

Table 1. Crystal data and structure refinement for structure2.

Identification code	structure2	
Empirical formula	C12 H10 Co N2 O6	
Formula weight	337.15	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 6.7145(5) Å	$\alpha = 90^\circ$.
	b = 13.0147(9) Å	$\beta = 90^\circ$.
	c = 13.2121(9) Å	$\gamma = 90^\circ$.
Volume	1154.57(14) Å ³	
Z	4	
Calculated density	1.940 Mg/m ³	
Absorption coefficient	1.520 mm ⁻¹	
F(000)	684	
Crystal size	0.20 x 0.05 x 0.04 mm ³	
Theta range for data collection	2.20 to 29.99°.	
Limiting indices	-9<=h<=9, -10<=k<=18, -17<=l<=18	
Reflections collected	9015	
Independent reflections	3282 [R(int) = 0.0306]	
Completeness to theta = 29.99°	98.6%	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.846	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	3282 / 4 / 207	
Goodness-of-fit on F ²	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0345, wR2 = 0.0739	
R indices (all data)	R1 = 0.0382, wR2 = 0.0752	
Absolute structure parameter	0.328(14)	
Largest diff. peak and hole	0.723 and -0.305 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	-586(1)	-1185(1)	171(1)	10(1)
O(1)	414(3)	2470(1)	3976(1)	13(1)
O(2)	2651(2)	1394(1)	4650(1)	16(1)
O(3)	-27(3)	4162(1)	-523(1)	19(1)
O(4)	595(3)	3728(1)	-2125(1)	21(1)
O(5)	-3524(3)	-1034(1)	673(1)	18(1)
O(6)	-1304(3)	-2073(1)	-1107(1)	16(1)
N(1)	392(3)	-340(1)	1450(1)	12(1)
C(1)	835(4)	-720(2)	2364(2)	15(1)
C(2)	1211(4)	-122(2)	3213(2)	13(1)
C(3)	1076(3)	940(2)	3106(2)	12(1)
C(4)	616(3)	1342(2)	2158(2)	12(1)
C(5)	307(3)	689(2)	1344(2)	10(1)
C(6)	-99(3)	1071(2)	309(2)	11(1)
C(7)	81(3)	2098(2)	48(2)	13(1)
C(8)	-187(3)	2406(2)	-949(2)	12(1)
C(9)	-705(4)	1662(2)	-1653(2)	15(1)
C(10)	-938(4)	651(2)	-1342(2)	14(1)
N(2)	-608(3)	347(1)	-385(1)	12(1)
C(11)	1442(3)	1651(2)	3984(2)	11(1)
C(12)	156(3)	3530(2)	-1225(2)	14(1)

Table 3. Bond lengths [Å] and angles [°] for struct2.

Co(1)-O(1)#1	2.0852(15)
Co(1)-O(5)	2.0902(18)
Co(1)-O(6)	2.1026(17)
Co(1)-O(2)#2	2.1056(16)
Co(1)-N(1)	2.1200(19)
Co(1)-N(2)	2.1243(19)
O(1)-C(11)	1.270(3)
O(1)-Co(1)#3	2.0852(15)
O(2)-C(11)	1.243(3)
O(2)-Co(1)#4	2.1056(16)
O(3)-C(12)	1.246(3)
O(4)-C(12)	1.252(3)
N(1)-C(1)	1.337(3)
N(1)-C(5)	1.349(3)
C(1)-C(2)	1.388(3)
C(2)-C(3)	1.393(3)
C(3)-C(4)	1.392(3)
C(3)-C(11)	1.504(3)
C(4)-C(5)	1.386(3)
C(5)-C(6)	1.480(3)
C(6)-N(2)	1.359(3)
C(6)-C(7)	1.385(3)
C(7)-C(8)	1.389(3)
C(8)-C(9)	1.387(3)
C(8)-C(12)	1.526(3)
C(9)-C(10)	1.387(3)
C(10)-N(2)	1.344(3)
O(1)#1-Co(1)-O(5)	87.69(7)
O(1)#1-Co(1)-O(6)	89.14(6)
O(5)-Co(1)-O(6)	95.16(7)
O(1)#1-Co(1)-O(2)#2	90.94(6)

O(5)-Co(1)-O(2)#2	177.86(7)
O(6)-Co(1)-O(2)#2	83.17(7)
O(1)#1-Co(1)-N(1)	89.27(6)
O(5)-Co(1)-N(1)	89.48(7)
O(6)-Co(1)-N(1)	175.03(8)
O(2)#2-Co(1)-N(1)	92.15(7)
O(1)#1-Co(1)-N(2)	167.17(6)
O(5)-Co(1)-N(2)	90.87(7)
O(6)-Co(1)-N(2)	103.68(7)
O(2)#2-Co(1)-N(2)	90.83(7)
N(1)-Co(1)-N(2)	77.97(7)
C(11)-O(1)-Co(1)#3	132.07(15)
C(11)-O(2)-Co(1)#4	151.30(15)
C(1)-N(1)-C(5)	118.06(19)
C(1)-N(1)-Co(1)	126.64(15)
C(5)-N(1)-Co(1)	114.76(14)
N(1)-C(1)-C(2)	124.2(2)
C(1)-C(2)-C(3)	117.5(2)
C(4)-C(3)-C(2)	118.6(2)
C(4)-C(3)-C(11)	120.0(2)
C(2)-C(3)-C(11)	121.5(2)
C(5)-C(4)-C(3)	120.1(2)
N(1)-C(5)-C(4)	121.43(19)
N(1)-C(5)-C(6)	115.99(19)
C(4)-C(5)-C(6)	122.58(19)
N(2)-C(6)-C(7)	121.5(2)
N(2)-C(6)-C(5)	115.87(19)
C(7)-C(6)-C(5)	122.57(19)
C(6)-C(7)-C(8)	120.2(2)
C(9)-C(8)-C(7)	117.9(2)
C(9)-C(8)-C(12)	123.2(2)
C(7)-C(8)-C(12)	118.9(2)
C(8)-C(9)-C(10)	119.5(2)
N(2)-C(10)-C(9)	122.6(2)
C(10)-N(2)-C(6)	118.18(19)

C(10)-N(2)-Co(1)	127.09(15)
C(6)-N(2)-Co(1)	114.58(14)
O(2)-C(11)-O(1)	125.9(2)
O(2)-C(11)-C(3)	119.2(2)
O(1)-C(11)-C(3)	114.91(19)
O(3)-C(12)-O(4)	126.5(2)
O(3)-C(12)-C(8)	116.12(19)
O(4)-C(12)-C(8)	117.4(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct2.

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)	14 (1)	8 (1)	9 (1)	0 (1)	0 (1)	0 (1)
O (1)	19 (1)	9 (1)	11 (1)	-1 (1)	-1 (1)	2 (1)
O (2)	16 (1)	17 (1)	14 (1)	-2 (1)	-3 (1)	1 (1)
O (3)	30 (1)	12 (1)	16 (1)	0 (1)	4 (1)	-4 (1)
O (4)	36 (1)	15 (1)	12 (1)	3 (1)	5 (1)	-2 (1)
O (5)	16 (1)	11 (1)	27 (1)	0 (1)	1 (1)	1 (1)
O (6)	19 (1)	19 (1)	11 (1)	0 (1)	1 (1)	-6 (1)
N (1)	14 (1)	10 (1)	12 (1)	0 (1)	1 (1)	1 (1)
C (1)	21 (1)	9 (1)	14 (1)	2 (1)	-1 (1)	-1 (1)
C (2)	17 (1)	11 (1)	10 (1)	1 (1)	-2 (1)	1 (1)
C (3)	13 (1)	11 (1)	11 (1)	-2 (1)	1 (1)	-1 (1)
C (4)	15 (1)	9 (1)	12 (1)	0 (1)	0 (1)	0 (1)
C (5)	11 (1)	9 (1)	10 (1)	0 (1)	1 (1)	1 (1)
C (6)	13 (1)	11 (1)	9 (1)	-1 (1)	0 (1)	0 (1)
C (7)	16 (1)	11 (1)	10 (1)	0 (1)	0 (1)	0 (1)
C (8)	12 (1)	12 (1)	13 (1)	1 (1)	1 (1)	1 (1)
C (9)	19 (1)	14 (1)	11 (1)	0 (1)	-1 (1)	0 (1)
C (10)	19 (1)	12 (1)	11 (1)	-3 (1)	-2 (1)	0 (1)
N (2)	14 (1)	11 (1)	11 (1)	-1 (1)	2 (1)	1 (1)
C (11)	14 (1)	9 (1)	9 (1)	0 (1)	1 (1)	-3 (1)
C (12)	14 (1)	12 (1)	16 (1)	1 (1)	-1 (1)	1 (1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct2.

	x	y	z	U(eq)
H(5A)	-4140(40)	-483(13)	570(20)	30(9)
H(5B)	-4430(40)	-1480(20)	730(30)	46(10)
H(6A)	-1100(50)	-1870(20)	-1699(9)	33(9)
H(6B)	-2534(9)	-2190(20)	-1130(20)	29(9)
H(1)	896	-1445	2436	17
H(2)	1549	-426	3843	16
H(4)	513	2064	2068	15
H(7)	388	2593	552	15
H(9)	-899	1843	-2343	18
H(10)	-1348	153	-1825	17

