

Table 1. Crystal data and structure refinement for structure13.

Identification code	structure13
Empirical formula	C39 H53.50 Co N7.50 O22.50
Formula weight	1046.32
Temperature	153 (2) K
Wavelength	0.71073 Å
Crystal system	Trigonal
Space group	R-3
Unit cell dimensions	a = 14.822 (2) Å .α = 90°. b = 14.822 (2) Å β = 90°. c = 37.527 (5) Å .γ = 120°.
Volume	7139.8 (17) Å ³
Z	6
Calculated density	1.460 Mg/m ³
Absorption coefficient	0.451 mm ⁻¹
F(000)	3282
Crystal size	0.20 x 0.18 x 0.06 mm ³
Theta range for data collection	1.92 to 25.00°.
Limiting indices	-17<=h<=17, -17<=k<=17, -44<=l<=44
Reflections collected	22589
Independent reflections	2802 [R(int) = 0.0575]
Completeness to theta = 25.00°	99.9%
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.874
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2802 / 1 / 235
Goodness-of-fit on F ²	1.418
Final R indices [I>2sigma(I)]	R1 = 0.0775, wR2 = 0.1984
R indices (all data)	R1 = 0.0953, wR2 = 0.2091
Largest diff. peak and hole	0.818 and -0.429 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct13. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	0	0	3580(1)	38(1)
N(1)	454(3)	1308(3)	3863(1)	45(1)
N(2)	1276(2)	962(3)	3306(1)	42(1)
C(1)	-36(4)	1437(4)	4143(1)	58(1)
C(2)	381(4)	2345(4)	4335(1)	59(1)
C(3)	1346(3)	3157(3)	4246(1)	48(1)
C(4)	1859(3)	3043(3)	3953(1)	41(1)
C(5)	1392(3)	2117(3)	3767(1)	38(1)
C(6)	1860(3)	1928(3)	3449(1)	39(1)
C(7)	2812(3)	2647(3)	3307(1)	42(1)
C(8)	3181(3)	2390(3)	3007(1)	48(1)
C(9)	2570(3)	1413(4)	2857(1)	51(1)
C(10)	1619(3)	720(4)	3011(1)	51(1)
C(11)	1876(4)	4168(4)	4458(1)	57(1)
C(12)	4247(4)	3152(5)	2863(1)	73(2)
O(1)	2680(3)	4887(2)	4328(1)	81(1)
O(2)	1458(3)	4205(3)	4735(1)	86(1)
O(3)	4670(3)	4048(3)	2972(1)	89(1)
O(4)	4648(3)	2771(3)	2654(1)	93(1)
O(5)	3333	6667	4611(2)	84(2)
O(6)	654(5)	2883(5)	5310(2)	182(3)
O(7)	-430(30)	840(20)	5046(8)	251(10)
O(8)	6317(3)	5590(3)	2605(1)	88(1)
O(9)	6667	3333	3208(6)	243(14)
O(10)	6667	3333	2811(5)	108(5)
O(11)	6667	3333	2480(4)	89(4)
O(12)	6667	3333	2019(8)	170(11)
N(3)	267(11)	5342(12)	4863(3)	114(5)
C(13)	822(19)	5908(18)	5178(8)	142(10)
C(14)	-679(14)	4360(20)	4931(8)	166(15)

Table 3. Bond lengths [Å] and angles [°] for struct13.

Co(1)-N(2)#1	1.993(3)
Co(1)-N(2)#2	1.993(3)
Co(1)-N(2)	1.993(3)
Co(1)-N(1)#1	2.010(3)
Co(1)-N(1)#2	2.010(3)
Co(1)-N(1)	2.010(3)
N(1)-C(1)	1.345(5)
N(1)-C(5)	1.354(5)
N(2)-C(10)	1.339(5)
N(2)-C(6)	1.360(5)
C(1)-C(2)	1.370(6)
C(2)-C(3)	1.373(6)
C(3)-C(4)	1.393(5)
C(3)-C(11)	1.522(6)
C(4)-C(5)	1.379(5)
C(5)-C(6)	1.476(5)
C(6)-C(7)	1.381(6)
C(7)-C(8)	1.385(5)
C(8)-C(9)	1.387(6)
C(8)-C(12)	1.510(7)
C(9)-C(10)	1.388(6)
C(11)-O(2)	1.226(5)
C(11)-O(1)	1.234(5)
C(12)-O(3)	1.221(6)
C(12)-O(4)	1.275(6)
O(7)-O(7)#3	1.691(19)
O(7)-O(7)#4	1.69(2)
O(9)-O(9)#5	0.94(5)
O(9)-O(10)	1.49(3)
O(10)-O(11)	1.24(2)
O(11)-O(12)	1.73(3)
N(3)-C(13)	1.444(19)
N(3)-C(14)	1.45(2)
N(2)#1-Co(1)-N(2)#2	95.77(12)
N(2)#1-Co(1)-N(2)	95.77(12)
N(2)#2-Co(1)-N(2)	95.77(12)
N(2)#1-Co(1)-N(1)#1	80.96(13)
N(2)#2-Co(1)-N(1)#1	88.92(13)
N(2)-Co(1)-N(1)#1	174.55(13)
N(2)#1-Co(1)-N(1)#2	174.55(13)
N(2)#2-Co(1)-N(1)#2	80.96(13)
N(2)-Co(1)-N(1)#2	88.92(13)
N(1)#1-Co(1)-N(1)#2	94.57(14)
N(2)#1-Co(1)-N(1)	88.92(13)
N(2)#2-Co(1)-N(1)	174.55(13)
N(2)-Co(1)-N(1)	80.96(13)
N(1)#1-Co(1)-N(1)	94.57(14)
N(1)#2-Co(1)-N(1)	94.57(14)
C(1)-N(1)-C(5)	118.1(4)
C(1)-N(1)-Co(1)	127.4(3)
C(5)-N(1)-Co(1)	114.4(2)
C(10)-N(2)-C(6)	118.8(4)
C(10)-N(2)-Co(1)	125.9(3)
C(6)-N(2)-Co(1)	115.2(2)
N(1)-C(1)-C(2)	122.6(4)
C(1)-C(2)-C(3)	119.6(4)

C(2)-C(3)-C(4)	118.6(4)
C(2)-C(3)-C(11)	122.2(4)
C(4)-C(3)-C(11)	119.2(4)
C(5)-C(4)-C(3)	119.2(4)
N(1)-C(5)-C(4)	121.9(3)
N(1)-C(5)-C(6)	114.8(3)
C(4)-C(5)-C(6)	123.3(4)
N(2)-C(6)-C(7)	121.8(3)
N(2)-C(6)-C(5)	114.0(3)
C(7)-C(6)-C(5)	124.2(3)
C(6)-C(7)-C(8)	119.5(4)
C(7)-C(8)-C(9)	118.4(4)
C(7)-C(8)-C(12)	119.6(4)
C(9)-C(8)-C(12)	121.9(4)
C(8)-C(9)-C(10)	119.8(4)
N(2)-C(10)-C(9)	121.7(4)
O(2)-C(11)-O(1)	125.9(4)
O(2)-C(11)-C(3)	117.7(4)
O(1)-C(11)-C(3)	116.3(4)
O(3)-C(12)-O(4)	126.1(5)
O(3)-C(12)-C(8)	118.0(4)
O(4)-C(12)-C(8)	115.8(5)
O(7)#3-O(7)-O(7)#4	115.9(14)
O(9)#5-O(9)-O(10)	179.996(2)
O(11)-O(10)-O(9)	180.000(5)
O(10)-O(11)-O(12)	180.000(6)
C(13)-N(3)-C(14)	115(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct13.
The anisotropic displacement factor exponent takes the form:
 $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	39(1)	39(1)	38(1)	0	0	19(1)
N(1)	46(2)	56(2)	38(2)	-9(2)	0(2)	28(2)
N(2)	41(2)	51(2)	39(2)	-14(2)	-6(1)	27(2)
C(1)	50(3)	67(3)	52(3)	-14(2)	7(2)	25(2)
C(2)	60(3)	68(3)	49(3)	-11(2)	15(2)	31(3)
C(3)	67(3)	48(2)	38(2)	-2(2)	8(2)	36(2)
C(4)	55(2)	45(2)	33(2)	3(2)	5(2)	32(2)
C(5)	47(2)	43(2)	32(2)	1(2)	3(2)	29(2)
C(6)	47(2)	50(2)	33(2)	-4(2)	-5(2)	34(2)
C(7)	49(2)	45(2)	39(2)	-1(2)	2(2)	28(2)
C(8)	51(2)	61(3)	41(2)	-2(2)	4(2)	33(2)
C(9)	54(3)	77(3)	36(2)	-12(2)	-2(2)	42(3)
C(10)	51(3)	67(3)	44(2)	-20(2)	-10(2)	37(2)
C(11)	81(3)	48(3)	45(2)	-1(2)	17(2)	33(3)
C(12)	75(4)	88(4)	50(3)	-5(3)	24(3)	36(3)
O(1)	112(3)	44(2)	65(2)	0(2)	49(2)	22(2)
O(2)	98(3)	67(2)	70(2)	-20(2)	40(2)	24(2)
O(3)	91(3)	67(2)	78(3)	-10(2)	34(2)	17(2)
O(4)	80(3)	104(3)	83(3)	-11(2)	31(2)	38(2)
O(5)	60(2)	60(2)	132(6)	0	0	30(1)
O(6)	184(6)	179(6)	76(3)	31(4)	-9(4)	10(5)
O(7)	260(20)	240(30)	270(20)	126(19)	179(15)	146(16)
O(8)	80(3)	77(3)	85(3)	-5(2)	7(2)	24(2)
O(9)	310(20)	310(20)	110(30)	0	0	154(10)
O(10)	120(8)	120(8)	85(12)	0	0	60(4)
O(11)	109(7)	109(7)	48(8)	0	0	54(4)
O(12)	90(8)	90(8)	330(40)	0	0	45(4)
N(3)	109(11)	191(15)	60(7)	-30(8)	10(6)	89(11)
C(13)	170(20)	170(20)	134(19)	-82(17)	-45(15)	127(19)
C(14)	53(10)	230(30)	170(30)	-130(20)	-19(13)	31(13)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct13.

	x	y	z	U(eq)
H(1)	-698	877	4211	70
H(2)	5	2412	4528	71
H(4)	2522	3597	3883	49
H(7)	3211	3313	3414	51
H(9)	2801	1220	2650	62
H(10)	1201	56	2904	61
H(3A)	707	5212	4728	137
H(3B)	98	5759	4731	137
H(13A)	1436	6565	5108	213
H(13B)	1041	5488	5315	213
H(13C)	364	6055	5325	213
H(14A)	-1011	4041	4703	249
H(14B)	-1158	4486	5074	249
H(14C)	-507	3891	5060	249

