Diaquabis[4-(dimethylamino)pyridine-κN^1]bis[2-(1,3-dioxo-2,3-dihydro-1H-isoindol-2-yl)acetato-κO^1]cobalt(II)

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In the mononuclear title complex, [Co($C_{10}H_6NO_4$)$_2$($C_7H_{10}N_2$)$_2$(H_2O)$_2$], the Co^{II} ion is located on an inversion centre and has a distorted octahedral coordination geometry of type CoN$_2$O$_4$ by two N atoms from the two 4-(dimethylamino)-pyridine (DMAP) ligands, two carboxylate O atoms from the two deprotonated N-phthaloylglycine (Nphgly) ligands [systematic name: 2-(1,3-dioxo-2,3-di-hydro-1H-isoindol-2-yl)acetate] and two coordination water molecules. In the crystal, O—H⋯O, C—H⋯O hydrogen bonds and π–π stacking interactions link the molecules into the supramolecular structure.

3D view

Chemical scheme
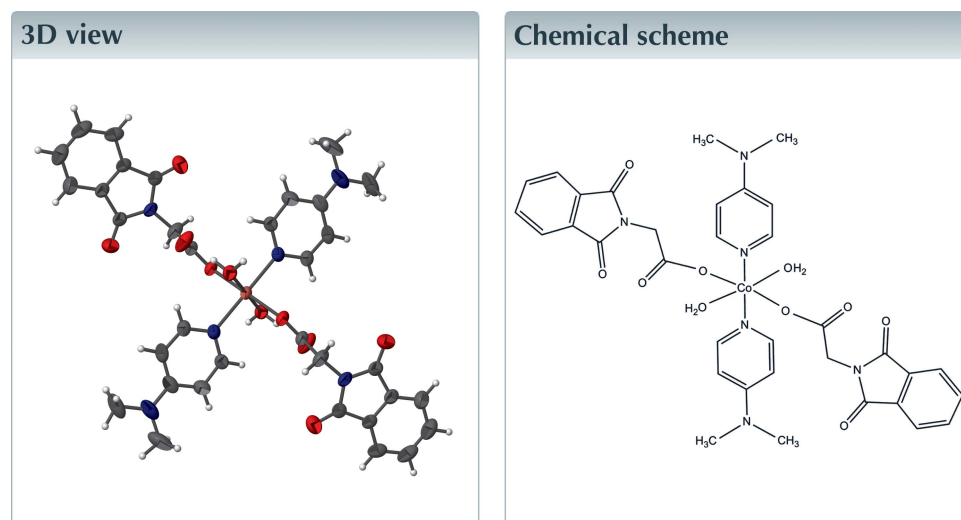
Structure description

Paramagnetic materials and extended structures based on transition metals have found wide applications in molecular magnetism (Pavlishchuk *et al.*, 2010, 2011; Moroz *et al.*, 2012). The Lewis base 4-dimethylaminopyridine (DMAP), a derivative of pyridine, finds use as a homogeneous catalyst in cellulose acylation for the synthesis of biodegradable plastics (Satgé *et al.*, 2004). DMAP is also known to form transition-metal complexes which exhibit luminescence properties (Araki *et al.*, 2005; Liu *et al.*, 2015). The possibility of combining the DMAP ligand with a wide variety of co-ligands leads to an extensive variety of coordination modes. We report here the synthesis and crystal structure of a cobalt(II) complex with 4-(dimethylamino)pyridine and N-phthaloylglycine.

In the title complex, the cobalt(II) ion is located on an inversion center. The complex comprises two deprotonated *N*-phthaloylglycine ligands in a monodentate coordination
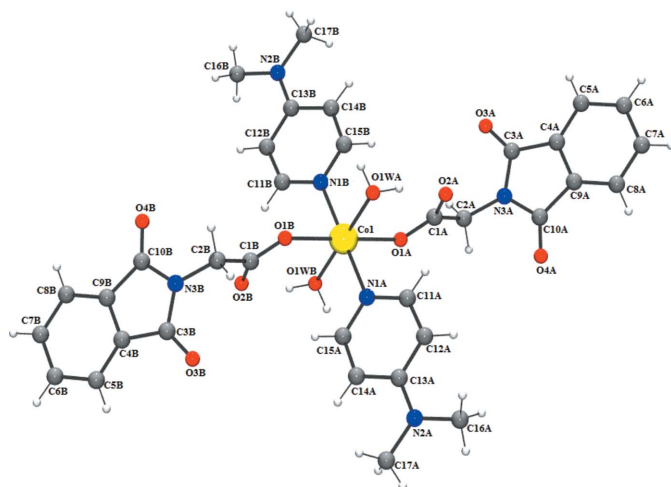
Table 1
Hydrogen-bond geometry (Å, °).

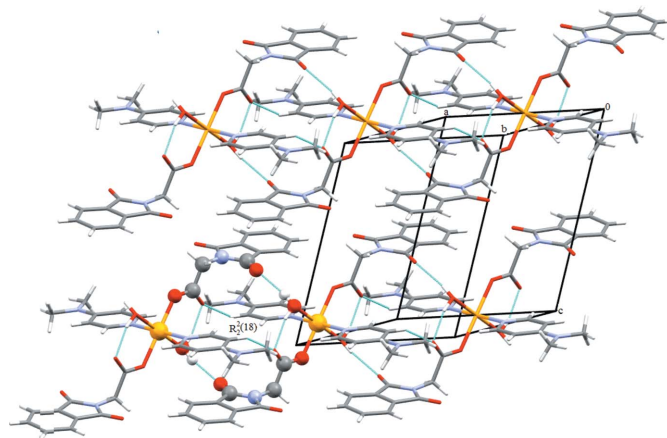| D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1W—H11W⋯O2A	0.86 (1)	1.83 (1)	2.648 (2)	158 (2)
O1W—H21W⋯O3A^i	0.85 (1)	2.02 (1)	2.853 (2)	168 (2)
C14A—H14A⋯O2A^{ii}	0.93	2.40	3.160 (3)	139

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

mode and two 4-(dimethylamino)pyridine ligands. The slightly distorted coordination sphere CoN₂O₄ coordination sphere is completed by two aqua ligands (Fig. 1). The four oxygen atoms occupy the equatorial plane of the complex in a *trans* configuration and the DMAP ligands are coordinated through their N atoms in the axial positions. The Co—N bond length of 2.1293 (16) Å is in agreement with those retrieved from literature (Guenifa *et al.*, 2013). The DMAP ligands are planar. The Co—O bond length of the Nphgly ligand is 2.0984 (13) Å and is shorter than that of the terminal aqua ligand of 2.1533 (14) Å. This is expected and is in agreement with bond lengths reported in the related structure of [Co(C₅HF₆O₂)₂(H₂O)₂]·2H₂O (Tominaga & Mochida, 2017). The dihedral angles formed between the mean planes through the four O atoms and the DMAP ring is 89.79 (1)°. Intramolecular O—H⋯O hydrogen bonding is observed between the carboxylate oxygen atoms and the coordinating water molecules, generating an $S(6)$ ring motif.

The complex cations are connected *via* C—H⋯O and O—H⋯O hydrogen bonds into infinite chains parallel to [100] (Fig. 2, Table 1). The O—H⋯O hydrogen bonds generate $R_2^2(18)$ motifs (Fig. 2). There are face-to-face π–π interactions between the benzene ring of the Nphgly ligand and the pyridine ring [$Cg3⋯Cg2(-1 + x, y, z) = 3.735$ (7) Å; $Cg2$ and $Cg3$ are the centroids of the NA1/CA11–CA15 and C4A–CA9 rings, respectively] (Fig. 3). This combination of hydrogen

Figure 2
Partial view of the crystal structure of the title compound showing the formation of $R_2^2(18)$ rings. The C—H⋯O and O—H⋯O hydrogen bonds are shown as dashed lines.

bonds and stacking interactions builds a three-dimensional network structure.

Synthesis and crystallization

CoCl₂·6H₂O (0.237 g, 1 mmol) was dissolved in an ethanol solution (20 ml). 4-(Dimethylamino)-pyridine (0.122 g, 1 mmol) was added to this solution and the mixture was stirred for 15 min to obtain a blue solution. Then *N*-phthaloylglycine (0.205 g, 1 mmol) was added and the mixture was stirred for additional 20 min. Single crystals suitable for X-ray diffraction were obtained from a methanol solution of the title complex by slow evaporation.

Figure 1
The molecular structure of the title compound with displacement spheres drawn at the 30% probability level. H atoms are shown as spheres of arbitrary radius.
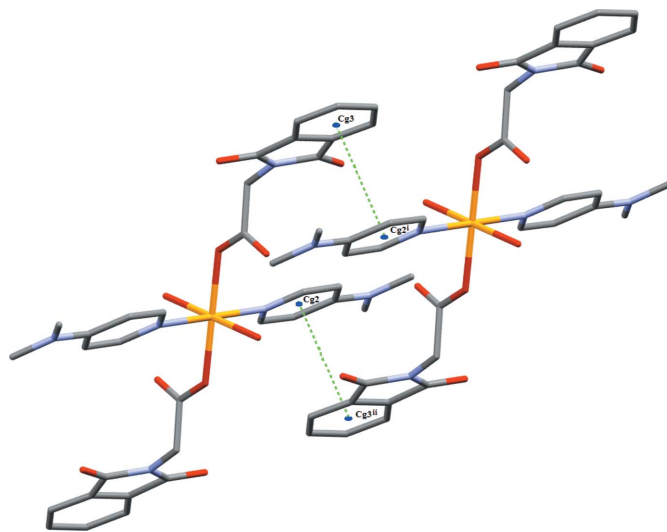

Figure 3
π–π interactions (dashed lines) between the 4-(dimethylamino)pyridine and benzene rings of *N*-phthaloylglycine in the title compound [symmetry codes: (i) = $-1 + x, y, z$; (ii) = $1 + x, y, z$].

Table 2
Experimental details.

Crystal data	
Chemical formula	[Co(C$_{10}$H$_6$NO$_4$)$_2$(C$_7$H$_{10}$N$_2$)$_2$-(H$_2$O)$_2$]
M_r	747.62
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	8.6830 (9), 10.2560 (11), 11.2980 (12)
α, β, γ (°)	83.547 (3), 72.194 (3), 68.901 (3)
V (Å^3)	893.70 (17)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.54
Crystal size (mm)	0.10 × 0.09 × 0.08
Data collection	
Diffractometer	Bruker APEXII QUAZAR CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.950, 0.970
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22559, 4629, 3658
R_{int}	0.060
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.677
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.114, 1.05
No. of reflections	4629
No. of parameters	238
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å^{-3})	0.32, −0.23

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *POVRay* (Persistence of Vision Team, 2004).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

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Crystal data

$[Co(C_{10}H_6NO_4)_2(C_7H_{10}N_2)_2(H_2O)_2]$	$Z = 1$
$M_r = 747.62$	$F(000) = 389$
Triclinic, $P\overline{1}$	$D_x = 1.389$ Mg m^{-3}
$a = 8.6830 (9)$ Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 10.2560 (11)$ Å	Cell parameters from 2690 reflections
$c = 11.2980 (12)$ Å	$\theta = 1.9–28.8°$
$\alpha = 83.547 (3)°$	$\mu = 0.54$ mm^{-1}
$\beta = 72.194 (3)°$	$T = 293$ K
$\gamma = 68.901 (3)°$	Prism, blue
$V = 893.70 (17)$ Å^3	$0.1 \times 0.09 \times 0.08$ mm

Data collection

Bruker APEXII QUAZAR CCD diffractometer	4629 independent reflections
Radiation source: ImuS	3658 reflections with $I > 2\sigma(I)$
f\ and ω scans	$R_{int} = 0.060$
Absorption correction: multi-scan (SADABS; Bruker, 2004)	$\theta_{max} = 28.8°$, $\theta_{min} = 1.9°$
$T_{min} = 0.950$, $T_{max} = 0.970$	$h = -11 \rightarrow 11$
22559 measured reflections	$k = -13 \rightarrow 13$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.040$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.114$	$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 0.3707P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
4629 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
238 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
3 restraints	
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
Co1	0.5000	1.0000	1.0000	0.03061 (12)
O1A	0.45480 (17)	0.99688 (14)	0.82838 (12)	0.0374 (3)
O1W	0.24026 (17)	1.13925 (15)	1.07614 (13)	0.0390 (3)
H11W	0.195 (3)	1.152 (3)	1.0160 (14)	0.059*
H21W	0.176 (3)	1.113 (3)	1.1393 (13)	0.059*
N1A	0.5758 (2)	1.17785 (17)	0.93996 (15)	0.0369 (4)
N3A	0.1690 (2)	1.0721 (2)	0.63725 (15)	0.0414 (4)
O2A	0.1816 (2)	1.1375 (2)	0.85983 (15)	0.0614 (5)
C3A	0.0278 (3)	1.0292 (2)	0.66807 (18)	0.0392 (4)
O3A	0.0192 (2)	0.92469 (18)	0.72650 (16)	0.0568 (4)
C4A	−0.1014 (2)	1.1350 (2)	0.61425 (18)	0.0382 (4)
C9A	−0.0343 (3)	1.2380 (2)	0.55858 (19)	0.0413 (5)
O4A	0.2396 (2)	1.2623 (2)	0.54431 (19)	0.0698 (5)
C15A	0.7243 (3)	1.1837 (2)	0.9467 (2)	0.0398 (4)
H15A	0.7944	1.1068	0.9803	0.048*
C1A	0.3167 (2)	1.0511 (2)	0.79943 (17)	0.0360 (4)
C10A	0.1395 (3)	1.2001 (2)	0.57571 (19)	0.0445 (5)
C13A	0.6808 (3)	1.4125 (2)	0.85706 (19)	0.0446 (5)
C5A	−0.2617 (3)	1.1408 (3)	0.6127 (2)	0.0505 (6)
H5A	−0.3076	1.0725	0.6510	0.061*
C2A	0.3226 (3)	1.0008 (3)	0.6763 (2)	0.0486 (5)
H2A1	0.4207	1.0130	0.6126	0.058*
H2A2	0.3406	0.9016	0.6828	0.058*
C11A	0.4790 (3)	1.2922 (2)	0.8915 (2)	0.0422 (5)
H11A	0.3746	1.2926	0.8852	0.051*
C6A	−0.3516 (3)	1.2532 (3)	0.5512 (3)	0.0628 (7)
H6A	−0.4598	1.2600	0.5476	0.075*
C14A	0.7810 (3)	1.2935 (2)	0.9083 (2)	0.0462 (5)
H14A	0.8862	1.2895	0.9161	0.055*
N2A	0.7346 (3)	1.5225 (2)	0.8160 (2)	0.0621 (6)
C12A	0.5239 (3)	1.4080 (2)	0.8508 (2)	0.0473 (5)
H12A	0.4501	1.4839	0.8189	0.057*
C8A	−0.1236 (3)	1.3495 (3)	0.4985 (2)	0.0576 (6)
H8A	−0.0784	1.4187	0.4614	0.069*
C7A	−0.2841 (3)	1.3549 (3)	0.4955 (3)	0.0665 (7)

H7A	−0.3476	1.4288	0.4549	0.080*
C17A	0.8965 (4)	1.5217 (3)	0.8262 (3)	0.0851 (10)
H17A	0.9144	1.6070	0.7923	0.128*
H17B	0.9885	1.4437	0.7809	0.128*
H17C	0.8944	1.5138	0.9121	0.128*
C16A	0.6279 (5)	1.6452 (3)	0.7642 (3)	0.0781 (9)
H16A	0.6856	1.7122	0.7397	0.117*
H16B	0.5198	1.6858	0.8257	0.117*
H16C	0.6076	1.6186	0.6931	0.117*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03132 (19)	0.03084 (19)	0.02919 (19)	−0.00865 (14)	−0.01154 (14)	0.00303 (13)
O1A	0.0352 (7)	0.0442 (8)	0.0327 (7)	−0.0094 (6)	−0.0153 (6)	0.0023 (6)
O1W	0.0374 (7)	0.0412 (8)	0.0356 (7)	−0.0113 (6)	−0.0099 (6)	0.0015 (6)
N1A	0.0391 (9)	0.0342 (8)	0.0355 (9)	−0.0106 (7)	−0.0113 (7)	0.0027 (7)
N3A	0.0377 (9)	0.0592 (11)	0.0321 (9)	−0.0177 (8)	−0.0166 (7)	0.0031 (8)
O2A	0.0413 (9)	0.0829 (12)	0.0446 (9)	0.0075 (8)	−0.0197 (7)	−0.0162 (8)
C3A	0.0415 (10)	0.0486 (11)	0.0269 (9)	−0.0165 (9)	−0.0067 (8)	−0.0030 (8)
O3A	0.0597 (10)	0.0536 (10)	0.0508 (10)	−0.0212 (8)	−0.0081 (8)	0.0090 (8)
C4A	0.0353 (10)	0.0508 (12)	0.0287 (9)	−0.0143 (9)	−0.0077 (8)	−0.0069 (8)
C9A	0.0408 (11)	0.0518 (12)	0.0333 (10)	−0.0160 (9)	−0.0137 (8)	0.0004 (9)
O4A	0.0642 (11)	0.0924 (14)	0.0743 (13)	−0.0521 (11)	−0.0290 (10)	0.0267 (11)
C15A	0.0382 (10)	0.0334 (10)	0.0438 (11)	−0.0092 (8)	−0.0105 (9)	0.0008 (8)
C1A	0.0334 (9)	0.0418 (10)	0.0308 (10)	−0.0093 (8)	−0.0117 (8)	0.0026 (8)
C10A	0.0456 (12)	0.0620 (14)	0.0334 (10)	−0.0264 (10)	−0.0149 (9)	0.0069 (9)
C13A	0.0542 (13)	0.0338 (10)	0.0352 (11)	−0.0148 (9)	0.0036 (9)	−0.0065 (8)
C5A	0.0376 (11)	0.0687 (15)	0.0472 (13)	−0.0214 (10)	−0.0056 (9)	−0.0155 (11)
C2A	0.0405 (11)	0.0639 (14)	0.0393 (11)	−0.0081 (10)	−0.0187 (9)	−0.0050 (10)
C11A	0.0429 (11)	0.0392 (10)	0.0413 (11)	−0.0100 (9)	−0.0138 (9)	0.0039 (8)
C6A	0.0345 (12)	0.090 (2)	0.0603 (16)	−0.0078 (12)	−0.0171 (11)	−0.0200 (14)
C14A	0.0395 (11)	0.0405 (11)	0.0548 (13)	−0.0141 (9)	−0.0059 (10)	−0.0063 (9)
N2A	0.0835 (16)	0.0378 (10)	0.0592 (13)	−0.0285 (10)	−0.0027 (11)	−0.0004 (9)
C12A	0.0577 (13)	0.0324 (10)	0.0412 (12)	−0.0062 (9)	−0.0120 (10)	0.0037 (8)
C8A	0.0572 (14)	0.0620 (15)	0.0525 (14)	−0.0174 (12)	−0.0219 (12)	0.0113 (11)
C7A	0.0504 (14)	0.0755 (18)	0.0601 (16)	0.0012 (13)	−0.0250 (12)	0.0009 (14)
C17A	0.086 (2)	0.0629 (18)	0.104 (3)	−0.0485 (17)	0.0064 (19)	−0.0085 (17)
C16A	0.120 (3)	0.0393 (13)	0.0609 (17)	−0.0300 (15)	−0.0058 (17)	0.0068 (12)

Geometric parameters (Å, °)

Co1—O1A	2.0984 (13)	C13A—N2A	1.354 (3)
Co1—O1A^i	2.0984 (13)	C13A—C14A	1.402 (3)
Co1—N1A	2.1293 (16)	C13A—C12A	1.404 (3)
Co1—N1A^i	2.1293 (16)	C5A—C6A	1.387 (4)
Co1—O1W^i	2.1533 (14)	C5A—H5A	0.9300
Co1—O1W	2.1533 (14)	C2A—H2A1	0.9700

O1A—C1A	1.254 (2)	C2A—H2A2	0.9700
O1W—H11W	0.859 (9)	C11A—C12A	1.369 (3)
O1W—H21W	0.848 (9)	C11A—H11A	0.9300
N1A—C15A	1.337 (3)	C6A—C7A	1.376 (4)
N1A—C11A	1.345 (2)	C6A—H6A	0.9300
N3A—C3A	1.383 (3)	C14A—H14A	0.9300
N3A—C10A	1.391 (3)	N2A—C17A	1.442 (4)
N3A—C2A	1.447 (3)	N2A—C16A	1.452 (4)
O2A—C1A	1.235 (2)	C12A—H12A	0.9300
C3A—O3A	1.208 (3)	C8A—C7A	1.385 (4)
C3A—C4A	1.482 (3)	C8A—H8A	0.9300
C4A—C5A	1.377 (3)	C7A—H7A	0.9300
C4A—C9A	1.386 (3)	C17A—H17A	0.9600
C9A—C8A	1.371 (3)	C17A—H17B	0.9600
C9A—C10A	1.485 (3)	C17A—H17C	0.9600
O4A—C10A	1.203 (3)	C16A—H16A	0.9600
C15A—C14A	1.363 (3)	C16A—H16B	0.9600
C15A—H15A	0.9300	C16A—H16C	0.9600
C1A—C2A	1.518 (3)		
O1A—Co1—O1A^i	180.0	N2A—C13A—C12A	123.2 (2)
O1A—Co1—N1A	89.62 (6)	C14A—C13A—C12A	115.20 (19)
O1A^i—Co1—N1A	90.38 (6)	C4A—C5A—C6A	117.0 (2)
O1A—Co1—N1A^i	90.38 (6)	C4A—C5A—H5A	121.5
O1A^i—Co1—N1A^i	89.62 (6)	C6A—C5A—H5A	121.5
N1A—Co1—N1A^i	180.0	N3A—C2A—C1A	114.20 (18)
O1A—Co1—O1W^i	88.93 (5)	N3A—C2A—H2A1	108.7
O1A^i—Co1—O1W^i	91.07 (5)	C1A—C2A—H2A1	108.7
N1A—Co1—O1W^i	91.28 (6)	N3A—C2A—H2A2	108.7
N1A^i—Co1—O1W^i	88.72 (6)	C1A—C2A—H2A2	108.7
O1A—Co1—O1W	91.07 (5)	H2A1—C2A—H2A2	107.6
O1A^i—Co1—O1W	88.93 (5)	N1A—C11A—C12A	124.4 (2)
N1A—Co1—O1W	88.72 (6)	N1A—C11A—H11A	117.8
N1A^i—Co1—O1W	91.28 (6)	C12A—C11A—H11A	117.8
O1W^i—Co1—O1W	180.0	C7A—C6A—C5A	121.4 (2)
C1A—O1A—Co1	128.90 (13)	C7A—C6A—H6A	119.3
Co1—O1W—H11W	104.0 (17)	C5A—C6A—H6A	119.3
Co1—O1W—H21W	118.6 (17)	C15A—C14A—C13A	120.1 (2)
H11W—O1W—H21W	108.2 (14)	C15A—C14A—H14A	120.0
C15A—N1A—C11A	114.92 (18)	C13A—C14A—H14A	120.0
C15A—N1A—Co1	122.42 (13)	C13A—N2A—C17A	120.6 (2)
C11A—N1A—Co1	122.66 (14)	C13A—N2A—C16A	120.6 (3)
C3A—N3A—C10A	112.13 (17)	C17A—N2A—C16A	118.8 (2)
C3A—N3A—C2A	124.14 (19)	C11A—C12A—C13A	120.2 (2)
C10A—N3A—C2A	123.40 (19)	C11A—C12A—H12A	119.9
O3A—C3A—N3A	124.6 (2)	C13A—C12A—H12A	119.9
O3A—C3A—C4A	129.3 (2)	C9A—C8A—C7A	117.1 (3)
N3A—C3A—C4A	106.07 (17)	C9A—C8A—H8A	121.5

C5A—C4A—C9A	121.4 (2)	C7A—C8A—H8A	121.5
C5A—C4A—C3A	130.6 (2)	C6A—C7A—C8A	121.5 (2)
C9A—C4A—C3A	107.97 (17)	C6A—C7A—H7A	119.2
C8A—C9A—C4A	121.6 (2)	C8A—C7A—H7A	119.2
C8A—C9A—C10A	130.4 (2)	N2A—C17A—H17A	109.5
C4A—C9A—C10A	107.96 (18)	N2A—C17A—H17B	109.5
N1A—C15A—C14A	125.17 (19)	H17A—C17A—H17B	109.5
N1A—C15A—H15A	117.4	N2A—C17A—H17C	109.5
C14A—C15A—H15A	117.4	H17A—C17A—H17C	109.5
O2A—C1A—O1A	127.18 (18)	H17B—C17A—H17C	109.5
O2A—C1A—C2A	118.74 (17)	N2A—C16A—H16A	109.5
O1A—C1A—C2A	114.08 (17)	N2A—C16A—H16B	109.5
O4A—C10A—N3A	124.7 (2)	H16A—C16A—H16B	109.5
O4A—C10A—C9A	129.6 (2)	N2A—C16A—H16C	109.5
N3A—C10A—C9A	105.73 (17)	H16A—C16A—H16C	109.5
N2A—C13A—C14A	121.6 (2)	H16B—C16A—H16C	109.5

Symmetry code: (i) $-x+1, -y+2, -z+2$.

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1W—H11W⋯O2A	0.86 (1)	1.83 (1)	2.648 (2)	158 (2)
O1W—H21W⋯O3A[ii]	0.85 (1)	2.02 (1)	2.853 (2)	168 (2)
C14A—H14A⋯O2A[iii]	0.93	2.40	3.160 (3)	139

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