	3.083(2)	163(2)
N(14)-H(14C)...N(13)#4	0.84(2)	2.20(2)	3.013(2)	163(2)
N(17)-H(17B)...N(12)#5	0.89(3)	2.26(3)	3.043(2)	145.6(17)
N(17)-H(17C)...N(7)#6	0.90(3)	2.17(3)	3.061(2)	170(2)
N(18)-H(18B)...N(11)#5	0.83(2)	2.27(3)	3.098(2)	175(2)
N(18)-H(18C)...O(1)#4	0.85(3)	2.30(3)	3.110(2)	160(2)

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

Fig. S9 ORTEP diagram of **7** with thermal displacement parameters drawn at 50% probability.

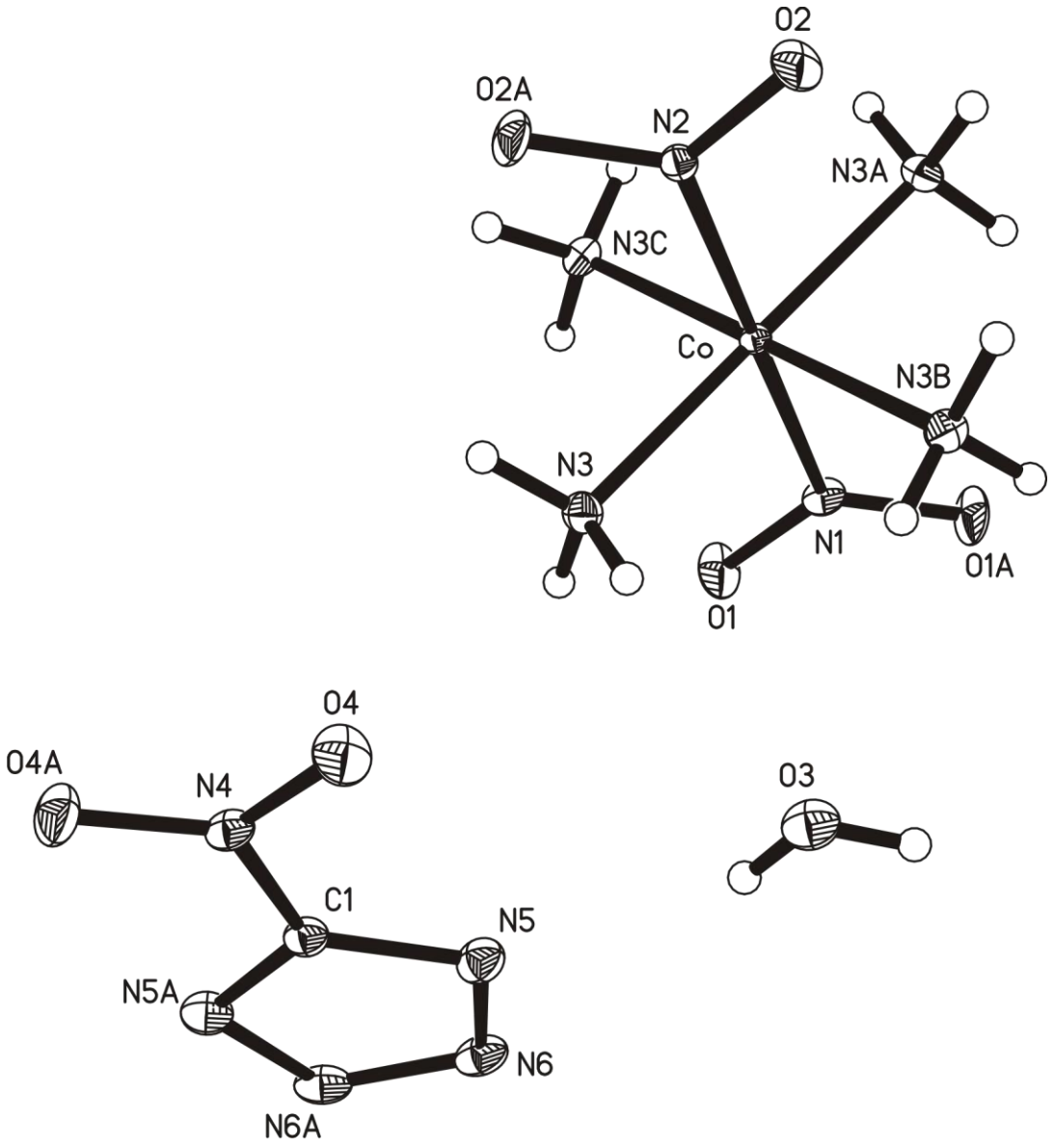

Fig. S10 Packing diagram of **7**. View along the *b* axis.

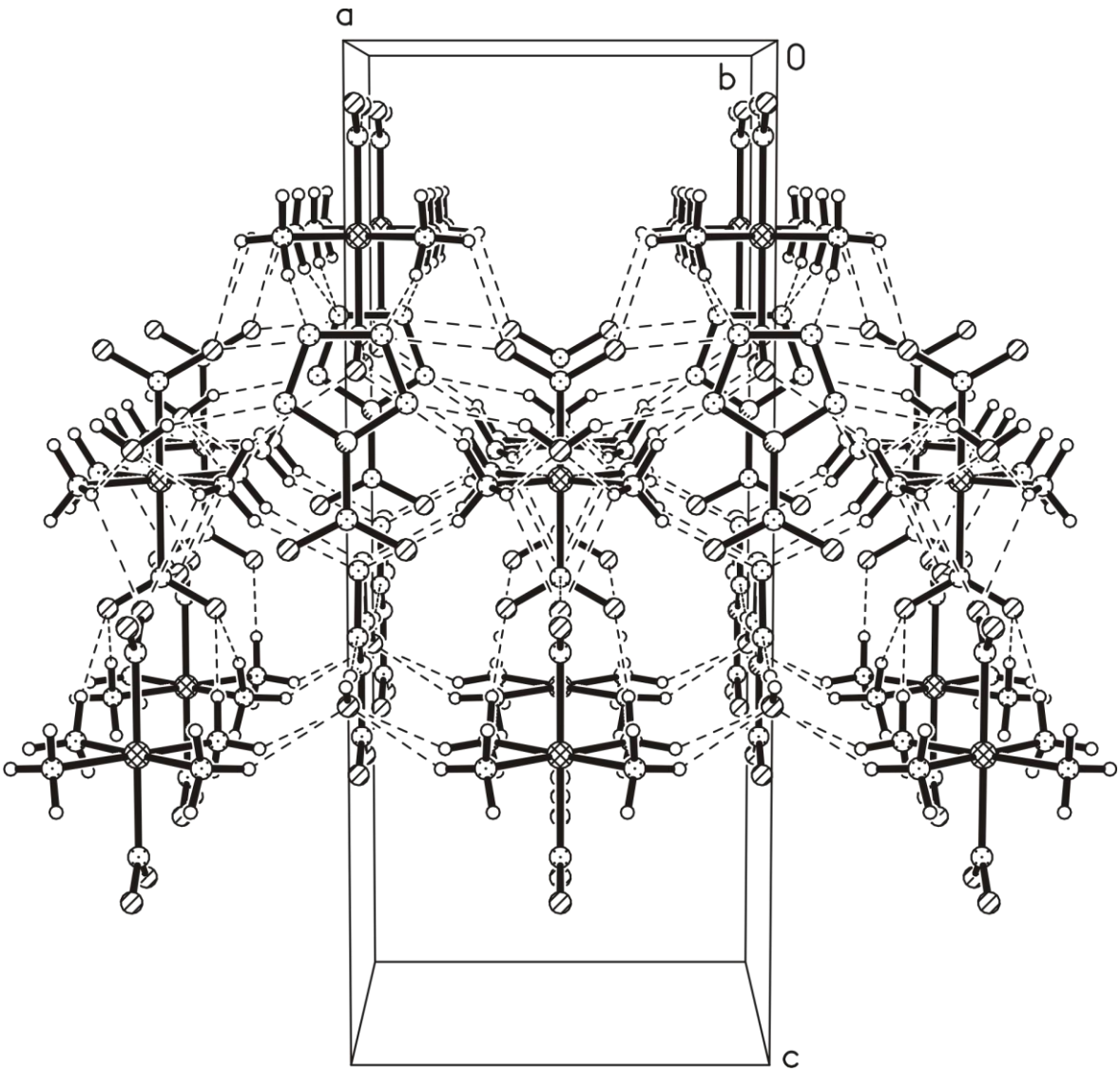

Table S13. Crystal data and structure refinement of **7**.

Identification code	ip115	
Empirical formula	$CH_{14}CoN_{11}O_7$	
Formula weight	351.12	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	$I4_1md$	
Unit cell dimensions	a = 7.8926(11) Å	α= 90°
	b = 7.8926(11) Å	β= 90°
	c = 19.125(4) Å	γ = 90°
Volume	1191.3(3) $Å^3$	
Z	4	
Density (calculated)	1.958 Mg/m^3	
Absorption coefficient	1.502 mm^{-1}	
F(000)	720	
Crystal size	0.42 x 0.41 x 0.24 mm^3	
Theta range for data collection	2.79 to 29.16°	
Index ranges	-10<=h<=10, -10<=k<=10, -26<=l<=26	
Reflections collected	6477	
Independent reflections	855 [R(int) = 0.0510]	
Completeness to theta = 29.00°	98.9 %	
Absorption correction	None	
Max. and min. transmission	0.7145 and 0.5711	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	855 / 2 / 67	
Goodness-of-fit on F^2	1.208	
Final R indices [I>2sigma(I)]	R1 = 0.0232, wR2 = 0.0565	
R indices (all data)	R1 = 0.0234, wR2 = 0.0566	
Absolute structure parameter	0.007(15)	
Largest diff. peak and hole	0.434 and -0.989 $e.Å^{-3}$	

Table S14. Bond lengths [Å] and angles [°]of **7**.

C(1)-N(5)	1.331(3)	N(1)-O(1)	1.235(2)
C(1)-N(5)#1	1.331(3)	N(1)-O(1)#4	1.235(2)
C(1)-N(4)	1.438(6)	N(2)-O(2)	1.234(3)
Co-N(1)	1.937(3)	N(2)-O(2)#4	1.234(3)
Co-N(2)	1.942(4)	N(4)-O(4)	1.228(2)
Co-N(3)	1.9537(10)	N(4)-O(4)#1	1.228(2)
Co-N(3)#2	1.9537(10)	N(5)-N(6)	1.333(3)
Co-N(3)#3	1.9537(10)	N(6)-N(6)#1	1.331(4)
Co-N(3)#4	1.9537(10)		
N(5)-C(1)-N(5)#1	114.5(3)	N(3)-Co-N(3)#4	179.47(13)
N(5)-C(1)-N(4)	122.77(17)	N(3)#2-Co-N(3)#4	91.88(8)
N(5)#1-C(1)-N(4)	122.77(17)	N(3)#3-Co-N(3)#4	88.12(8)
N(1)-Co-N(2)	180.0	O(1)-N(1)-O(1)#4	120.4(3)
N(1)-Co-N(3)	89.73(6)	O(1)-N(1)-Co	119.82(17)
N(2)-Co-N(3)	90.27(6)	O(1)#4-N(1)-Co	119.82(17)
N(1)-Co-N(3)#2	89.73(6)	O(2)-N(2)-O(2)#4	119.5(4)
N(2)-Co-N(3)#2	90.27(6)	O(2)-N(2)-Co	120.26(18)
N(3)-Co-N(3)#2	88.12(8)	O(2)#4-N(2)-Co	120.26(18)
N(1)-Co-N(3)#3	89.73(6)	O(4)-N(4)-O(4)#1	125.1(3)
N(2)-Co-N(3)#3	90.27(6)	O(4)-N(4)-C(1)	117.44(16)
N(3)-Co-N(3)#3	91.88(8)	O(4)#1-N(4)-C(1)	117.45(16)
N(3)#2-Co-N(3)#3	179.47(13)	C(1)-N(5)-N(6)	102.9(2)
N(1)-Co-N(3)#4	89.73(6)	N(6)#1-N(6)-N(5)	109.90(12)
N(2)-Co-N(3)#4	90.27(6)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+0,z+0 #2 -x+0,y+0,z+0 #3 x,-y+1,z

#4 -x+0,-y+1,z+0

Table S15. Hydrogen bonds [Å and °] of **7**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3A)...O(1)	0.91	2.33	2.901(2)	120.3
N(3)-H(3A)...O(2)#5	0.91	2.53	3.380(2)	154.9
N(3)-H(3B)...N(6)#6	0.91	2.30	3.156(2)	157.0
N(3)-H(3B)...O(2)#4	0.91	2.41	2.929(3)	116.2
N(3)-H(3C)...O(3)	0.91	2.27	3.0820(17)	148.4
N(3)-H(3C)...O(1)#6	0.91	2.49	3.047(2)	120.0
O(3)-HW1...N(5)	0.794(19)	2.22(2)	2.960(2)	155(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+0,z+0 #2 -x+0,y+0,z+0 #3 x,-y+1,z

#4 -x+0,-y+1,z+0 #5 y-1/2,-x,z-1/4 #6 y+0,-x+1/2,z+1/4

Fig. S11 ORTEP diagram of **9** with thermal displacement parameters drawn at 50% probability.

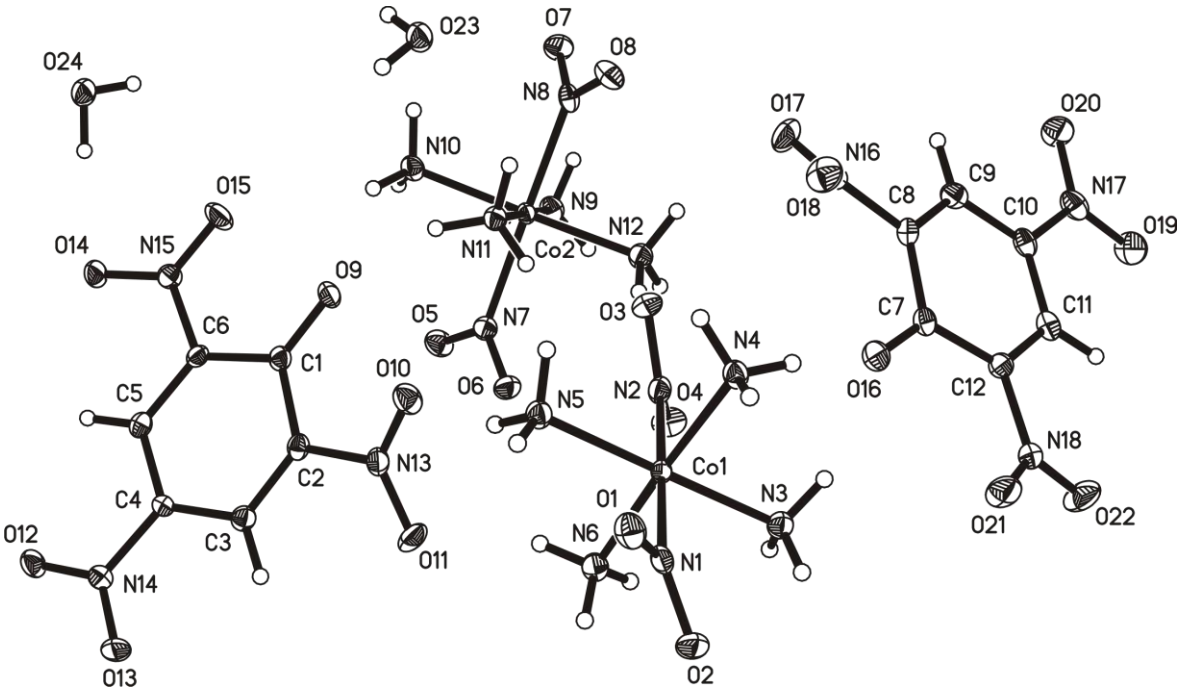

Fig. S12 Packing diagram of **9**. View along the *a* axis.

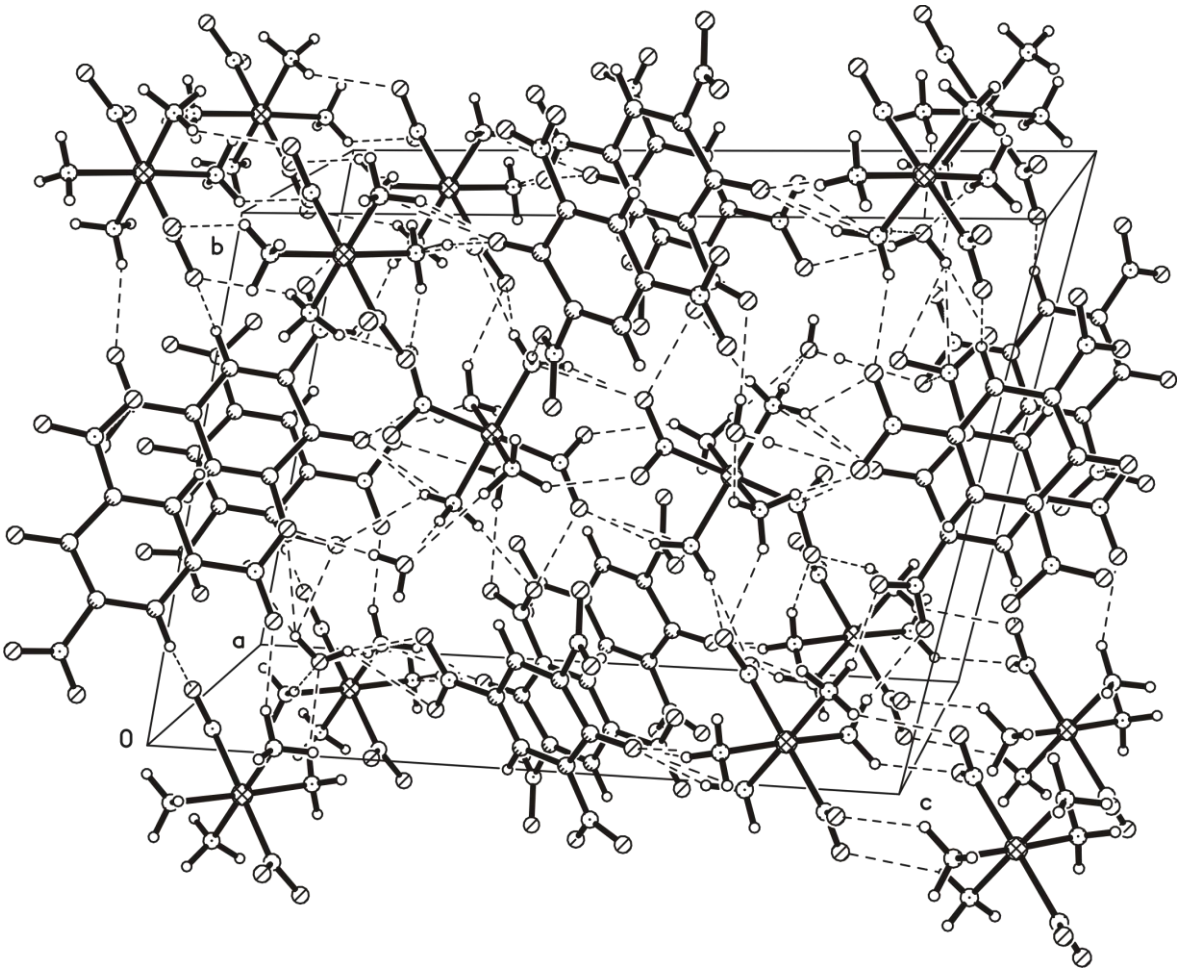

Table S16. Crystal data and structure refinement of **9**.

Identification code	magd08	
Empirical formula	$C_6H_{16}CoN_9O_{12}$	
Formula weight	465.18	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.8481(3) Å	α= 75.421(3)°
	b = 13.4859(5) Å	β= 89.746(3)°
	c = 18.5624(6) Å	γ = 85.199(3)°
Volume	1653.03(11) $Å^3$	
Z	4	
Density (calculated)	1.869 Mg/m^3	
Absorption coefficient	8.991 mm^{-1}	
F(000)	952	
Crystal size	0.08 x 0.05 x 0.03 mm^3	
Theta range for data collection	3.40 to 76.02°	
Index ranges	-8<=h<=8, -16<=k<=16, -23<=l<=23	
Reflections collected	42643	
Independent reflections	6845 [R(int) = 0.0528]	
Completeness to theta = 76.02°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.87767	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6845 / 0 / 521	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0566, wR2 = 0.1527	
R indices (all data)	R1 = 0.0599, wR2 = 0.1553	
Largest diff. peak and hole	1.327 and -0.790 $e.Å^{-3}$	

Table S17. Bond lengths [Å] and angles [°]of **9**.

Co(1)-N(2)	1.931(3)	C(8)-N(16)	1.461(5)
Co(1)-N(1)	1.943(3)	C(9)-C(10)	1.396(5)
Co(1)-N(3)	1.956(3)	C(10)-C(11)	1.381(5)
Co(1)-N(4)	1.962(3)	C(10)-N(17)	1.442(4)
Co(1)-N(6)	1.965(3)	C(11)-C(12)	1.391(5)
Co(1)-N(5)	1.967(3)	C(12)-N(18)	1.443(5)
Co(2)-N(8)	1.936(3)	N(1)-O(2)	1.240(4)
Co(2)-N(7)	1.942(3)	N(1)-O(1)	1.242(4)
Co(2)-N(12)	1.958(3)	N(2)-O(4)	1.235(4)
Co(2)-N(11)	1.959(3)	N(2)-O(3)	1.251(4)
Co(2)-N(10)	1.968(3)	N(7)-O(5)	1.235(4)
Co(2)-N(9)	1.973(3)	N(7)-O(6)	1.254(4)
C(1)-O(9)	1.234(4)	N(8)-O(8)	1.241(4)
C(1)-C(6)	1.456(5)	N(8)-O(7)	1.243(4)
C(1)-C(2)	1.465(5)	N(13)-O(10)	1.230(4)
C(2)-C(3)	1.366(5)	N(13)-O(11)	1.239(4)
C(2)-N(13)	1.450(4)	N(14)-O(13)	1.230(4)
C(3)-C(4)	1.393(5)	N(14)-O(12)	1.240(4)
C(4)-C(5)	1.390(5)	N(15)-O(15)	1.219(4)
C(4)-N(14)	1.443(4)	N(15)-O(14)	1.245(4)
C(5)-C(6)	1.378(5)	N(16)-O(18)	1.231(4)
C(6)-N(15)	1.453(4)	N(16)-O(17)	1.231(4)
C(7)-O(16)	1.241(4)	N(17)-O(19)	1.237(5)
C(7)-C(12)	1.452(5)	N(17)-O(20)	1.239(4)
C(7)-C(8)	1.456(5)	N(18)-O(22)	1.235(4)
C(8)-C(9)	1.367(5)	N(18)-O(21)	1.238(4)
N(2)-Co(1)-N(1)	179.39(13)	N(2)-Co(1)-N(5)	89.52(13)
N(2)-Co(1)-N(3)	89.54(13)	N(1)-Co(1)-N(5)	89.88(13)
N(1)-Co(1)-N(3)	91.06(13)	N(3)-Co(1)-N(5)	179.06(13)
N(2)-Co(1)-N(4)	90.37(13)	N(4)-Co(1)-N(5)	90.71(13)
N(1)-Co(1)-N(4)	89.66(13)	N(6)-Co(1)-N(5)	91.46(13)
N(3)-Co(1)-N(4)	89.27(13)	N(8)-Co(2)-N(7)	179.05(13)
N(2)-Co(1)-N(6)	90.31(13)	N(8)-Co(2)-N(12)	88.60(13)
N(1)-Co(1)-N(6)	89.68(13)	N(7)-Co(2)-N(12)	90.87(13)
N(3)-Co(1)-N(6)	88.57(13)	N(8)-Co(2)-N(11)	90.34(13)
N(4)-Co(1)-N(6)	177.73(13)	N(7)-Co(2)-N(11)	90.42(13)

N(12)-Co(2)-N(11)	88.54(13)	C(10)-C(11)-C(12)	119.2(3)
N(8)-Co(2)-N(10)	89.91(13)	C(11)-C(12)-N(18)	116.1(3)
N(7)-Co(2)-N(10)	90.66(13)	C(11)-C(12)-C(7)	123.5(3)
N(12)-Co(2)-N(10)	177.05(14)	N(18)-C(12)-C(7)	120.3(3)
N(11)-Co(2)-N(10)	88.94(13)	O(2)-N(1)-O(1)	120.1(3)
N(8)-Co(2)-N(9)	90.39(13)	O(2)-N(1)-Co(1)	119.9(2)
N(7)-Co(2)-N(9)	88.86(13)	O(1)-N(1)-Co(1)	120.0(2)
N(12)-Co(2)-N(9)	92.81(13)	O(4)-N(2)-O(3)	120.3(3)
N(11)-Co(2)-N(9)	178.48(13)	O(4)-N(2)-Co(1)	120.5(2)
N(10)-Co(2)-N(9)	89.74(13)	O(3)-N(2)-Co(1)	119.2(2)
O(9)-C(1)-C(6)	124.9(3)	O(5)-N(7)-O(6)	120.0(3)
O(9)-C(1)-C(2)	123.6(3)	O(5)-N(7)-Co(2)	120.8(2)
C(6)-C(1)-C(2)	111.5(3)	O(6)-N(7)-Co(2)	119.3(2)
C(3)-C(2)-N(13)	116.1(3)	O(8)-N(8)-O(7)	120.3(3)
C(3)-C(2)-C(1)	124.6(3)	O(8)-N(8)-Co(2)	119.7(2)
N(13)-C(2)-C(1)	119.2(3)	O(7)-N(8)-Co(2)	120.0(2)
C(2)-C(3)-C(4)	119.0(3)	O(10)-N(13)-O(11)	123.0(3)
C(5)-C(4)-C(3)	121.4(3)	O(10)-N(13)-C(2)	118.9(3)
C(5)-C(4)-N(14)	118.7(3)	O(11)-N(13)-C(2)	118.1(3)
C(3)-C(4)-N(14)	119.8(3)	O(13)-N(14)-O(12)	122.9(3)
C(6)-C(5)-C(4)	118.9(3)	O(13)-N(14)-C(4)	119.3(3)
C(5)-C(6)-N(15)	116.0(3)	O(12)-N(14)-C(4)	117.8(3)
C(5)-C(6)-C(1)	124.4(3)	O(15)-N(15)-O(14)	122.4(3)
N(15)-C(6)-C(1)	119.5(3)	O(15)-N(15)-C(6)	120.0(3)
O(16)-C(7)-C(12)	125.5(3)	O(14)-N(15)-C(6)	117.6(3)
O(16)-C(7)-C(8)	122.6(3)	O(18)-N(16)-O(17)	123.6(3)
C(12)-C(7)-C(8)	111.9(3)	O(18)-N(16)-C(8)	117.8(3)
C(9)-C(8)-C(7)	125.4(3)	O(17)-N(16)-C(8)	118.6(3)
C(9)-C(8)-N(16)	117.2(3)	O(19)-N(17)-O(20)	122.6(3)
C(7)-C(8)-N(16)	117.4(3)	O(19)-N(17)-C(10)	118.8(3)
C(8)-C(9)-C(10)	117.9(3)	O(20)-N(17)-C(10)	118.6(3)
C(11)-C(10)-C(9)	122.0(3)	O(22)-N(18)-O(21)	121.9(3)
C(11)-C(10)-N(17)	118.6(3)	O(22)-N(18)-C(12)	118.7(3)
C(9)-C(10)-N(17)	119.4(3)	O(21)-N(18)-C(12)	119.4(3)

Table S18. Hydrogen bonds [Å and °] of **9**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3A)...O(13)#1	0.91	2.28	3.050(4)	141.9
N(3)-H(3B)...O(16)	0.91	1.94	2.808(4)	159.0
N(3)-H(3C)...O(24)#2	0.91	2.26	3.149(4)	166.7
N(4)-H(4A)...O(24)#3	0.91	2.26	3.043(4)	144.5
N(4)-H(4B)...O(6)#4	0.91	2.21	3.067(4)	156.9
N(4)-H(4C)...O(16)	0.91	2.02	2.882(4)	156.6
N(5)-H(5A)...O(2)#5	0.91	2.39	3.132(4)	138.6
N(5)-H(5B)...O(10)	0.91	2.17	3.048(4)	160.7
N(5)-H(5C)...O(6)#4	0.91	2.23	3.084(4)	155.5
N(6)-H(6A)...O(1)#5	0.91	2.33	3.020(4)	132.7
N(6)-H(6C)...O(11)	0.91	2.22	3.083(4)	157.8
N(10)-H(10B)...O(9)	0.91	2.10	2.908(4)	147.4
N(10)-H(10C)...O(23)#6	0.91	2.16	3.065(4)	179.0
N(11)-H(11B)...O(3)	0.91	2.28	3.078(4)	146.8
N(11)-H(11C)...O(9)	0.91	2.01	2.829(4)	148.7
N(12)-H(12B)...O(18)#6	0.91	2.09	2.993(4)	173.2
N(12)-H(12C)...O(4)	0.91	2.33	3.181(4)	155.4
O(23)-H(23A)...O(12)#7	0.80(7)	2.11(7)	2.886(4)	161(6)
O(23)-H(23B)...O(21)#8	0.75(7)	2.22(7)	2.957(4)	171(7)
O(24)-H(24A)...O(14)	0.93(7)	2.03(7)	2.947(4)	168(6)
O(24)-H(24B)...O(20)#9	0.79(7)	2.26(7)	3.035(4)	166(7)

Symmetry transformations used to generate equivalent atoms:

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

#5 -x+2,-y+2,-z #6 x-1,y,z #7 -x+1,-y+1,-z

#8 x,y-1,z #9 -x+1,-y+1,-z+1

Fig. S13 ORTEP diagram of **10** with thermal displacement parameters drawn at 50% probability.

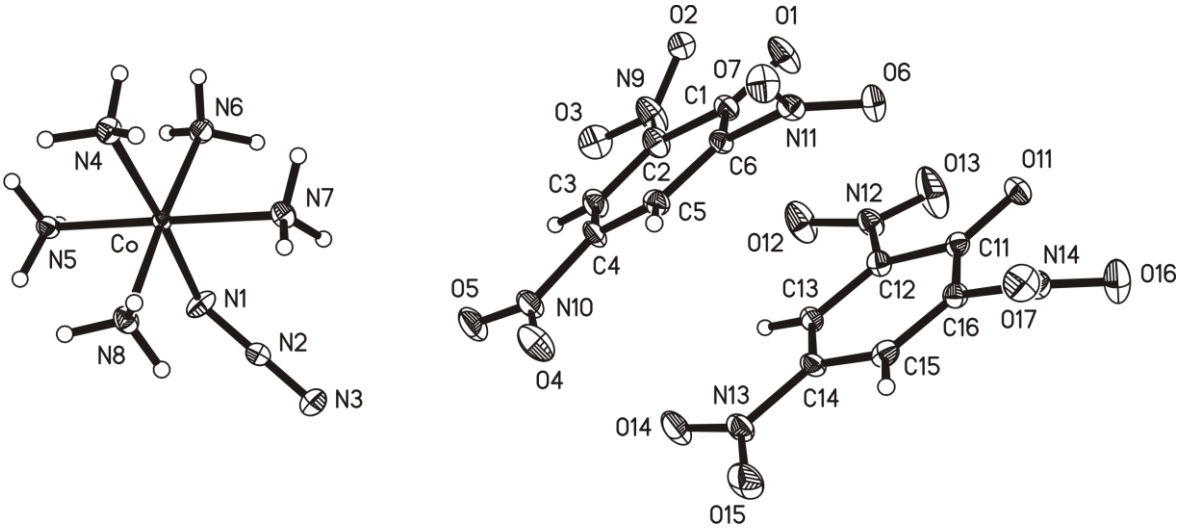

Fig. S14 Packing diagram of **10**. View along the *b* axis.

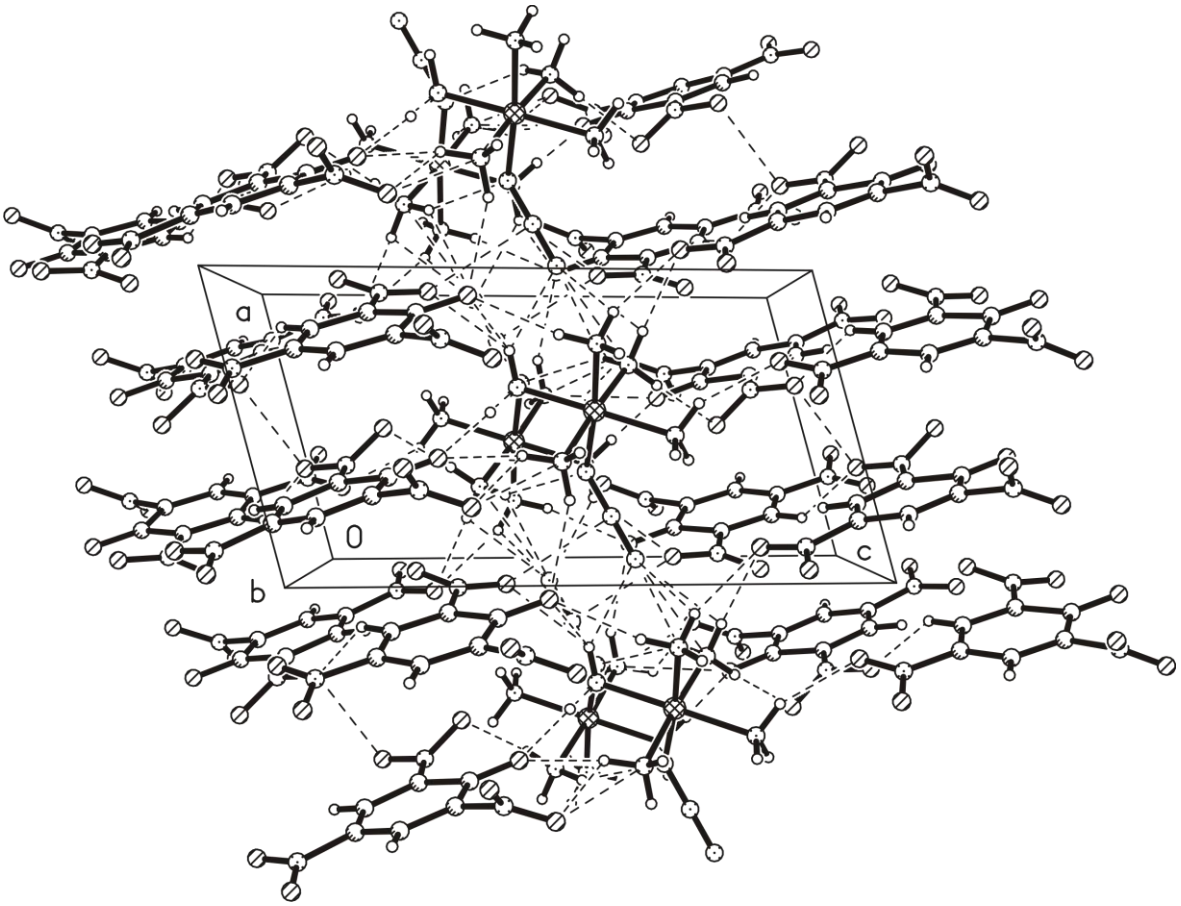

Table S19. Crystal data and structure refinement of **10**.

Identification code	ip152	
Empirical formula	$C_{12}H_{19}CoN_{14}O_{14}$	
Formula weight	642.30	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.0622(14) Å	α= 98.33(3)°
	b = 12.888(3) Å	β= 104.80(3)°
	c = 13.299(3) Å	γ = 90.52(3)°
Volume	1156.6(4) $Å^3$	
Z	2	
Density (calculated)	1.844 Mg/m^3	
Absorption coefficient	0.845 mm^{-1}	
F(000)	656	
Crystal size	0.29 x 0.13 x 0.09 mm^3	
Theta range for data collection	2.08 to 29.23°	
Index ranges	-9<=h<=9, -16<=k<=17, -18<=l<=18	
Reflections collected	14708	
Independent reflections	6204 [R(int) = 0.0511]	
Completeness to theta = 29.00°	99.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6204 / 33 / 374	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0512, wR2 = 0.0924	
R indices (all data)	R1 = 0.0797, wR2 = 0.0998	
Largest diff. peak and hole	0.751 and -0.575 $e.Å^{-3}$	

Table S20. Bond lengths [Å] and angles [°]of **10**.

Co-N(5)	1.945(2)	N(14)-O(17)	1.233(3)
Co-N(1)	1.950(3)	N(14)-C(16)	1.453(3)
Co-N(8)	1.961(2)	O(1)-C(1)	1.240(3)
Co-N(4)	1.967(2)	N(9)-O(2')	1.211(6)
Co-N(6)	1.975(2)	N(9)-O(3)	1.223(5)
Co-N(7)	1.980(2)	N(9)-O(2)	1.257(6)
N(1)-N(2)	1.212(3)	N(9)-O(3')	1.268(6)
N(2)-N(3)	1.148(3)	N(9)-C(2)	1.454(4)
N(10)-O(4)	1.229(3)	O(11)-C(11)	1.242(3)
N(10)-O(5)	1.241(3)	C(1)-C(6)	1.445(4)
N(10)-C(4)	1.448(3)	C(1)-C(2)	1.456(4)
N(11)-O(6)	1.225(3)	C(2)-C(3)	1.377(4)
N(11)-O(7)	1.230(3)	C(3)-C(4)	1.383(4)
N(11)-C(6)	1.461(3)	C(4)-C(5)	1.385(4)
N(12)-O(13)	1.207(3)	C(5)-C(6)	1.365(3)
N(12)-O(12)	1.230(3)	C(11)-C(16)	1.457(3)
N(12)-C(12)	1.458(3)	C(11)-C(12)	1.457(3)
N(13)-O(15)	1.235(3)	C(12)-C(13)	1.377(3)
N(13)-O(14)	1.236(3)	C(13)-C(14)	1.385(4)
N(13)-C(14)	1.439(3)	C(14)-C(15)	1.391(4)
N(14)-O(16)	1.227(3)	C(15)-C(16)	1.365(3)
N(5)-Co-N(1)	85.43(10)	N(2)-N(1)-Co	116.68(18)
N(5)-Co-N(8)	91.32(9)	N(3)-N(2)-N(1)	178.8(3)
N(1)-Co-N(8)	90.89(10)	O(4)-N(10)-O(5)	123.1(2)
N(5)-Co-N(4)	89.65(10)	O(4)-N(10)-C(4)	118.9(2)
N(1)-Co-N(4)	175.08(9)	O(5)-N(10)-C(4)	118.0(2)
N(8)-Co-N(4)	89.33(10)	O(6)-N(11)-O(7)	123.4(2)
N(5)-Co-N(6)	90.66(9)	O(6)-N(11)-C(6)	119.2(2)
N(1)-Co-N(6)	86.76(10)	O(7)-N(11)-C(6)	117.4(2)
N(8)-Co-N(6)	176.79(11)	O(13)-N(12)-O(12)	122.5(2)
N(4)-Co-N(6)	93.20(10)	O(13)-N(12)-C(12)	119.3(2)
N(5)-Co-N(7)	178.09(11)	O(12)-N(12)-C(12)	118.2(2)
N(1)-Co-N(7)	92.93(10)	O(15)-N(13)-O(14)	122.7(2)
N(8)-Co-N(7)	89.67(9)	O(15)-N(13)-C(14)	118.7(2)
N(4)-Co-N(7)	91.99(10)	O(14)-N(13)-C(14)	118.5(2)
N(6)-Co-N(7)	88.27(9)	O(16)-N(14)-O(17)	123.2(2)

O(16)-N(14)-C(16)	119.0(2)	C(3)-C(4)-N(10)	119.8(2)
O(17)-N(14)-C(16)	117.8(2)	C(5)-C(4)-N(10)	117.7(2)
O(2')-N(9)-O(3)	120.0(4)	C(6)-C(5)-C(4)	117.5(2)
O(2')-N(9)-O(2)	15.0(4)	C(5)-C(6)-C(1)	125.9(2)
O(3)-N(9)-O(2)	116.7(4)	C(5)-C(6)-N(11)	116.3(2)
O(2')-N(9)-O(3')	118.5(5)	C(1)-C(6)-N(11)	117.8(2)
O(3)-N(9)-O(3')	30.4(3)	O(11)-C(11)-C(16)	123.7(2)
O(2)-N(9)-O(3')	124.3(4)	O(11)-C(11)-C(12)	125.2(2)
O(2')-N(9)-C(2)	120.9(4)	C(16)-C(11)-C(12)	111.0(2)
O(3)-N(9)-C(2)	118.1(3)	C(13)-C(12)-C(11)	124.2(2)
O(2)-N(9)-C(2)	119.0(3)	C(13)-C(12)-N(12)	115.8(2)
O(3')-N(9)-C(2)	116.5(3)	C(11)-C(12)-N(12)	120.0(2)
O(1)-C(1)-C(6)	123.0(2)	C(12)-C(13)-C(14)	119.1(2)
O(1)-C(1)-C(2)	125.6(2)	C(13)-C(14)-C(15)	121.8(2)
C(6)-C(1)-C(2)	111.4(2)	C(13)-C(14)-N(13)	118.9(2)
C(3)-C(2)-N(9)	116.9(2)	C(15)-C(14)-N(13)	119.3(2)
C(3)-C(2)-C(1)	123.9(2)	C(16)-C(15)-C(14)	118.1(2)
N(9)-C(2)-C(1)	119.2(2)	C(15)-C(16)-N(14)	116.7(2)
C(2)-C(3)-C(4)	118.7(2)	C(15)-C(16)-C(11)	125.7(2)
C(3)-C(4)-C(5)	122.4(2)	N(14)-C(16)-C(11)	117.6(2)

Table S21. Hydrogen bonds [Å and °] of **10**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(4)-H(4A)...O(5)#1	0.91	2.33	3.205(3)	162.3
N(4)-H(4A)...N(3)#1	0.91	2.52	3.053(3)	118.0
N(4)-H(4B)...O(7)#2	0.91	2.23	3.103(3)	160.0
N(4)-H(4B)...O(6)#2	0.91	2.64	3.446(3)	147.6
N(4)-H(4C)...O(11)#3	0.91	2.24	3.099(3)	156.8
N(4)-H(4C)...O(16)#3	0.91	2.58	3.283(3)	134.1
N(5)-H(5A)...N(1)#4	0.91	2.10	3.009(3)	173.0
N(5)-H(5A)...N(2)#4	0.91	2.66	3.490(3)	151.6
N(5)-H(5B)...O(11)#3	0.91	2.21	3.002(3)	145.9
N(5)-H(5B)...N(3)#1	0.91	2.37	3.001(3)	126.1
N(5)-H(5B)...O(13)#3	0.91	2.53	3.120(3)	122.8
N(5)-H(5C)...O(1)#5	0.91	1.95	2.835(3)	164.7
N(6)-H(6A)...N(1)#4	0.91	2.50	3.340(3)	153.9
N(6)-H(6B)...O(2)#6	0.91	2.52	3.391(7)	159.7
N(6)-H(6C)...O(5)#1	0.91	2.29	3.192(4)	174.0
N(7)-H(7A)...N(2)	0.91	2.40	2.853(3)	110.9
N(7)-H(7A)...O(5)	0.91	2.59	3.269(3)	131.8
N(7)-H(7B)...O(17)#7	0.91	2.20	3.088(3)	164.4
N(7)-H(7B)...O(7)#2	0.91	2.49	2.964(3)	113.0
N(7)-H(7C)...O(14)#1	0.91	2.22	3.014(3)	146.0
N(8)-H(8A)...O(1)#5	0.91	1.97	2.844(3)	159.1
N(8)-H(8A)...O(6)#5	0.91	2.45	2.950(3)	114.6
N(8)-H(8B)...O(16)#7	0.91	2.49	3.276(3)	144.9
N(8)-H(8C)...O(11)#5	0.91	2.27	3.100(3)	150.9
N(8)-H(8C)...N(2)	0.91	2.52	3.032(3)	116.1

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+3,-y+1,-z+1 #5 x,y,z-1 #6 -x+3,-y+1,-z+2

#7 -x+2,-y+2,-z+2

Fig. S15 ORTEP diagram of **12** with thermal displacement parameters drawn at 50% probability.

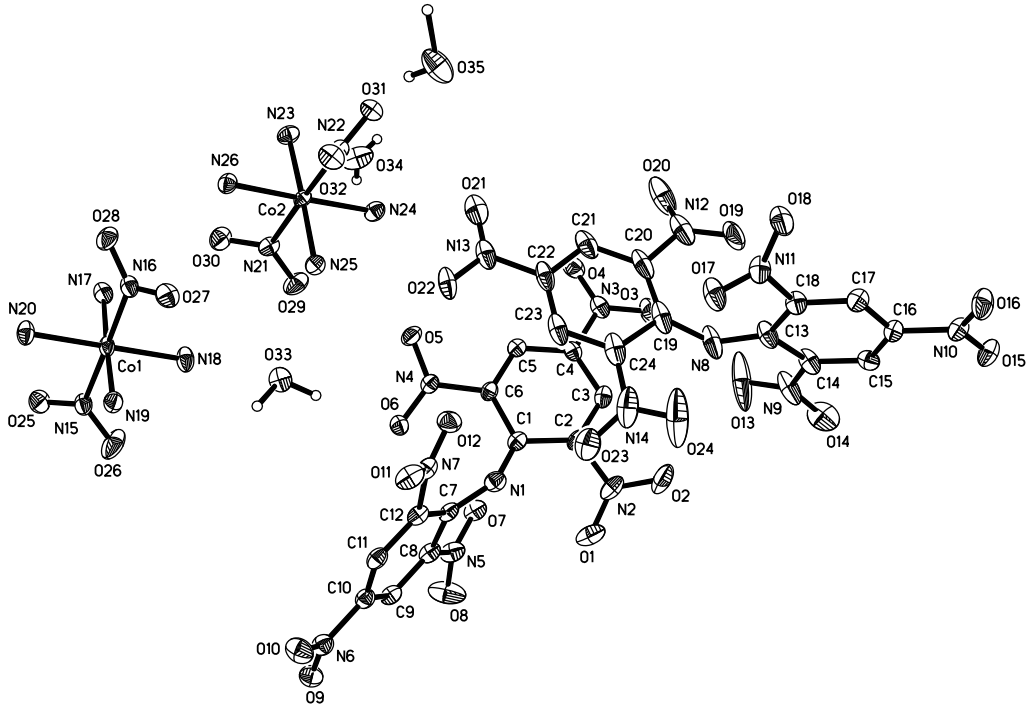

Fig. S16 Packing diagram of **12**. View along the *a* axis.

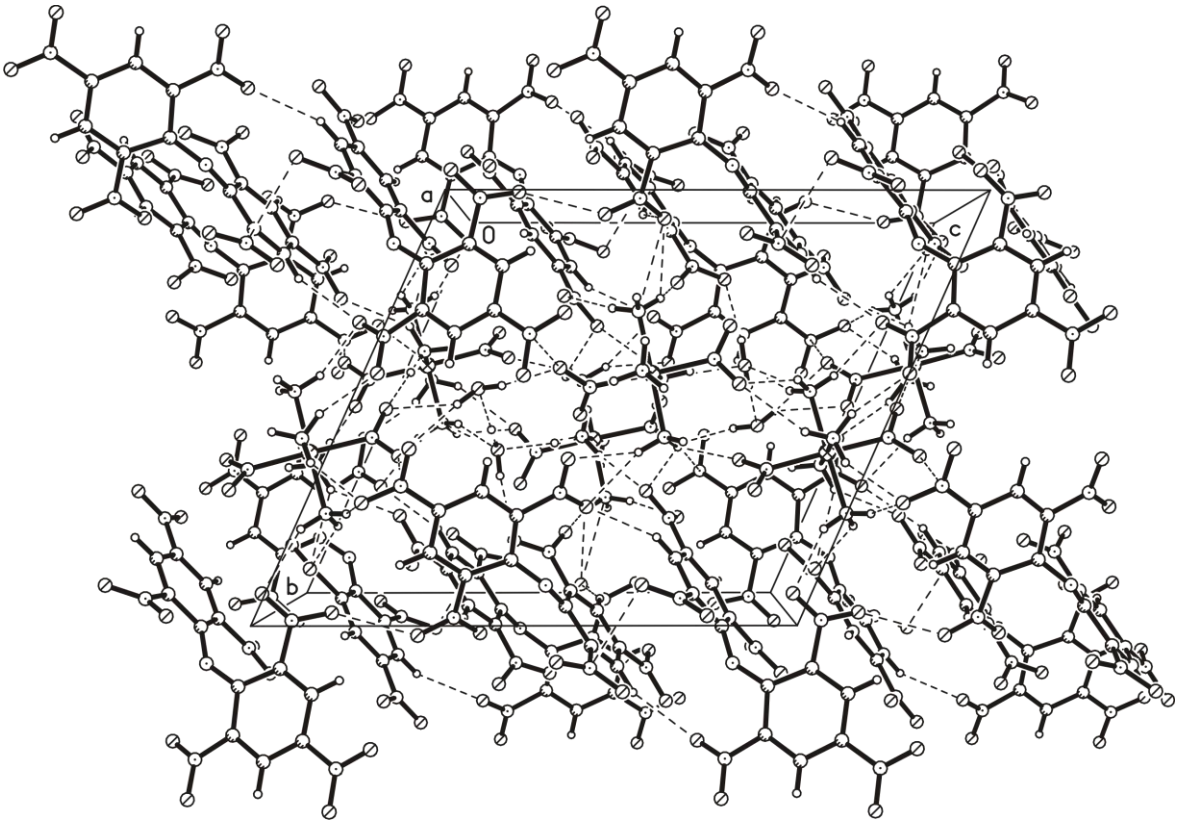

Table S22. Crystal data and structure refinement of **12**.

Identification code	magd20	
Empirical formula	C_{24} H_{38} Co_2 N_{26} O_{35}	
Formula weight	1368.59	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.6374(3) Å	α= 113.942(2)°
	b = 13.7368(3) Å	β= 90.678(2)°
	c = 15.6996(4) Å	γ = 89.527(2)°
Volume	2490.71(10) $Å^3$	
Z	2	
Density (calculated)	1.825 Mg/m^3	
Absorption coefficient	6.434 mm^{-1}	
F(000)	1396	
Crystal size	0.12 x 0.10 x 0.03 mm^3	
Theta range for data collection	3.50 to 75.88°	
Index ranges	-13<=h<=15, -17<=k<=17, -18<=l<=19	
Reflections collected	32362	
Independent reflections	10298 [R(int) = 0.0329]	
Completeness to theta = 72.50°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8304 and 0.5123	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10298 / 6 / 819	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0378, wR2 = 0.0942	
R indices (all data)	R1 = 0.0405, wR2 = 0.0964	
Largest diff. peak and hole	0.778 and -0.779 $e.Å^{-3}$	

Table S23. Bond lengths [Å] and angles [°]of **12**.

Co(1)-N(16)	1.9300(18)	C(15)-C(16)	1.382(3)
Co(1)-N(15)	1.9352(18)	C(16)-C(17)	1.386(3)
Co(1)-N(19)	1.953(2)	C(16)-N(10)	1.440(3)
Co(1)-N(20)	1.9543(18)	C(17)-C(18)	1.370(3)
Co(1)-N(17)	1.961(2)	C(18)-N(11)	1.459(3)
Co(1)-N(18)	1.9618(18)	C(19)-N(8)	1.314(3)
Co(2)-N(22)	1.9327(17)	C(19)-C(20)	1.435(4)
Co(2)-N(24)	1.9418(18)	C(19)-C(24)	1.444(3)
Co(2)-N(21)	1.9424(18)	C(20)-C(21)	1.382(4)
Co(2)-N(26)	1.9535(18)	C(20)-N(12)	1.450(3)
Co(2)-N(23)	1.9548(18)	C(21)-C(22)	1.386(3)
Co(2)-N(25)	1.9573(17)	C(22)-C(23)	1.384(4)
C(1)-N(1)	1.292(3)	C(22)-N(13)	1.453(3)
C(1)-C(2)	1.445(3)	C(23)-C(24)	1.374(3)
C(1)-C(6)	1.453(3)	C(24)-N(14)	1.463(4)
C(2)-C(3)	1.368(3)	O(1)-N(2)	1.232(3)
C(2)-N(2)	1.459(3)	O(2)-N(2)	1.223(3)
C(3)-C(4)	1.392(3)	O(3)-N(3)	1.241(3)
C(4)-C(5)	1.388(3)	O(4)-N(3)	1.233(3)
C(4)-N(3)	1.444(3)	O(5)-N(4)	1.233(2)
C(5)-C(6)	1.378(3)	O(6)-N(4)	1.235(2)
C(6)-N(4)	1.451(2)	O(7)-N(5)	1.235(3)
C(7)-N(1)	1.312(3)	O(8)-N(5)	1.222(3)
C(7)-C(8)	1.433(3)	O(9)-N(6)	1.239(3)
C(7)-C(12)	1.437(3)	O(10)-N(6)	1.226(3)
C(8)-C(9)	1.375(3)	O(11)-N(7)	1.231(2)
C(8)-N(5)	1.454(3)	O(12)-N(7)	1.231(2)
C(9)-C(10)	1.386(3)	O(13)-N(9)	1.202(3)
C(10)-C(11)	1.381(3)	O(14)-N(9)	1.232(3)
C(10)-N(6)	1.442(3)	O(15)-N(10)	1.234(3)
C(11)-C(12)	1.376(3)	O(16)-N(10)	1.232(3)
C(12)-N(7)	1.454(3)	O(17)-N(11)	1.198(4)
C(13)-N(8)	1.295(3)	O(18)-N(11)	1.217(4)
C(13)-C(18)	1.442(3)	O(17')-N(11)	1.304(4)
C(13)-C(14)	1.447(3)	O(18')-N(11)	1.217(5)
C(14)-C(15)	1.371(3)	O(19)-N(12)	1.223(3)
C(14)-N(9)	1.453(3)	O(20)-N(12)	1.239(4)

O(21)-N(13)	1.228(3)	O(27)-N(16)	1.248(2)
O(22)-N(13)	1.236(3)	O(28)-N(16)	1.235(3)
O(23)-N(14)	1.226(3)	O(29)-N(21)	1.237(2)
O(24)-N(14)	1.224(3)	O(30)-N(21)	1.241(2)
O(25)-N(15)	1.232(2)	O(31)-N(22)	1.246(2)
O(26)-N(15)	1.229(3)	O(32)-N(22)	1.240(2)

N(16)-Co(1)-N(15)	178.50(8)	C(2)-C(1)-C(6)	112.42(18)
N(16)-Co(1)-N(19)	89.54(8)	C(3)-C(2)-C(1)	124.64(19)
N(15)-Co(1)-N(19)	89.96(8)	C(3)-C(2)-N(2)	115.58(19)
N(16)-Co(1)-N(20)	90.25(8)	C(1)-C(2)-N(2)	119.78(19)
N(15)-Co(1)-N(20)	88.35(8)	C(2)-C(3)-C(4)	118.87(19)
N(19)-Co(1)-N(20)	91.11(8)	C(5)-C(4)-C(3)	121.13(19)
N(16)-Co(1)-N(17)	89.62(8)	C(5)-C(4)-N(3)	119.25(19)
N(15)-Co(1)-N(17)	90.91(8)	C(3)-C(4)-N(3)	119.61(18)
N(19)-Co(1)-N(17)	178.25(8)	C(6)-C(5)-C(4)	119.46(19)
N(20)-Co(1)-N(17)	90.43(8)	C(5)-C(6)-N(4)	115.66(17)
N(16)-Co(1)-N(18)	90.96(8)	C(5)-C(6)-C(1)	123.41(18)
N(15)-Co(1)-N(18)	90.46(8)	N(4)-C(6)-C(1)	120.80(17)
N(19)-Co(1)-N(18)	90.54(9)	N(1)-C(7)-C(8)	124.02(19)
N(20)-Co(1)-N(18)	177.96(8)	N(1)-C(7)-C(12)	121.7(2)
N(17)-Co(1)-N(18)	87.94(9)	C(8)-C(7)-C(12)	113.24(19)
N(22)-Co(2)-N(24)	89.35(8)	C(9)-C(8)-C(7)	123.57(19)
N(22)-Co(2)-N(21)	178.71(8)	C(9)-C(8)-N(5)	115.92(19)
N(24)-Co(2)-N(21)	89.53(8)	C(7)-C(8)-N(5)	120.47(19)
N(22)-Co(2)-N(26)	90.11(7)	C(8)-C(9)-C(10)	118.7(2)
N(24)-Co(2)-N(26)	178.88(8)	C(11)-C(10)-C(9)	121.9(2)
N(21)-Co(2)-N(26)	91.02(8)	C(11)-C(10)-N(6)	119.66(19)
N(22)-Co(2)-N(23)	91.32(8)	C(9)-C(10)-N(6)	118.44(19)
N(24)-Co(2)-N(23)	91.41(8)	C(12)-C(11)-C(10)	118.45(19)
N(21)-Co(2)-N(23)	89.35(8)	C(11)-C(12)-C(7)	123.78(19)
N(26)-Co(2)-N(23)	87.62(8)	C(11)-C(12)-N(7)	116.99(18)
N(22)-Co(2)-N(25)	89.27(7)	C(7)-C(12)-N(7)	119.18(19)
N(24)-Co(2)-N(25)	90.07(8)	N(8)-C(13)-C(18)	126.6(2)
N(21)-Co(2)-N(25)	90.09(7)	N(8)-C(13)-C(14)	121.0(2)
N(26)-Co(2)-N(25)	90.90(8)	C(18)-C(13)-C(14)	112.2(2)
N(23)-Co(2)-N(25)	178.41(8)	C(15)-C(14)-C(13)	124.1(2)
N(1)-C(1)-C(2)	120.55(19)	C(15)-C(14)-N(9)	115.9(2)
N(1)-C(1)-C(6)	126.54(19)	C(13)-C(14)-N(9)	119.9(2)

C(14)-C(15)-C(16)	119.21(19)	O(11)-N(7)-C(12)	118.49(18)
C(15)-C(16)-C(17)	121.1(2)	O(12)-N(7)-C(12)	118.76(17)
C(15)-C(16)-N(10)	119.68(19)	C(13)-N(8)-C(19)	140.8(2)
C(17)-C(16)-N(10)	119.24(19)	O(13)-N(9)-O(14)	122.6(2)
C(18)-C(17)-C(16)	119.2(2)	O(13)-N(9)-C(14)	120.3(2)
C(17)-C(18)-C(13)	124.2(2)	O(14)-N(9)-C(14)	117.1(2)
C(17)-C(18)-N(11)	115.55(19)	O(16)-N(10)-O(15)	122.29(19)
C(13)-C(18)-N(11)	120.27(19)	O(16)-N(10)-C(16)	118.96(18)
N(8)-C(19)-C(20)	126.2(2)	O(15)-N(10)-C(16)	118.75(19)
N(8)-C(19)-C(24)	120.1(3)	O(17)-N(11)-O(18')	84.5(3)
C(20)-C(19)-C(24)	112.7(2)	O(17)-N(11)-O(18)	127.2(3)
C(21)-C(20)-C(19)	124.0(2)	O(18')-N(11)-O(18)	63.2(3)
C(21)-C(20)-N(12)	115.9(3)	O(17)-N(11)-O(17')	68.4(3)
C(19)-C(20)-N(12)	120.1(2)	O(18')-N(11)-O(17')	117.9(3)
C(20)-C(21)-C(22)	118.8(3)	O(18)-N(11)-O(17')	90.3(3)
C(23)-C(22)-C(21)	121.4(2)	O(17)-N(11)-C(18)	117.4(2)
C(23)-C(22)-N(13)	120.1(2)	O(18')-N(11)-C(18)	121.9(3)
C(21)-C(22)-N(13)	118.5(3)	O(18)-N(11)-C(18)	115.0(2)
C(24)-C(23)-C(22)	119.0(2)	O(17')-N(11)-C(18)	120.2(2)
C(23)-C(24)-C(19)	124.1(3)	O(19)-N(12)-O(20)	122.0(2)
C(23)-C(24)-N(14)	117.2(2)	O(19)-N(12)-C(20)	120.0(3)
C(19)-C(24)-N(14)	118.7(2)	O(20)-N(12)-C(20)	118.0(2)
C(1)-N(1)-C(7)	144.46(19)	O(21)-N(13)-O(22)	123.5(2)
O(2)-N(2)-O(1)	123.5(2)	O(21)-N(13)-C(22)	118.3(2)
O(2)-N(2)-C(2)	117.1(2)	O(22)-N(13)-C(22)	118.2(2)
O(1)-N(2)-C(2)	119.4(2)	O(24)-N(14)-O(23)	123.3(3)
O(4)-N(3)-O(3)	123.14(19)	O(24)-N(14)-C(24)	119.8(3)
O(4)-N(3)-C(4)	118.97(18)	O(23)-N(14)-C(24)	117.0(2)
O(3)-N(3)-C(4)	117.88(19)	O(26)-N(15)-O(25)	118.55(19)
O(5)-N(4)-O(6)	122.50(17)	O(26)-N(15)-Co(1)	119.59(16)
O(5)-N(4)-C(6)	118.18(17)	O(25)-N(15)-Co(1)	121.86(15)
O(6)-N(4)-C(6)	119.31(17)	O(28)-N(16)-O(27)	120.23(18)
O(8)-N(5)-O(7)	123.00(19)	O(28)-N(16)-Co(1)	120.11(14)
O(8)-N(5)-C(8)	118.66(19)	O(27)-N(16)-Co(1)	119.65(14)
O(7)-N(5)-C(8)	118.34(18)	O(29)-N(21)-O(30)	119.49(18)
O(10)-N(6)-O(9)	123.81(19)	O(29)-N(21)-Co(2)	120.41(15)
O(10)-N(6)-C(10)	118.11(19)	O(30)-N(21)-Co(2)	120.10(14)
O(9)-N(6)-C(10)	118.08(18)	O(32)-N(22)-O(31)	119.71(17)
O(11)-N(7)-O(12)	122.72(18)	O(32)-N(22)-Co(2)	120.01(14)

O(31)-N(22)-Co(2) 120.27(13)

Table S24. Hydrogen bonds [Å and °] of **12**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(17)-H(17A)...O(14)#1	0.91	2.09	2.965(3)	160.5
N(17)-H(17C)...O(9)#2	0.91	2.18	3.017(2)	153.1
N(18)-H(18B)...O(33)	0.91	2.05	2.911(3)	157.6
N(19)-H(19A)...O(26)#2	0.91	2.01	2.892(3)	161.3
N(23)-H(23B)...O(34)	0.91	2.08	2.981(3)	171.0
N(25)-H(25A)...O(33)	0.91	2.06	2.924(3)	159.2

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

Fig. S17 ORTEP diagram of **13** with thermal displacement parameters drawn at 50% probability.

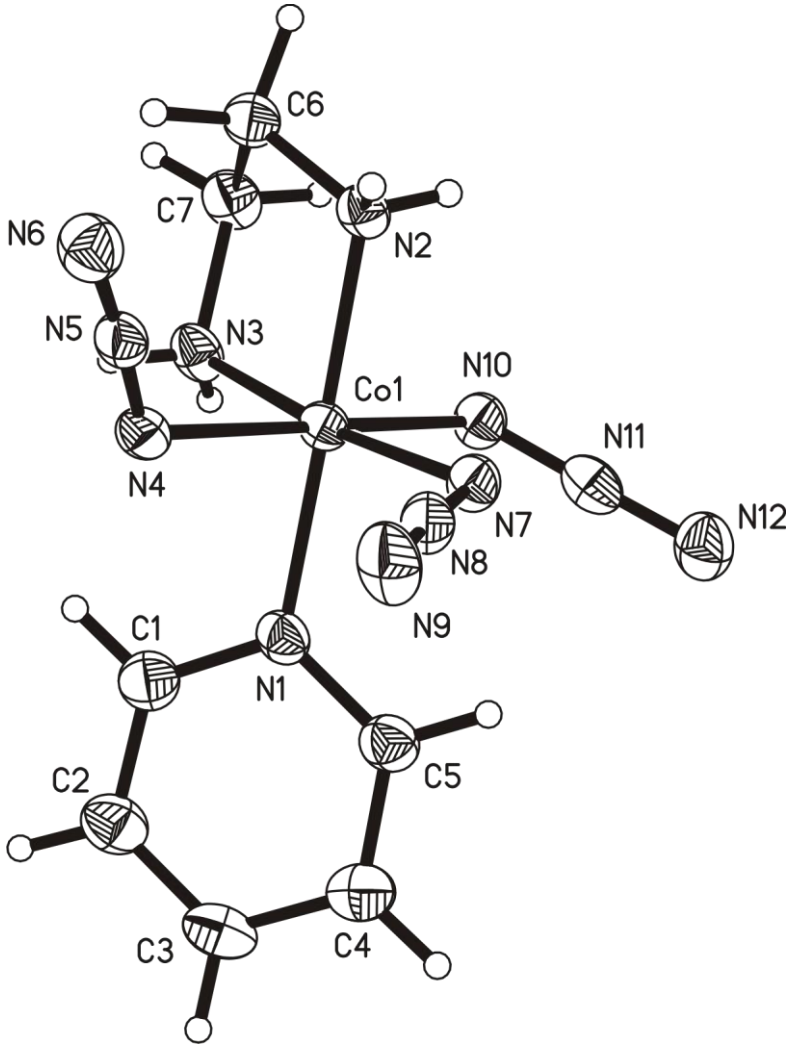

Fig. S18 Packing diagram of **13**. View along the *a* axis.

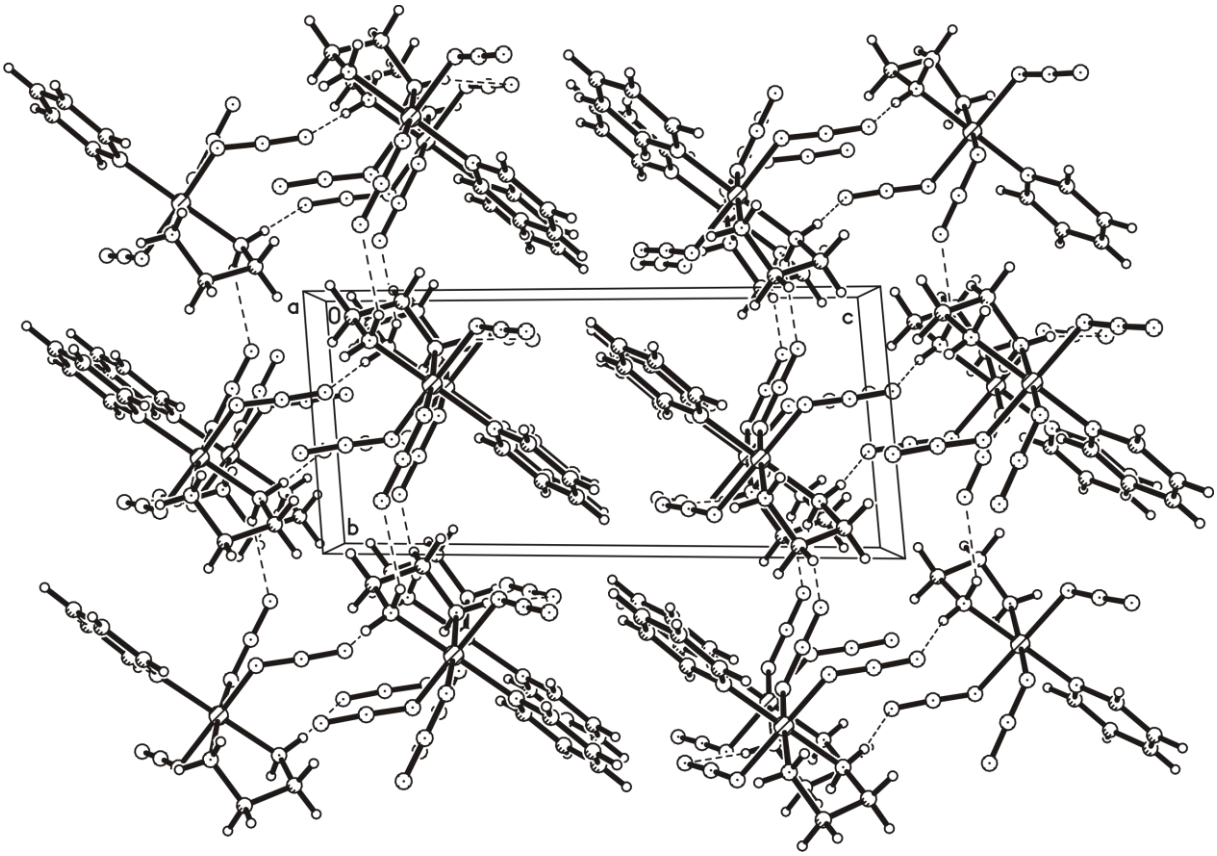

Table S25. Crystal data and structure refinement of **13**.

Identification code	fred01	
Empirical formula	$C_7 H_{13} Co N_{12}$	
Formula weight	324.19	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.2607(12) Å	α= 84.600(14)°
	b = 6.8540(12) Å	β= 79.945(15)°
	c = 15.006(2) Å	γ = 85.933(15)°
Volume	630.22(19) $Å^3$	
Z	2	
Density (calculated)	1.709 Mg/m^3	
Absorption coefficient	10.826 mm^{-1}	
F(000)	332	
Crystal size	0.20 x 0.03 x 0.01 mm^3	
Theta range for data collection	6.01 to 75.86°	
Index ranges	-7<=h<=7, -8<=k<=8, -18<=l<=17	
Reflections collected	10826	
Independent reflections	2563 [R(int) = 0.0649]	
Completeness to theta = 72.50°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.21909	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2563 / 6 / 197	
Goodness-of-fit on F^2	0.955	
Final R indices [I>2sigma(I)]	R1 = 0.0386, wR2 = 0.0834	
R indices (all data)	R1 = 0.0519, wR2 = 0.0880	
Largest diff. peak and hole	0.442 and -0.363 $e.Å^{-3}$	

Table S26. Bond lengths [Å] and angles [°]of **13**.

Co(1)-N(4)	1.946(2)	N(8)-N(9)	1.160(3)
Co(1)-N(2)	1.948(2)	N(10)-N(11)	1.195(3)
Co(1)-N(7)	1.962(2)	N(11)-N(12)	1.176(4)
Co(1)-N(10)	1.969(2)	C(1)-C(2)	1.381(4)
Co(1)-N(3)	1.973(2)	C(1)-H(1)	0.9500
Co(1)-N(1)	1.975(2)	C(2)-C(3)	1.377(5)
N(1)-C(1)	1.335(4)	C(2)-H(2)	0.9500
N(1)-C(5)	1.352(4)	C(3)-C(4)	1.392(4)
N(2)-C(6)	1.479(3)	C(3)-H(3)	0.9500
N(2)-H(01)	0.839(19)	C(4)-C(5)	1.393(4)
N(2)-H(02)	0.847(19)	C(4)-H(4)	0.9500
N(3)-C(7)	1.487(4)	C(5)-H(5)	0.9500
N(3)-H(03)	0.841(19)	C(6)-C(7)	1.509(4)
N(3)-H(04)	0.839(19)	C(6)-H(6A)	0.9900
N(4)-N(5)	1.200(3)	C(6)-H(6B)	0.9900
N(5)-N(6)	1.163(3)	C(7)-H(7A)	0.9900
N(7)-N(8)	1.204(3)	C(7)-H(7B)	0.9900
N(4)-Co(1)-N(2)	93.11(10)	C(6)-N(2)-H(01)	112.8(19)
N(4)-Co(1)-N(7)	94.14(10)	Co(1)-N(2)-H(01)	113(2)
N(2)-Co(1)-N(7)	89.00(10)	C(6)-N(2)-H(02)	107(2)
N(4)-Co(1)-N(10)	174.59(10)	Co(1)-N(2)-H(02)	107(2)
N(2)-Co(1)-N(10)	88.72(10)	H(01)-N(2)-H(02)	106(3)
N(7)-Co(1)-N(10)	90.98(10)	C(7)-N(3)-Co(1)	108.60(18)
N(4)-Co(1)-N(3)	88.59(10)	C(7)-N(3)-H(03)	109(2)
N(2)-Co(1)-N(3)	85.10(11)	Co(1)-N(3)-H(03)	112(2)
N(7)-Co(1)-N(3)	173.63(11)	C(7)-N(3)-H(04)	110(2)
N(10)-Co(1)-N(3)	86.49(10)	Co(1)-N(3)-H(04)	106(2)
N(4)-Co(1)-N(1)	86.30(10)	H(03)-N(3)-H(04)	111(3)
N(2)-Co(1)-N(1)	179.39(10)	N(5)-N(4)-Co(1)	121.75(19)
N(7)-Co(1)-N(1)	91.17(10)	N(6)-N(5)-N(4)	176.3(3)
N(10)-Co(1)-N(1)	91.86(10)	N(8)-N(7)-Co(1)	118.92(19)
N(3)-Co(1)-N(1)	94.74(10)	N(9)-N(8)-N(7)	176.1(3)
C(1)-N(1)-C(5)	117.7(3)	N(11)-N(10)-Co(1)	121.18(19)
C(1)-N(1)-Co(1)	121.2(2)	N(12)-N(11)-N(10)	177.4(3)
C(5)-N(1)-Co(1)	120.9(2)	N(1)-C(1)-C(2)	123.4(3)
C(6)-N(2)-Co(1)	110.46(18)	N(1)-C(1)-H(1)	118.3

C(2)-C(1)-H(1)	118.3	N(2)-C(6)-C(7)	105.8(2)
C(3)-C(2)-C(1)	119.1(3)	N(2)-C(6)-H(6A)	110.6
C(3)-C(2)-H(2)	120.5	C(7)-C(6)-H(6A)	110.6
C(1)-C(2)-H(2)	120.5	N(2)-C(6)-H(6B)	110.6
C(2)-C(3)-C(4)	118.9(3)	C(7)-C(6)-H(6B)	110.6
C(2)-C(3)-H(3)	120.5	H(6A)-C(6)-H(6B)	108.7
C(4)-C(3)-H(3)	120.5	N(3)-C(7)-C(6)	106.6(2)
C(3)-C(4)-C(5)	118.4(3)	N(3)-C(7)-H(7A)	110.4
C(3)-C(4)-H(4)	120.8	C(6)-C(7)-H(7A)	110.4
C(5)-C(4)-H(4)	120.8	N(3)-C(7)-H(7B)	110.4
N(1)-C(5)-C(4)	122.6(3)	C(6)-C(7)-H(7B)	110.4
N(1)-C(5)-H(5)	118.7	H(7A)-C(7)-H(7B)	108.6
C(4)-C(5)-H(5)	118.7		

Table S27. Hydrogen bonds [Å and °] of **13**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(01)...N(6)#1	0.839(19)	2.30(2)	3.072(3)	153(3)
N(2)-H(02)...N(9)#2	0.847(19)	2.36(2)	3.086(3)	144(3)
N(3)-H(03)...N(12)#3	0.841(19)	2.37(2)	3.125(4)	150(3)

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