

Table 1. Crystal data and structure refinement for struct12.

Identification code	struct12	
Empirical formula	C12 H22 Co N2 O12	
Formula weight	445.25	
Temperature	173 (2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pccn	
Unit cell dimensions	a = 6.3780 (10) Å b = 12.938 (2) Å c = 21.558 (3) Å	$\alpha = 90^\circ$. $\beta = 90^\circ$. $\gamma = 90^\circ$.
Volume	1778.9 (5) Å ³	
Z	4	
Calculated density	1.662 Mg/m ³	
Absorption coefficient	1.032 mm ⁻¹	
F(000)	924	
Crystal size	0.4 x 0.1 x 0.1 mm ³	
Theta range for data collection	1.89 to 28.42°.	
Limiting indices	-8<=h<=8, -17<=k<=17, -28<=l<=28	
Reflections collected	20361	
Independent reflections	2151 [R(int) = 0.0655]	
Completeness to theta = 28.42°	95.6%	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.842	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2151 / 8 / 147	
Goodness-of-fit on F ²	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0413, wR2 = 0.0973	
R indices (all data)	R1 = 0.0572, wR2 = 0.1022	
Largest diff. peak and hole	0.532 and -0.228 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct12. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	2500	2500	3447(1)	17(1)
N(1)	793(3)	3089(2)	4212(1)	17(1)
C(1)	1534(3)	2816(2)	4772(1)	15(1)
C(2)	522(3)	3115(2)	5315(1)	18(1)
C(3)	-1269(3)	3714(2)	5286(1)	18(1)
C(4)	-2036(4)	3989(2)	4708(1)	20(1)
C(5)	-960(4)	3660(2)	4188(1)	21(1)
C(6)	-2311(4)	4077(2)	5874(1)	20(1)
O(1)	757(3)	1176(1)	3416(1)	30(1)
O(2)	4440(3)	2032(2)	2714(1)	27(1)
O(3)	-1293(3)	3984(2)	6367(1)	30(1)
O(4)	-4120(3)	4452(1)	5834(1)	25(1)
O(5)	-2204(3)	-1088(2)	3290(1)	29(1)
O(6)	-2220(3)	731(1)	2572(1)	25(1)

Table 3. Bond lengths [Å] and angles [°] for struct12.

Co(1)-O(1)#1	2.0430(18)
Co(1)-O(1)	2.0430(18)
Co(1)-O(2)	2.0962(18)
Co(1)-O(2)#1	2.0962(18)
Co(1)-N(1)#1	2.1193(19)
Co(1)-N(1)	2.1193(19)
N(1)-C(5)	1.341(3)
N(1)-C(1)	1.344(3)
C(1)-C(2)	1.391(3)
C(1)-C(1)#1	1.478(4)
C(2)-C(3)	1.382(3)
C(3)-C(4)	1.383(3)
C(3)-C(6)	1.507(3)
C(4)-C(5)	1.382(3)
C(6)-O(3)	1.251(3)
C(6)-O(4)	1.255(3)
O(1)#1-Co(1)-O(1)	176.35(11)
O(1)#1-Co(1)-O(2)	84.09(7)
O(1)-Co(1)-O(2)	93.15(8)
O(1)#1-Co(1)-O(2)#1	93.15(8)
O(1)-Co(1)-O(2)#1	84.09(7)
O(2)-Co(1)-O(2)#1	82.17(10)
O(1)#1-Co(1)-N(1)#1	92.69(8)
O(1)-Co(1)-N(1)#1	90.15(7)
O(2)-Co(1)-N(1)#1	100.37(7)
O(2)#1-Co(1)-N(1)#1	173.85(7)
O(1)#1-Co(1)-N(1)	90.15(7)
O(1)-Co(1)-N(1)	92.69(8)
O(2)-Co(1)-N(1)	173.85(7)
O(2)#1-Co(1)-N(1)	100.37(7)
N(1)#1-Co(1)-N(1)	77.68(10)
C(5)-N(1)-C(1)	118.25(19)
C(5)-N(1)-Co(1)	126.58(16)
C(1)-N(1)-Co(1)	115.11(15)
N(1)-C(1)-C(2)	121.26(19)
N(1)-C(1)-C(1)#1	116.01(12)
C(2)-C(1)-C(1)#1	122.73(13)
C(3)-C(2)-C(1)	120.1(2)
C(2)-C(3)-C(4)	118.5(2)
C(2)-C(3)-C(6)	120.0(2)
C(4)-C(3)-C(6)	121.5(2)
C(5)-C(4)-C(3)	118.4(2)
N(1)-C(5)-C(4)	123.5(2)
O(3)-C(6)-O(4)	125.0(2)
O(3)-C(6)-C(3)	117.2(2)
O(4)-C(6)-C(3)	117.8(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct12.
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)	16 (1)	21 (1)	15 (1)	0	0	3 (1)
N (1)	16 (1)	20 (1)	15 (1)	2 (1)	0 (1)	2 (1)
C (1)	12 (1)	15 (1)	18 (1)	-1 (1)	0 (1)	-1 (1)
C (2)	18 (1)	22 (1)	14 (1)	1 (1)	-2 (1)	1 (1)
C (3)	14 (1)	19 (1)	20 (1)	-2 (1)	0 (1)	-1 (1)
C (4)	15 (1)	23 (1)	21 (1)	1 (1)	0 (1)	5 (1)
C (5)	21 (1)	25 (1)	18 (1)	2 (1)	-2 (1)	4 (1)
C (6)	19 (1)	23 (1)	17 (1)	0 (1)	2 (1)	2 (1)
O (1)	36 (1)	24 (1)	31 (1)	10 (1)	-19 (1)	-7 (1)
O (2)	24 (1)	37 (1)	19 (1)	-8 (1)	-1 (1)	8 (1)
O (3)	22 (1)	51 (1)	19 (1)	-3 (1)	0 (1)	12 (1)
O (4)	19 (1)	33 (1)	23 (1)	-4 (1)	1 (1)	10 (1)
O (5)	20 (1)	43 (1)	25 (1)	-5 (1)	2 (1)	-5 (1)
O (6)	25 (1)	31 (1)	19 (1)	2 (1)	1 (1)	-1 (1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct12.

	x	y	z	U(eq)
H(2C)	1062	2907	5706	21
H(4)	-3271	4394	4670	24
H(5C)	-1492	3847	3792	25
H(1A)	910 (50)	637 (17)	3606 (13)	45
H(1B)	-30 (40)	1090 (20)	3128 (11)	45
H(2A)	3800 (40)	1830 (20)	2392 (10)	40
H(2B)	5510 (30)	1670 (20)	2766 (13)	40
H(5A)	-3350 (30)	-1030 (20)	3475 (13)	44
H(5B)	-1400 (40)	-900 (20)	3559 (11)	44
H(6A)	-1880 (40)	780 (20)	2201 (9)	37
H(6B)	-2350 (40)	117 (15)	2685 (13)	37

