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(Adamantane-1,3-dicarboxylato-κO)-aquabis(1,10-phenanthroline-$\kappa^2 N,N'$)-cobalt(II) tetrahydrate

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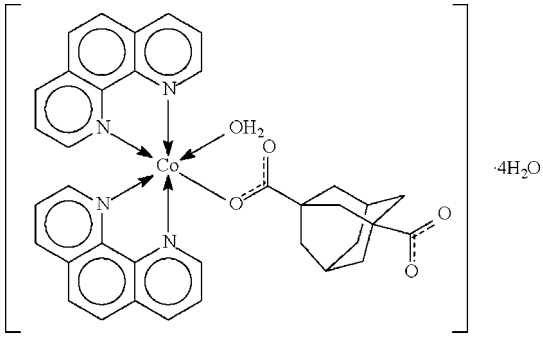
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.167; data-to-parameter ratio = 17.1.

The Co^{II} atom in the racemic title compound, $[Co(C_{12}H_{14}O_4)(C_{12}H_8N_2)_2(H_2O)]\cdot 4H_2O$, is chelated by two N-heterocycles; it is also linked datively to a water molecule and covalently to a single O atom of the dicarboxylate dianion to yield a *cis*-CoO_2N_4 octahedral geometry. A plausible O—H···O hydrogen-bonding scheme results in the component species being linked into a chain.

Related literature

There are no examples of metal derivatives of this dicarboxylic acid according to the Cambridge Structural Database (Version 5.28; May 2007; Allen, 2002). For the structure of the free acid, see: Glidewell & Ferguson (1996).



Experimental

Crystal data

$[Co(C_{12}H_{14}O_4)(C_{12}H_8N_2)_2(H_2O)]\cdot 4H_2O$
M_r = 731.65
Triclinic, $P\overline{1}$
a = 8.9902 (2) Å
b = 13.2497 (2) Å
c = 15.6671 (2) Å
α = 69.277 (1)°
β = 77.067 (1)°
γ = 87.328 (1)°
V = 1700.12 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.57 mm^{-1}
T = 295 (2) K
0.39 × 0.31 × 0.09 mm

Data collection

Bruker APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.813, T_{max} = 0.951
29003 measured reflections
7692 independent reflections
6662 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.167
S = 1.06
7692 reflections
451 parameters
24 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1	2.114 (2)	Co1—N2	2.288 (2)
Co1—O1*w*	2.134 (2)	Co1—N3	2.293 (2)
Co1—N1	2.281 (2)	Co1—N4	2.294 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1*w*—H1*w*1···O2	0.85	1.82	2.599 (3)	152
O1*w*—H1*w*2···O2*w*	0.85	2.10	2.656 (3)	122
O2*w*—H2*w*1···O4^{i}	0.86	1.86	2.712 (3)	176
O2*w*—H2*w*2···O4*w*^{ii}	0.86	2.37	3.113 (5)	145
O3*w*—H3*w*1···O4^{iii}	0.86	2.06	2.895 (4)	164
O3*w*—H3*w*2···O4*w*	0.86	2.08	2.913 (5)	164
O4*w*—H4*w*1···O3^{iv}	0.85	1.84	2.695 (3)	178
O5*w*—H5*w*1···O3^{iv}	0.86	1.96	2.814 (4)	173
O5*w*—H5*w*2···O3*w*	0.86	2.36	3.211 (5)	174

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x+2, -y+1, -z+1$; (iii) $x, y-1, z$; (iv) $x+1, y-1, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2477).

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supplementary materials

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(Adamantane-1,3-dicarboxylato-κO)aquabis(1,10-phenanthroline-$\kappa^2 N,N'$)cobalt(II) tetrahydrate

G.-L. Zhao, X. Shi and S. W. Ng

Comment

The crystal structures of an enormous number of metal(II) dicarboxylates have been reported (CSD Version 5.28, May 2007; Allen, 2002). However, there is no example of a metal 1,3-adamantanedicarboxylate; the crystal structure of the dicarboxylic acid itself has been known for some time (Glidewell & Ferguson, 1996).

The cobalt(II) atom in the title compound, (I), (Fig. 1), is chelated by two *N*-heterocycles; it is also linked datively to a water molecule and covalently to a single O atom of the dicarboxylate dianion in an all-*cis* octahedral geometry (Table 1). The mononuclear complex exists as as a zwitterion (*i.e.* formal Co^+ and free $-CO_2^-$ carboxyate anion in the same molecule). The component species of (I) are linked into a chain by ay of O—H···O interactions (Table 2).

Experimental

Cobalt diacetate tetrahydrate (1 mmol), 1,3-adamantanedicarboxylic acid (1 mmol) and 1,10-phenanthroline (2 mmol) were dissolved in ethanol (50 ml). The solution was set aside for the growth of the yellow plates of (I), which were isolated after a week.

Refinement

The carbon-bound H atoms were positioned geometrically (C–H = 0.93–0.97 Å), and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The H atoms of water were placed (O—H = 0.85 Å) to generate a chemically plausible hydrogen bonding scheme and refined as riding with U_{iso}(H) = 1.2U_{eq}(O). In the resulting scheme, which should be regarded as tentative, the O4w water molecule forms only one hydrogen bond.

Figures

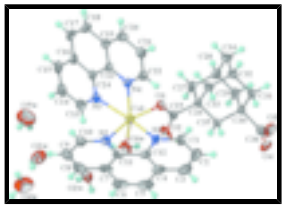


Fig. 1. **Figure 1**. View of the molecular structure of (I); displacement ellipsoids are drawn at the 50% probabilty level and hydrogen atoms as spheres of arbitrary radius.

(Adamantane-1,3-dicarboxylato-κ*O*)aquabis(1,10-phenanthroline-\ κ^2*N*,*N*')cobalt(II) tetrahydrate

Crystal data

$[Co(C_{12}H_{14}O_4)(C_{12}H_8N_2)_2(H_2O)]\cdot 4H_2O$ $Z = 2$

M_r = 731.65	F_{000} = 766
Triclinic, $P\bar{1}$	D_x = 1.429 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.9902 (2) Å	Cell parameters from 7731 reflections
b = 13.2497 (2) Å	θ = 2.5–27.4º
c = 15.6671 (2) Å	μ = 0.57 mm^{-1}
α = 69.277 (1)º	T = 295 (2) K
β = 77.067 (1)º	Plate, yellow
γ = 87.328 (1)º	0.39 × 0.31 × 0.09 mm
V = 1700.12 (5) Å^3	

Data collection

Bruker APEX II CCD diffractometer	7692 independent reflections
Radiation source: fine-focus sealed tube	6662 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.022
T = 295(2) K	θ_{max} = 27.4º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→11
T_{min} = 0.813, T_{max} = 0.951	k = −17→17
29003 measured reflections	l = −20→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.050	H-atom parameters constrained
$wR(F^2)$ = 0.167	$w = 1/[\sigma^2(F_o^2) + (0.0966P)^2 + 1.4193P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001
7692 reflections	$\Delta\rho_{max}$ = 0.70 e Å^{-3}
451 parameters	$\Delta\rho_{min}$ = −0.77 e Å^{-3}
24 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Co1	0.77668 (4)	0.73276 (3)	0.75869 (2)	0.03448 (13)
O1	0.6078 (2)	0.83204 (14)	0.80147 (12)	0.0363 (4)
O2	0.4719 (3)	0.8737 (2)	0.69354 (19)	0.0733 (9)
O3	0.1345 (3)	1.27607 (18)	0.67492 (17)	0.0592 (6)

O4	0.3830 (2)	1.29932 (16)	0.61730 (14)	0.0505 (5)
O1w	0.6634 (3)	0.73629 (19)	0.65170 (16)	0.0555 (6)
H1w1	0.5867	0.7761	0.6530	0.083*
H1w2	0.6335	0.6725	0.6609	0.083*
O2w	0.6797 (4)	0.6062 (2)	0.55445 (16)	0.0676 (7)
H2w1	0.6602	0.6391	0.5006	0.101*
H2w2	0.7708	0.5826	0.5469	0.101*
O3w	0.6600 (3)	0.3795 (2)	0.6404 (2)	0.0763 (8)
H3w1	0.5898	0.3520	0.6253	0.114*
H3w2	0.7455	0.3718	0.6058	0.114*
O4w	0.9756 (4)	0.3754 (3)	0.5430 (2)	0.1015 (11)
H4w1	1.0274	0.3433	0.5838	0.152*
H4w2	0.9818	0.3394	0.5057	0.152*
O5w	0.8633 (4)	0.3016 (4)	0.7950 (3)	0.1137 (13)
H5w1	0.9500	0.2925	0.7622	0.171*
H5w2	0.8028	0.3231	0.7571	0.171*
N1	0.9384 (2)	0.87944 (17)	0.67661 (14)	0.0344 (4)
N2	0.9945 (2)	0.67309 (17)	0.68646 (14)	0.0340 (4)
N3	0.6912 (2)	0.55917 (16)	0.84887 (14)	0.0309 (4)
N4	0.8511 (2)	0.68960 (15)	0.89783 (13)	0.0273 (4)
C1	0.9074 (4)	0.9812 (2)	0.6682 (2)	0.0433 (6)
H1	0.8163	0.9948	0.7036	0.052*
C2	1.0050 (4)	1.0683 (2)	0.6089 (2)	0.0517 (7)
H2	0.9787	1.1384	0.6045	0.062*
C3	1.1392 (4)	1.0497 (3)	0.5574 (2)	0.0532 (8)
H3	1.2055	1.1072	0.5175	0.064*
C4	1.1780 (3)	0.9432 (2)	0.56434 (18)	0.0434 (6)
C5	1.3174 (3)	0.9163 (3)	0.5126 (2)	0.0559 (9)
H5	1.3870	0.9712	0.4717	0.067*
C6	1.3490 (3)	0.8135 (3)	0.5221 (2)	0.0554 (8)
H6	1.4412	0.7983	0.4887	0.066*
C7	1.2439 (3)	0.7268 (3)	0.58235 (18)	0.0450 (6)
C8	1.2697 (4)	0.6184 (3)	0.5932 (2)	0.0544 (8)
H8	1.3625	0.5992	0.5637	0.065*
C9	1.1598 (4)	0.5413 (3)	0.6466 (2)	0.0520 (7)
H9	1.1757	0.4693	0.6534	0.062*
C10	1.0223 (3)	0.5719 (2)	0.69122 (19)	0.0413 (6)
H10	0.9463	0.5189	0.7261	0.050*
C11	1.1034 (3)	0.7501 (2)	0.63264 (16)	0.0341 (5)
C12	1.0721 (3)	0.8606 (2)	0.62498 (16)	0.0342 (5)
C13	0.6101 (3)	0.4955 (2)	0.8254 (2)	0.0394 (5)
H13	0.5920	0.5200	0.7654	0.047*
C14	0.5510 (3)	0.3934 (2)	0.8872 (2)	0.0452 (6)
H14	0.4945	0.3517	0.8682	0.054*
C15	0.5765 (3)	0.3556 (2)	0.9748 (2)	0.0412 (6)
H15	0.5365	0.2883	1.0165	0.049*
C16	0.6643 (3)	0.41909 (18)	1.00232 (18)	0.0333 (5)
C17	0.6976 (3)	0.3850 (2)	1.09303 (19)	0.0409 (6)
H17	0.6602	0.3181	1.1368	0.049*

C18	0.7823 (3)	0.4483 (2)	1.11631 (18)	0.0400 (6)
H18	0.8045	0.4237	1.1753	0.048*
C19	0.8386 (3)	0.55296 (19)	1.05137 (16)	0.0310 (5)
C20	0.9240 (3)	0.6234 (2)	1.07304 (18)	0.0371 (5)
H20	0.9488	0.6020	1.1313	0.045*
C21	0.9700 (3)	0.7228 (2)	1.00833 (19)	0.0380 (5)
H21	1.0273	0.7698	1.0216	0.046*
C22	0.9300 (3)	0.75346 (19)	0.92164 (18)	0.0342 (5)
H22	0.9604	0.8221	0.8785	0.041*
C23	0.8062 (2)	0.58983 (17)	0.96187 (15)	0.0260 (4)
C24	0.7189 (2)	0.52079 (17)	0.93618 (16)	0.0278 (4)
C25	0.5087 (3)	0.88646 (18)	0.76021 (16)	0.0290 (4)
C26	0.4244 (2)	0.96943 (17)	0.79885 (15)	0.0249 (4)
C27	0.2706 (3)	0.91488 (18)	0.86213 (18)	0.0342 (5)
H27A	0.2136	0.8921	0.8260	0.041*
H27B	0.2895	0.8513	0.9127	0.041*
C28	0.1772 (3)	0.99344 (19)	0.90258 (17)	0.0347 (5)
H28A	0.0802	0.9578	0.9426	0.042*
C29	0.1454 (3)	1.09256 (19)	0.82272 (17)	0.0321 (5)
H29A	0.0854	1.1423	0.8482	0.039*
H29B	0.0871	1.0707	0.7866	0.039*
C30	0.2957 (2)	1.14894 (17)	0.75907 (15)	0.0262 (4)
C31	0.3852 (3)	1.18280 (18)	0.81816 (16)	0.0303 (5)
H31A	0.4809	1.2190	0.7789	0.036*
H31B	0.3265	1.2329	0.8437	0.036*
C32	0.4172 (3)	1.0835 (2)	0.89789 (16)	0.0320 (5)
H32A	0.4746	1.1062	0.9348	0.038*
C33	0.5125 (3)	1.00539 (19)	0.85689 (16)	0.0300 (5)
H33A	0.6087	1.0408	0.8177	0.036*
H33B	0.5347	0.9428	0.9072	0.036*
C34	0.2674 (3)	1.0273 (2)	0.96088 (17)	0.0397 (6)
H34A	0.2082	1.0759	0.9882	0.048*
H34B	0.2880	0.9642	1.0113	0.048*
C35	0.3915 (2)	1.06957 (17)	0.71942 (15)	0.0259 (4)
H35A	0.3368	1.0477	0.6817	0.031*
H35B	0.4872	1.1052	0.6795	0.031*
C36	0.2686 (3)	1.24950 (19)	0.67744 (17)	0.0344 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0349 (2)	0.0314 (2)	0.0364 (2)	0.00510 (14)	−0.00779 (14)	−0.01162 (14)
O1	0.0384 (9)	0.0373 (9)	0.0373 (9)	0.0179 (7)	−0.0151 (7)	−0.0164 (7)
O2	0.1009 (19)	0.0826 (17)	0.0847 (17)	0.0644 (16)	−0.0679 (16)	−0.0664 (15)
O3	0.0485 (12)	0.0522 (12)	0.0643 (14)	0.0218 (10)	−0.0229 (11)	−0.0017 (10)
O4	0.0548 (12)	0.0409 (10)	0.0415 (11)	0.0051 (9)	−0.0130 (9)	0.0037 (8)
O1w	0.0627 (13)	0.0641 (14)	0.0657 (14)	0.0315 (11)	−0.0372 (11)	−0.0439 (12)
O2w	0.114 (2)	0.0533 (13)	0.0486 (12)	0.0234 (13)	−0.0352 (13)	−0.0253 (11)

O3w	0.0752 (17)	0.0716 (17)	0.0724 (17)	−0.0151 (14)	−0.0187 (14)	−0.0103 (13)
O4w	0.085 (2)	0.138 (3)	0.086 (2)	0.031 (2)	−0.0518 (18)	−0.029 (2)
O5w	0.092 (2)	0.147 (3)	0.102 (3)	0.049 (2)	−0.014 (2)	−0.054 (2)
N1	0.0387 (11)	0.0315 (10)	0.0309 (10)	0.0000 (8)	−0.0064 (8)	−0.0091 (8)
N2	0.0368 (10)	0.0351 (10)	0.0297 (10)	0.0074 (8)	−0.0076 (8)	−0.0117 (8)
N3	0.0287 (9)	0.0299 (9)	0.0362 (10)	0.0006 (7)	−0.0074 (8)	−0.0142 (8)
N4	0.0239 (8)	0.0238 (8)	0.0323 (9)	0.0004 (7)	−0.0041 (7)	−0.0086 (7)
C1	0.0518 (15)	0.0335 (13)	0.0440 (14)	0.0004 (11)	−0.0118 (12)	−0.0122 (11)
C2	0.072 (2)	0.0324 (13)	0.0526 (17)	−0.0076 (13)	−0.0249 (16)	−0.0089 (12)
C3	0.0631 (19)	0.0504 (16)	0.0394 (15)	−0.0260 (14)	−0.0178 (14)	−0.0004 (12)
C4	0.0434 (14)	0.0561 (16)	0.0275 (12)	−0.0148 (12)	−0.0114 (10)	−0.0067 (11)
C5	0.0390 (14)	0.088 (3)	0.0316 (13)	−0.0221 (15)	−0.0024 (11)	−0.0101 (14)
C6	0.0347 (14)	0.093 (3)	0.0340 (14)	−0.0021 (15)	−0.0008 (11)	−0.0203 (15)
C7	0.0339 (12)	0.0724 (19)	0.0304 (12)	0.0074 (12)	−0.0069 (10)	−0.0211 (13)
C8	0.0452 (15)	0.081 (2)	0.0447 (16)	0.0286 (16)	−0.0123 (13)	−0.0339 (16)
C9	0.0604 (18)	0.0557 (17)	0.0480 (16)	0.0275 (15)	−0.0182 (14)	−0.0277 (14)
C10	0.0466 (14)	0.0398 (13)	0.0396 (13)	0.0137 (11)	−0.0126 (11)	−0.0162 (11)
C11	0.0299 (11)	0.0466 (14)	0.0252 (11)	0.0034 (10)	−0.0062 (9)	−0.0121 (10)
C12	0.0351 (12)	0.0418 (13)	0.0251 (11)	−0.0037 (10)	−0.0089 (9)	−0.0090 (9)
C13	0.0387 (13)	0.0388 (13)	0.0463 (14)	−0.0006 (10)	−0.0115 (11)	−0.0205 (11)
C14	0.0378 (13)	0.0367 (13)	0.0696 (19)	−0.0038 (11)	−0.0100 (13)	−0.0296 (13)
C15	0.0349 (12)	0.0249 (11)	0.0602 (17)	−0.0037 (9)	−0.0029 (11)	−0.0148 (11)
C16	0.0278 (10)	0.0234 (10)	0.0452 (13)	0.0015 (8)	−0.0018 (9)	−0.0118 (10)
C17	0.0442 (14)	0.0246 (11)	0.0418 (14)	0.0008 (10)	−0.0031 (11)	−0.0010 (10)
C18	0.0450 (14)	0.0337 (12)	0.0331 (12)	0.0033 (10)	−0.0082 (11)	−0.0025 (10)
C19	0.0293 (11)	0.0294 (11)	0.0311 (11)	0.0048 (9)	−0.0058 (9)	−0.0081 (9)
C20	0.0374 (12)	0.0439 (14)	0.0326 (12)	0.0049 (10)	−0.0112 (10)	−0.0149 (10)
C21	0.0364 (12)	0.0386 (13)	0.0441 (14)	−0.0029 (10)	−0.0101 (11)	−0.0197 (11)
C22	0.0331 (11)	0.0288 (11)	0.0388 (13)	−0.0038 (9)	−0.0066 (10)	−0.0099 (9)
C23	0.0215 (9)	0.0242 (10)	0.0309 (11)	0.0036 (7)	−0.0037 (8)	−0.0096 (8)
C24	0.0233 (9)	0.0233 (10)	0.0354 (11)	0.0039 (8)	−0.0038 (8)	−0.0108 (9)
C25	0.0316 (11)	0.0251 (10)	0.0310 (11)	0.0062 (8)	−0.0079 (9)	−0.0104 (8)
C26	0.0254 (10)	0.0238 (9)	0.0257 (10)	0.0056 (8)	−0.0077 (8)	−0.0083 (8)
C27	0.0320 (11)	0.0254 (10)	0.0397 (13)	0.0017 (9)	−0.0029 (10)	−0.0079 (9)
C28	0.0276 (11)	0.0313 (11)	0.0369 (12)	0.0013 (9)	0.0025 (9)	−0.0079 (10)
C29	0.0254 (10)	0.0322 (11)	0.0416 (13)	0.0072 (9)	−0.0094 (9)	−0.0159 (10)
C30	0.0281 (10)	0.0238 (10)	0.0286 (10)	0.0064 (8)	−0.0102 (8)	−0.0099 (8)
C31	0.0341 (11)	0.0284 (10)	0.0335 (11)	0.0026 (9)	−0.0101 (9)	−0.0158 (9)
C32	0.0352 (11)	0.0392 (12)	0.0291 (11)	0.0088 (10)	−0.0135 (9)	−0.0182 (10)
C33	0.0308 (11)	0.0361 (11)	0.0270 (10)	0.0092 (9)	−0.0126 (9)	−0.0130 (9)
C34	0.0444 (14)	0.0444 (14)	0.0261 (11)	0.0128 (11)	−0.0031 (10)	−0.0116 (10)
C35	0.0303 (10)	0.0249 (10)	0.0244 (10)	0.0063 (8)	−0.0099 (8)	−0.0093 (8)
C36	0.0454 (13)	0.0266 (11)	0.0344 (12)	0.0107 (10)	−0.0166 (10)	−0.0111 (9)

Geometric parameters (Å, °)

Co1—O1	2.114 (2)	C13—C14	1.400 (4)
Co1—O1w	2.134 (2)	C13—H13	0.9300
Co1—N1	2.281 (2)	C14—C15	1.352 (4)

Co1—N2	2.288 (2)	C14—H14	0.9300
Co1—N3	2.293 (2)	C15—C16	1.410 (3)
Co1—N4	2.294 (2)	C15—H15	0.9300
C25—O1	1.264 (3)	C16—C24	1.406 (3)
C25—O2	1.231 (3)	C16—C17	1.427 (4)
C36—O3	1.246 (3)	C17—C18	1.348 (4)
C36—O4	1.253 (3)	C17—H17	0.9300
O1w—H1w1	0.85	C18—C19	1.432 (3)
O1w—H1w2	0.85	C18—H18	0.9300
O2w—H2w1	0.86	C19—C23	1.405 (3)
O2w—H2w2	0.86	C19—C20	1.408 (3)
O3w—H3w1	0.86	C20—C21	1.362 (4)
O3w—H3w2	0.86	C20—H20	0.9300
O4w—H4w1	0.85	C21—C22	1.398 (4)
O4w—H4w2	0.87	C21—H21	0.9300
O5w—H5w1	0.86	C22—H22	0.9300
O5w—H5w2	0.86	C23—C24	1.443 (3)
N1—C1	1.330 (3)	C25—C26	1.529 (3)
N1—C12	1.357 (3)	C26—C33	1.531 (3)
N2—C10	1.331 (3)	C26—C35	1.535 (3)
N2—C11	1.352 (3)	C26—C27	1.546 (3)
N3—C13	1.331 (3)	C27—C28	1.529 (3)
N3—C24	1.357 (3)	C27—H27A	0.9700
N4—C22	1.325 (3)	C27—H27B	0.9700
N4—C23	1.359 (3)	C28—C29	1.528 (3)
C1—C2	1.392 (4)	C28—C34	1.533 (4)
C1—H1	0.9300	C28—H28A	0.9800
C2—C3	1.358 (5)	C29—C30	1.530 (3)
C2—H2	0.9300	C29—H29A	0.9700
C3—C4	1.409 (5)	C29—H29B	0.9700
C3—H3	0.9300	C30—C31	1.538 (3)
C4—C12	1.401 (4)	C30—C35	1.540 (3)
C4—C5	1.436 (5)	C30—C36	1.540 (3)
C5—C6	1.341 (5)	C31—C32	1.528 (3)
C5—H5	0.9300	C31—H31A	0.9700
C6—C7	1.427 (5)	C31—H31B	0.9700
C6—H6	0.9300	C32—C34	1.524 (4)
C7—C8	1.401 (5)	C32—C33	1.536 (3)
C7—C11	1.414 (3)	C32—H32A	0.9800
C8—C9	1.356 (5)	C33—H33A	0.9700
C8—H8	0.9300	C33—H33B	0.9700
C9—C10	1.395 (4)	C34—H34A	0.9700
C9—H9	0.9300	C34—H34B	0.9700
C10—H10	0.9300	C35—H35A	0.9700
C11—C12	1.445 (4)	C35—H35B	0.9700
O1—Co1—O1w	89.16 (7)	C17—C18—H18	119.6
O1—Co1—N1	90.53 (8)	C19—C18—H18	119.6
O1w—Co1—N1	98.86 (9)	C23—C19—C20	117.3 (2)
O1—Co1—N2	163.25 (8)	C23—C19—C18	119.6 (2)

O1w—Co1—N2	91.39 (8)	C20—C19—C18	123.1 (2)
N1—Co1—N2	72.85 (8)	C21—C20—C19	119.7 (2)
O1—Co1—N3	105.30 (7)	C21—C20—H20	120.2
O1w—Co1—N3	92.71 (9)	C19—C20—H20	120.2
N1—Co1—N3	160.55 (8)	C20—C21—C22	119.1 (2)
N2—Co1—N3	91.39 (7)	C20—C21—H21	120.5
O1—Co1—N4	89.86 (7)	C22—C21—H21	120.5
O1w—Co1—N4	164.05 (9)	N4—C22—C21	123.3 (2)
N1—Co1—N4	97.07 (7)	N4—C22—H22	118.3
N2—Co1—N4	94.11 (7)	C21—C22—H22	118.3
N3—Co1—N4	72.22 (7)	N4—C23—C19	122.8 (2)
C25—O1—Co1	130.01 (15)	N4—C23—C24	117.70 (19)
Co1—O1w—H1w1	109.6	C19—C23—C24	119.5 (2)
Co1—O1w—H1w2	109.5	N3—C24—C16	123.2 (2)
H1w1—O1w—H1w2	109.4	N3—C24—C23	117.56 (19)
H2w1—O2w—H2w2	108.6	C16—C24—C23	119.2 (2)
H3w1—O3w—H3w2	107.0	O2—C25—O1	124.1 (2)
H4w1—O4w—H4w2	108.0	O2—C25—C26	118.2 (2)
H5w1—O5w—H5w2	106.2	O1—C25—C26	117.65 (19)
C1—N1—C12	118.0 (2)	C25—C26—C33	112.78 (17)
C1—N1—Co1	126.02 (19)	C25—C26—C35	110.93 (17)
C12—N1—Co1	115.71 (16)	C33—C26—C35	108.73 (17)
C10—N2—C11	117.8 (2)	C25—C26—C27	106.81 (18)
C10—N2—Co1	126.68 (18)	C33—C26—C27	108.89 (19)
C11—N2—Co1	115.51 (16)	C35—C26—C27	108.59 (18)
C13—N3—C24	117.5 (2)	C28—C27—C26	110.27 (19)
C13—N3—Co1	126.11 (17)	C28—C27—H27A	109.6
C24—N3—Co1	116.30 (14)	C26—C27—H27A	109.6
C22—N4—C23	117.8 (2)	C28—C27—H27B	109.6
C22—N4—Co1	126.09 (16)	C26—C27—H27B	109.6
C23—N4—Co1	116.12 (14)	H27A—C27—H27B	108.1
N1—C1—C2	123.0 (3)	C29—C28—C27	109.4 (2)
N1—C1—H1	118.5	C29—C28—C34	110.0 (2)
C2—C1—H1	118.5	C27—C28—C34	109.1 (2)
C3—C2—C1	119.2 (3)	C29—C28—H28A	109.4
C3—C2—H2	120.4	C27—C28—H28A	109.4
C1—C2—H2	120.4	C34—C28—H28A	109.4
C2—C3—C4	120.0 (3)	C28—C29—C30	110.18 (18)
C2—C3—H3	120.0	C28—C29—H29A	109.6
C4—C3—H3	120.0	C30—C29—H29A	109.6
C12—C4—C3	117.0 (3)	C28—C29—H29B	109.6
C12—C4—C5	119.4 (3)	C30—C29—H29B	109.6
C3—C4—C5	123.7 (3)	H29A—C29—H29B	108.1
C6—C5—C4	121.3 (3)	C29—C30—C31	108.37 (19)
C6—C5—H5	119.4	C29—C30—C35	109.55 (18)
C4—C5—H5	119.4	C31—C30—C35	108.49 (17)
C5—C6—C7	121.3 (3)	C29—C30—C36	111.84 (19)
C5—C6—H6	119.4	C31—C30—C36	109.32 (18)
C7—C6—H6	119.4	C35—C30—C36	109.21 (18)

C8—C7—C11	117.1 (3)	C32—C31—C30	110.08 (18)
C8—C7—C6	123.6 (3)	C32—C31—H31A	109.6
C11—C7—C6	119.3 (3)	C30—C31—H31A	109.6
C9—C8—C7	120.2 (3)	C32—C31—H31B	109.6
C9—C8—H8	119.9	C30—C31—H31B	109.6
C7—C8—H8	119.9	H31A—C31—H31B	108.2
C8—C9—C10	118.9 (3)	C34—C32—C31	110.0 (2)
C8—C9—H9	120.6	C34—C32—C33	109.7 (2)
C10—C9—H9	120.6	C31—C32—C33	109.38 (18)
N2—C10—C9	123.3 (3)	C34—C32—H32A	109.2
N2—C10—H10	118.3	C31—C32—H32A	109.2
C9—C10—H10	118.3	C33—C32—H32A	109.2
N2—C11—C7	122.6 (3)	C26—C33—C32	109.86 (17)
N2—C11—C12	118.1 (2)	C26—C33—H33A	109.7
C7—C11—C12	119.3 (2)	C32—C33—H33A	109.7
N1—C12—C4	122.9 (3)	C26—C33—H33B	109.7
N1—C12—C11	117.7 (2)	C32—C33—H33B	109.7
C4—C12—C11	119.4 (2)	H33A—C33—H33B	108.2
N3—C13—C14	122.9 (3)	C32—C34—C28	109.04 (19)
N3—C13—H13	118.6	C32—C34—H34A	109.9
C14—C13—H13	118.6	C28—C34—H34A	109.9
C15—C14—C13	119.8 (2)	C32—C34—H34B	109.9
C15—C14—H14	120.1	C28—C34—H34B	109.9
C13—C14—H14	120.1	H34A—C34—H34B	108.3
C14—C15—C16	119.5 (2)	C26—C35—C30	110.72 (17)
C14—C15—H15	120.2	C26—C35—H35A	109.5
C16—C15—H15	120.2	C30—C35—H35A	109.5
C24—C16—C15	117.1 (2)	C26—C35—H35B	109.5
C24—C16—C17	119.7 (2)	C30—C35—H35B	109.5
C15—C16—C17	123.1 (2)	H35A—C35—H35B	108.1
C18—C17—C16	121.1 (2)	O3—C36—O4	124.0 (2)
C18—C17—H17	119.4	O3—C36—C30	118.1 (2)
C16—C17—H17	119.4	O4—C36—C30	118.0 (2)
C17—C18—C19	120.9 (2)		
O1w—Co1—O1—C25	−14.0 (2)	C24—N3—C13—C14	1.4 (4)
N1—Co1—O1—C25	84.9 (2)	Co1—N3—C13—C14	−174.56 (19)
N2—Co1—O1—C25	78.1 (3)	N3—C13—C14—C15	−0.4 (4)
N3—Co1—O1—C25	−106.5 (2)	C13—C14—C15—C16	−0.9 (4)
N4—Co1—O1—C25	−178.0 (2)	C14—C15—C16—C24	1.1 (4)
O1—Co1—N1—C1	−1.6 (2)	C14—C15—C16—C17	−179.5 (2)
O1w—Co1—N1—C1	87.7 (2)	C24—C16—C17—C18	−0.8 (4)
N2—Co1—N1—C1	176.4 (2)	C15—C16—C17—C18	179.9 (3)
N3—Co1—N1—C1	−146.5 (2)	C16—C17—C18—C19	1.5 (4)
N4—Co1—N1—C1	−91.5 (2)	C17—C18—C19—C23	−0.6 (4)
O1—Co1—N1—C12	−174.87 (16)	C17—C18—C19—C20	178.2 (3)
O1w—Co1—N1—C12	−85.65 (17)	C23—C19—C20—C21	0.6 (4)
N2—Co1—N1—C12	3.07 (16)	C18—C19—C20—C21	−178.2 (2)
N3—Co1—N1—C12	40.2 (3)	C19—C20—C21—C22	0.6 (4)
N4—Co1—N1—C12	95.21 (16)	C23—N4—C22—C21	0.7 (3)

O1—Co1—N2—C10	−172.9 (2)	Co1—N4—C22—C21	179.00 (18)
O1w—Co1—N2—C10	−81.2 (2)	C20—C21—C22—N4	−1.3 (4)
N1—Co1—N2—C10	179.9 (2)	C22—N4—C23—C19	0.6 (3)
N3—Co1—N2—C10	11.5 (2)	Co1—N4—C23—C19	−177.88 (16)
N4—Co1—N2—C10	83.8 (2)	C22—N4—C23—C24	179.4 (2)
O1—Co1—N2—C11	6.0 (3)	Co1—N4—C23—C24	0.9 (2)
O1w—Co1—N2—C11	97.68 (17)	C20—C19—C23—N4	−1.2 (3)
N1—Co1—N2—C11	−1.17 (16)	C18—C19—C23—N4	177.6 (2)
N3—Co1—N2—C11	−169.58 (17)	C20—C19—C23—C24	−180.0 (2)
N4—Co1—N2—C11	−97.31 (16)	C18—C19—C23—C24	−1.1 (3)
O1—Co1—N3—C13	94.0 (2)	C13—N3—C24—C16	−1.1 (3)
O1w—Co1—N3—C13	4.1 (2)	Co1—N3—C24—C16	175.24 (17)
N1—Co1—N3—C13	−122.6 (3)	C13—N3—C24—C23	−179.7 (2)
N2—Co1—N3—C13	−87.4 (2)	Co1—N3—C24—C23	−3.4 (2)
N4—Co1—N3—C13	178.8 (2)	C15—C16—C24—N3	−0.1 (3)
O1—Co1—N3—C24	−82.01 (16)	C17—C16—C24—N3	−179.5 (2)
O1w—Co1—N3—C24	−171.88 (16)	C15—C16—C24—C23	178.5 (2)
N1—Co1—N3—C24	61.5 (3)	C17—C16—C24—C23	−0.9 (3)
N2—Co1—N3—C24	96.67 (16)	N4—C23—C24—N3	1.7 (3)
N4—Co1—N3—C24	2.80 (15)	C19—C23—C24—N3	−179.50 (19)
O1—Co1—N4—C22	−74.12 (19)	N4—C23—C24—C16	−176.99 (19)
O1w—Co1—N4—C22	−160.5 (2)	C19—C23—C24—C16	1.8 (3)
N1—Co1—N4—C22	16.4 (2)	Co1—O1—C25—O2	15.9 (4)
N2—Co1—N4—C22	89.59 (19)	Co1—O1—C25—C26	−167.12 (15)
N3—Co1—N4—C22	179.7 (2)	O2—C25—C26—C33	−160.6 (3)
O1—Co1—N4—C23	104.25 (15)	O1—C25—C26—C33	22.3 (3)
O1w—Co1—N4—C23	17.8 (3)	O2—C25—C26—C35	−38.4 (3)
N1—Co1—N4—C23	−165.24 (15)	O1—C25—C26—C35	144.5 (2)
N2—Co1—N4—C23	−92.03 (15)	O2—C25—C26—C27	79.8 (3)
N3—Co1—N4—C23	−1.89 (14)	O1—C25—C26—C27	−97.3 (2)
C12—N1—C1—C2	0.4 (4)	C25—C26—C27—C28	−179.01 (19)
Co1—N1—C1—C2	−172.8 (2)	C33—C26—C27—C28	58.9 (2)
N1—C1—C2—C3	−0.6 (4)	C35—C26—C27—C28	−59.3 (2)
C1—C2—C3—C4	0.0 (4)	C26—C27—C28—C29	60.2 (3)
C2—C3—C4—C12	0.7 (4)	C26—C27—C28—C34	−60.2 (3)
C2—C3—C4—C5	−179.9 (3)	C27—C28—C29—C30	−59.8 (3)
C12—C4—C5—C6	−0.9 (4)	C34—C28—C29—C30	60.1 (2)
C3—C4—C5—C6	179.8 (3)	C28—C29—C30—C31	−59.4 (2)
C4—C5—C6—C7	1.5 (4)	C28—C29—C30—C35	58.7 (2)
C5—C6—C7—C8	178.5 (3)	C28—C29—C30—C36	179.98 (19)
C5—C6—C7—C11	0.3 (4)	C29—C30—C31—C32	59.5 (2)
C11—C7—C8—C9	3.0 (4)	C35—C30—C31—C32	−59.3 (2)
C6—C7—C8—C9	−175.3 (3)	C36—C30—C31—C32	−178.34 (19)
C7—C8—C9—C10	−0.9 (4)	C30—C31—C32—C34	−60.3 (2)
C11—N2—C10—C9	2.6 (4)	C30—C31—C32—C33	60.2 (2)
Co1—N2—C10—C9	−178.6 (2)	C25—C26—C33—C32	−176.82 (19)
C8—C9—C10—N2	−2.1 (4)	C35—C26—C33—C32	59.7 (2)
C10—N2—C11—C7	−0.2 (3)	C27—C26—C33—C32	−58.4 (2)
Co1—N2—C11—C7	−179.19 (18)	C34—C32—C33—C26	60.4 (2)

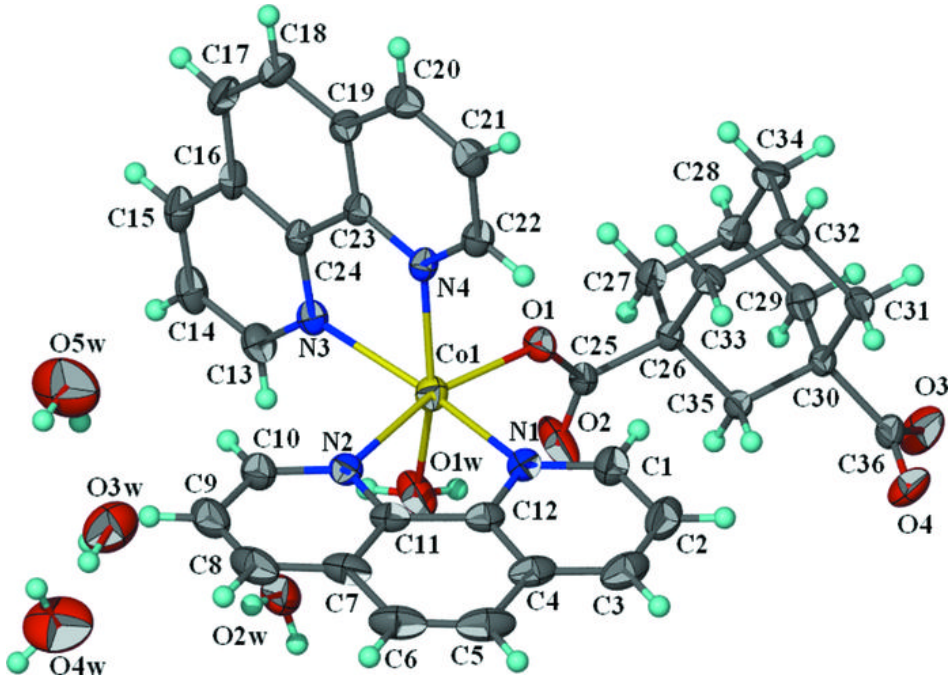
C10—N2—C11—C12	178.2 (2)	C31—C32—C33—C26	−60.4 (2)
Co1—N2—C11—C12	−0.8 (3)	C31—C32—C34—C28	59.3 (2)
C8—C7—C11—N2	−2.5 (4)	C33—C32—C34—C28	−61.0 (2)
C6—C7—C11—N2	175.8 (2)	C29—C28—C34—C32	−59.2 (2)
C8—C7—C11—C12	179.1 (2)	C27—C28—C34—C32	60.9 (3)
C6—C7—C11—C12	−2.6 (4)	C25—C26—C35—C30	175.56 (18)
C1—N1—C12—C4	0.4 (3)	C33—C26—C35—C30	−59.9 (2)
Co1—N1—C12—C4	174.31 (18)	C27—C26—C35—C30	58.5 (2)
C1—N1—C12—C11	−178.5 (2)	C29—C30—C35—C26	−58.7 (2)
Co1—N1—C12—C11	−4.6 (3)	C31—C30—C35—C26	59.5 (2)
C3—C4—C12—N1	−1.0 (4)	C36—C30—C35—C26	178.53 (18)
C5—C4—C12—N1	179.6 (2)	C29—C30—C36—O3	3.6 (3)
C3—C4—C12—C11	177.9 (2)	C31—C30—C36—O3	−116.4 (3)
C5—C4—C12—C11	−1.5 (3)	C35—C30—C36—O3	125.0 (2)
N2—C11—C12—N1	3.6 (3)	C29—C30—C36—O4	−176.1 (2)
C7—C11—C12—N1	−177.9 (2)	C31—C30—C36—O4	63.9 (3)
N2—C11—C12—C4	−175.3 (2)	C35—C30—C36—O4	−54.6 (3)
C7—C11—C12—C4	3.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w1···O2	0.85	1.82	2.599 (3)	152
O1w—H1w2···O2w	0.85	2.10	2.656 (3)	122
O2w—H2w1···O4^{i}	0.86	1.86	2.712 (3)	176
O2w—H2w2···O4w^{ii}	0.86	2.37	3.113 (5)	145
O3w—H3w1···O4^{iii}	0.86	2.06	2.895 (4)	164
O3w—H3w2···O4w	0.86	2.08	2.913 (5)	164
O4w—H4w1···O3^{iv}	0.85	1.84	2.695 (3)	178
O5w—H5w1···O3^{iv}	0.86	1.96	2.814 (4)	173
O5w—H5w2···O3w	0.86	2.36	3.211 (5)	174

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) *x*, *y*−1, *z*; (iv) *x*+1, *y*−1, *z*.

Fig. 1


C18
C17
C20
C19
C21
C16
C15
C22
C23
C24
N4
C14
N3
Co1
O1
C25
C13
C26
C27
C28
C34
C32
C29
C31
C33
C35
C30
O3
O5w
C10
N2
N1
O2
C1
C36
O4
O3w
C9
O1w
C12
C11
C2
C8
C7
C4
C3
O2w
C6
C5
O4w