

Table 1. Crystal data and structure refinement for structure6.

Identification code	structure6
Empirical formula	C22 H23 Co N4 O8
Formula weight	530.37
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 10.4189(10) Å α = 90°. b = 18.3762(18) Å β = 110.124(2)°. c = 12.5348(12) Å γ = 90°.
Volume	2253.4(4) Å ³
Z	4
Calculated density	1.563 Mg/m ³
Absorption coefficient	0.819 mm ⁻¹
F(000)	1096
Crystal size	0.15 x 0.05 x 0.03 mm ³
Theta range for data collection	2.05 to 28.52°.
Limiting indices	-13<=h<=13, -20<=k<=23, -16<=l<=16
Reflections collected	13903
Independent reflections	5195 [R(int) = 0.0806]
Completeness to theta = 28.52°	90.7%
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.868
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5195 / 8 / 348
Goodness-of-fit on F ²	1.059
Final R indices [I>2sigma(I)]	R1 = 0.0783, wR2 = 0.1227
R indices (all data)	R1 = 0.1227, wR2 = 0.1374
Largest diff. peak and hole	0.790 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 struct6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	4959(1)	1196(1)	2573(1)	13(1)
C(1)	5335(5)	-443(2)	3214(4)	22(1)
C(2)	5263(5)	-1180(2)	3031(4)	21(1)
C(3)	4654(4)	-1435(2)	1941(4)	14(1)
C(4)	4107(4)	-939(2)	1069(3)	15(1)
C(5)	4183(4)	-201(2)	1322(3)	12(1)
C(6)	3597(4)	367(2)	445(3)	14(1)
C(7)	2874(4)	197(2)	-671(3)	13(1)
C(8)	2372(4)	750(2)	-1461(3)	13(1)
C(9)	2618(4)	1459(2)	-1080(3)	16(1)
C(10)	3343(5)	1594(2)	53(4)	20(1)
C(11)	4581(4)	-2248(2)	1675(4)	16(1)
C(12)	1564(4)	585(2)	-2707(4)	17(1)
C(13)	2180(5)	1810(2)	2441(4)	24(1)
C(14)	1001(5)	1932(3)	2675(5)	34(1)
C(15)	801(5)	1526(3)	3543(5)	40(1)
C(16)	1778(5)	1012(3)	4119(4)	37(1)
C(17)	2901(5)	930(3)	3788(4)	31(1)
C(18)	976(6)	-1558(3)	781(5)	38(1)
C(19)	427(5)	-1001(3)	21(4)	34(1)
C(20)	318(5)	-307(2)	403(4)	23(1)
C(21)	822(5)	-211(3)	1566(4)	29(1)
C(22)	1365(5)	-796(3)	2266(4)	33(1)
N(1)	4798(4)	45(2)	2392(3)	16(1)
N(2)	3829(4)	1060(2)	816(3)	15(1)
N(3)	3118(4)	1321(2)	2968(3)	18(1)
N(4)	1449(4)	-1463(2)	1910(4)	33(1)
O(1)	4145(4)	-2427(1)	648(2)	27(1)
O(2)	4987(3)	-2670(1)	2517(2)	18(1)
O(3)	1469(3)	-73(2)	-2994(2)	24(1)
O(4)	1069(3)	1111(2)	-3333(2)	25(1)

O (5)	6028 (3)	1134 (2)	4346 (2)	19 (1)
O (6)	6761 (3)	1169 (2)	2237 (3)	24 (1)
O (8)	1349 (4)	-732 (2)	-4958 (3)	42 (1)
O (7)	2179 (4)	-2332 (2)	-1567 (3)	32 (1)

Table 3. Bond lengths [Å] and angles [°] for struct6.

Co(1)-O(6)	2.061(3)
Co(1)-O(2) #1	2.089(2)
Co(1)-O(5)	2.118(3)
Co(1)-N(2)	2.125(3)
Co(1)-N(1)	2.127(3)
Co(1)-N(3)	2.152(4)
C(1)-N(1)	1.335(5)
C(1)-C(2)	1.372(5)
C(2)-C(3)	1.376(5)
C(3)-C(4)	1.386(5)
C(3)-C(11)	1.526(5)
C(4)-C(5)	1.389(5)
C(5)-N(1)	1.350(5)
C(5)-C(6)	1.486(5)
C(6)-N(2)	1.349(5)
C(6)-C(7)	1.377(5)
C(7)-C(8)	1.390(5)
C(8)-C(9)	1.381(5)
C(8)-C(12)	1.528(5)
C(9)-C(10)	1.383(5)
C(10)-N(2)	1.341(5)
C(11)-O(1)	1.254(5)
C(11)-O(2)	1.260(5)
C(12)-O(4)	1.240(5)
C(12)-O(3)	1.256(5)
C(13)-N(3)	1.325(5)
C(13)-C(14)	1.376(6)
C(14)-C(15)	1.392(7)
C(15)-C(16)	1.395(7)
C(16)-C(17)	1.377(7)
C(17)-N(3)	1.335(5)
C(18)-N(4)	1.340(6)
C(18)-C(19)	1.381(7)
C(19)-C(20)	1.382(6)
C(20)-C(21)	1.381(6)

C (20) -C (20) #2	1.506 (9)
C (21) -C (22)	1.379 (6)
C (22) -N (4)	1.318 (6)
O (2) -Co (1) #3	2.089 (2)
O (6) -Co (1) -O (2) #1	88.27 (12)
O (6) -Co (1) -O (5)	91.50 (13)
O (2) #1-Co (1) -O (5)	95.49 (11)
O (6) -Co (1) -N (2)	90.23 (13)
O (2) #1-Co (1) -N (2)	94.38 (11)
O (5) -Co (1) -N (2)	170.03 (11)
O (6) -Co (1) -N (1)	89.90 (13)
O (2) #1-Co (1) -N (1)	171.33 (12)
O (5) -Co (1) -N (1)	93.03 (12)
N (2) -Co (1) -N (1)	77.15 (12)
O (6) -Co (1) -N (3)	175.03 (13)
O (2) #1-Co (1) -N (3)	87.04 (12)
O (5) -Co (1) -N (3)	87.31 (13)
N (2) -Co (1) -N (3)	91.77 (13)
N (1) -Co (1) -N (3)	94.98 (12)
N (1) -C (1) -C (2)	123.4 (4)
C (1) -C (2) -C (3)	118.8 (4)
C (2) -C (3) -C (4)	118.9 (3)
C (2) -C (3) -C (11)	121.4 (3)
C (4) -C (3) -C (11)	119.7 (4)
C (3) -C (4) -C (5)	119.1 (4)
N (1) -C (5) -C (4)	121.6 (4)
N (1) -C (5) -C (6)	115.7 (3)
C (4) -C (5) -C (6)	122.7 (4)
N (2) -C (6) -C (7)	122.3 (4)
N (2) -C (6) -C (5)	115.4 (3)
C (7) -C (6) -C (5)	122.3 (3)
C (6) -C (7) -C (8)	119.9 (3)
C (9) -C (8) -C (7)	117.6 (4)
C (9) -C (8) -C (12)	120.8 (3)
C (7) -C (8) -C (12)	121.6 (3)
C (8) -C (9) -C (10)	119.6 (4)

N(2)-C(10)-C(9)	122.7(4)
O(1)-C(11)-O(2)	126.7(4)
O(1)-C(11)-C(3)	117.0(3)
O(2)-C(11)-C(3)	116.3(4)
O(4)-C(12)-O(3)	126.5(4)
O(4)-C(12)-C(8)	117.1(4)
O(3)-C(12)-C(8)	116.4(4)
N(3)-C(13)-C(14)	124.3(4)
C(13)-C(14)-C(15)	117.7(5)
C(14)-C(15)-C(16)	119.2(5)
C(17)-C(16)-C(15)	117.5(5)
N(3)-C(17)-C(16)	124.1(5)
N(4)-C(18)-C(19)	123.2(5)
C(18)-C(19)-C(20)	120.6(5)
C(21)-C(20)-C(19)	115.8(4)
C(21)-C(20)-C(20)#2	122.2(5)
C(19)-C(20)-C(20)#2	122.0(5)
C(22)-C(21)-C(20)	119.8(5)
N(4)-C(22)-C(21)	124.8(5)
C(1)-N(1)-C(5)	118.1(3)
C(1)-N(1)-Co(1)	126.1(3)
C(5)-N(1)-Co(1)	115.6(2)
C(10)-N(2)-C(6)	117.8(4)
C(10)-N(2)-Co(1)	126.3(3)
C(6)-N(2)-Co(1)	115.9(3)
C(13)-N(3)-C(17)	117.2(4)
C(13)-N(3)-Co(1)	121.4(3)
C(17)-N(3)-Co(1)	121.4(3)
C(22)-N(4)-C(18)	115.8(4)
C(11)-O(2)-Co(1)#3	125.2(3)

Symmetry transformations used to generate equivalent atoms:

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

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct6.

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)	20 (1)	8 (1)	9 (1)	0 (1)	1 (1)	0 (1)
C (1)	32 (3)	16 (2)	10 (2)	-1 (2)	-2 (2)	2 (2)
C (2)	33 (3)	11 (2)	14 (2)	3 (2)	3 (2)	1 (2)
C (3)	13 (2)	10 (2)	18 (2)	0 (2)	5 (2)	-2 (2)
C (4)	16 (2)	14 (2)	14 (2)	-2 (2)	3 (2)	-2 (2)
C (5)	11 (2)	14 (2)	10 (2)	0 (2)	1 (2)	-1 (2)
C (6)	15 (2)	10 (2)	15 (2)	0 (2)	4 (2)	-1 (2)
C (7)	17 (2)	9 (2)	11 (2)	-2 (2)	3 (2)	-1 (2)
C (8)	9 (2)	17 (2)	11 (2)	-3 (2)	2 (2)	1 (2)
C (9)	21 (2)	14 (2)	11 (2)	7 (2)	2 (2)	4 (2)
C (10)	29 (3)	11 (2)	17 (2)	-2 (2)	5 (2)	1 (2)
C (11)	14 (2)	13 (2)	18 (2)	0 (2)	3 (2)	0 (2)
C (12)	13 (2)	21 (2)	17 (2)	0 (2)	4 (2)	2 (2)
C (13)	26 (3)	18 (2)	23 (2)	-5 (2)	4 (2)	-5 (2)
C (14)	23 (3)	30 (3)	45 (3)	-16 (2)	7 (3)	-2 (2)
C (15)	28 (3)	48 (3)	48 (4)	-19 (3)	19 (3)	-10 (3)
C (16)	33 (3)	46 (3)	33 (3)	-3 (2)	15 (3)	-6 (2)
C (17)	32 (3)	33 (3)	25 (3)	3 (2)	5 (2)	0 (2)
C (18)	40 (4)	31 (3)	39 (3)	-4 (2)	8 (3)	-1 (2)
C (19)	34 (3)	40 (3)	24 (3)	-6 (2)	3 (2)	-7 (2)
C (20)	19 (3)	34 (3)	21 (3)	-4 (2)	11 (2)	-8 (2)
C (21)	28 (3)	40 (3)	18 (3)	-5 (2)	8 (2)	-8 (2)
C (22)	28 (3)	52 (3)	22 (3)	0 (2)	14 (2)	-3 (3)
N (1)	19 (2)	11 (2)	13 (2)	-2 (1)	1 (2)	-2 (1)
N (2)	20 (2)	11 (2)	14 (2)	2 (1)	6 (2)	-2 (1)
N (3)	22 (2)	12 (2)	16 (2)	-3 (1)	2 (2)	-1 (2)
N (4)	26 (3)	39 (2)	34 (3)	2 (2)	12 (2)	-5 (2)
O (1)	47 (2)	12 (2)	14 (2)	0 (1)	-1 (2)	0 (1)
O (2)	25 (2)	13 (1)	13 (2)	2 (1)	0 (1)	-1 (1)
O (3)	29 (2)	22 (2)	15 (2)	-4 (1)	-3 (1)	6 (1)
O (4)	32 (2)	21 (2)	14 (2)	4 (1)	-3 (1)	6 (1)

O (5)	25 (2)	11 (2)	16 (2)	-3 (1)	0 (1)	1 (1)
O (6)	26 (2)	17 (2)	29 (2)	7 (2)	8 (2)	3 (2)
O (8)	25 (2)	75 (3)	18 (2)	-19 (2)	-3 (2)	13 (2)
O (7)	31 (2)	32 (2)	27 (2)	5 (2)	2 (2)	0 (2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct6.

	x	y	z	U(eq)
H(1)	5790	-271	3964	26
H(2)	5627	-1509	3647	25
H(4)	3685	-1102	309	18
H(7)	2719	-297	-900	15
H(9)	2291	1852	-1594	20
H(10)	3503	2084	302	24
H(13)	2332	2096	1864	28
H(14)	346	2280	2259	41
H(15)	8	1599	3740	48
H(16)	1674	728	4717	44
H(17)	3562	574	4166	37
H(18)	1020	-2031	490	46
H(19)	120	-1097	-772	41
H(21)	795	255	1884	34
H(22)	1702	-712	3062	39
H(5A)	5960(50)	1570(10)	4520(40)	45(16)
H(5B)	6858(19)	1020(30)	4550(50)	70(20)
H(6A)	7150(40)	1535(15)	2090(40)	24(14)
H(6B)	7380(40)	860(20)	2480(40)	55(19)
H(8A)	1170(50)	-510(20)	-4450(30)	24(14)
H(8B)	610(30)	-850(30)	-5450(30)	47(17)
H(7B)	2100(60)	-2709(19)	-1970(40)	60(20)
H(7A)	2760(40)	-2410(30)	-920(20)	48(18)