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ISSN 2414-3146

Di-μ-aqua-bis[aqua(2,2′-bipyridine)(4-nitrobenzoato)cobalt(II)] bis(4-nitrobenzoate)

Bikshandarkoil R. Srinivasan, Sarvesh S. Harmalkar, Luann R. D'Souza and Sunder N. Dhuri*

School of Chemical Sciences, Goa University, Goa 403206, India. *Correspondence e-mail: sndhuri@unigoa.ac.in

Received 27 May 2020
Accepted 13 June 2020

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

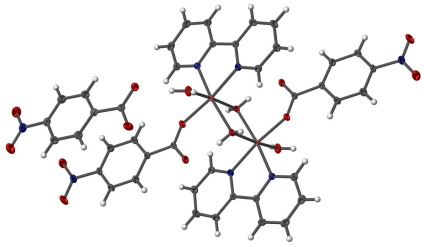
Keywords: crystal structure; bimetallic complex; divalent-metal 4-nitrobenzoate; hydrogen bonds.

CCDC reference: 2009578

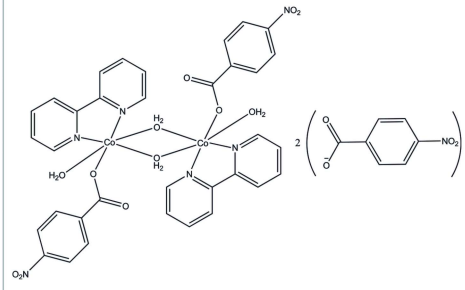
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Co_2(C_7H_4NO_4)_2(C_{10}H_8N_2)_2(H_2O)_4](C_7H_4NO_4)_2$, consists of a centrosymmetric bimetallic complex charge-balanced by free 4-nitrobenzoate anions. The Co^{II} ion exhibits a distorted *cis*-CoN_2O_4 octahedral coordination environment and the Co···Co separation is 3.326 (2) Å. In the crystal, the dications and anions are linked by O—H···O and C—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

As part of an ongoing research program we are investigating the structural aspects of mixed-ligand compounds of divalent-metal 4-nitrobenzoates. Recently we described the structure of $[Co(H_2O)_2(DMSO)_2(C_7H_4NO_4)](C_7H_4NO_4)$ **2** (DMSO = dimethylsulfoxide; $C_7H_4NO_4$ = 4-nitrobenzoate) containing a bidentate as well as a free 4-nitrobenzoate anion (Srinivasan *et al.*, 2020). Our attempts to replace the *cis*-aqua ligands of **2** with 2,2′-bipyridine has resulted in the isolation of the diaqua-bridged title dinuclear compound. The Cambridge Structural Database (CSD, version 5.40, update September 2019; Groom *et al.*, 2016) lists the structures of several cobalt 4-nitrobenzoates: of these, more than a dozen are mononuclear cobalt compounds (Srinivasan *et al.*, 2004, 2020; Chakravorty *et al.*, 2011) while only four dinuclear compounds of 4-nitrobenzoate are known to date (Singh *et al.*, 2007; Jung *et al.*, 2009; Yang *et al.*, 2011; Wang & Qi, 2014). The title compound is a new addition to the list of dimeric cobalt 4-nitrobenzoates.

The structure of the title compound, **1**, consists of a crystallographically unique cobaltous ion and a 2,2′-bipyridine molecule, two crystallographically independent 4-nitrobenzoate ions and two unique aqua ligands (one terminal, one bridging). The Co^{II} ion, one 4-nitrobenzoate ion, one 2,2′-bipyridine molecule and each of a terminal and bridging water molecule build up one half of a dimeric dicationic species

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2W—H2B···O5^{i}	0.84 (2)	1.67 (2)	2.5101 (13)	173 (2)
O2W—H2A···O3	0.79 (2)	1.88 (2)	2.6483 (13)	164 (2)
O1W—H1B···O3^{ii}	0.82 (2)	2.04 (2)	2.8477 (14)	174 (2)
O1W—H1A···O6^{iii}	0.81 (2)	1.88 (2)	2.6803 (14)	171 (2)
C21—H21···O2^{iv}	0.93	2.48	3.2219 (17)	137
C17—H17···O5^{i}	0.93	2.24	3.1679 (16)	172
C16—H16···O2^{v}	0.93	2.57	3.4644 (17)	160
C14—H14···O6^{vi}	0.93	2.41	3.3126 (16)	164
C9—H9···O7^{vii}	0.93	2.64	3.5467 (18)	164

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

$[Co_2(H_2O)_2(C_{10}H_8N_2)_2(C_7H_4NO_4)_2(\mu_2\text{-}H_2O)_2]^{2+}$, the other half being generated by inversion symmetry (Fig. 1). The crystallographic inversion centre is situated at the midpoint of the line connecting the Co^{II} atoms in the dimer. A charge-balancing 4-nitrobenzoate ion completes the structure.

In the centrosymmetric dimer, each Co^{II} ion exhibits a distorted octahedral environment and is bonded to a terminal aqua ligand, a monodentate 4-nitrobenzoate ligand disposed *cis* to the terminal aqua ligand and a bidentate 2,2′-bipyridine molecule. A pair of *cis*-aqua ligands bridges the metal centres

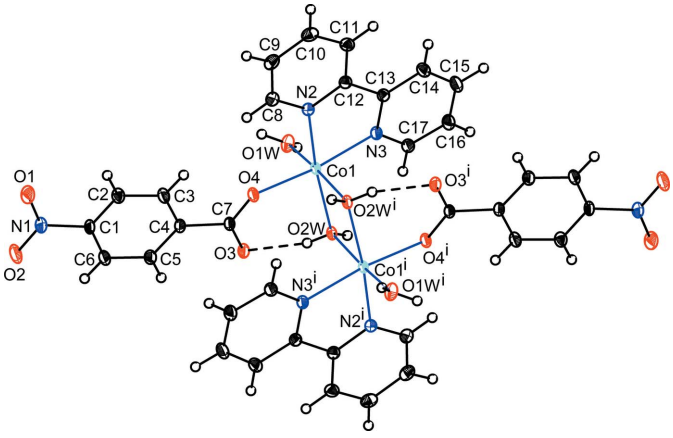


Figure 1
The dinuclear dication in **1** with displacement ellipsoids drawn at the 50% probability level. Intramolecular hydrogen bonds are shown as broken lines [Symmetry code: (i) $1-x, 1-y, 1-z$.]

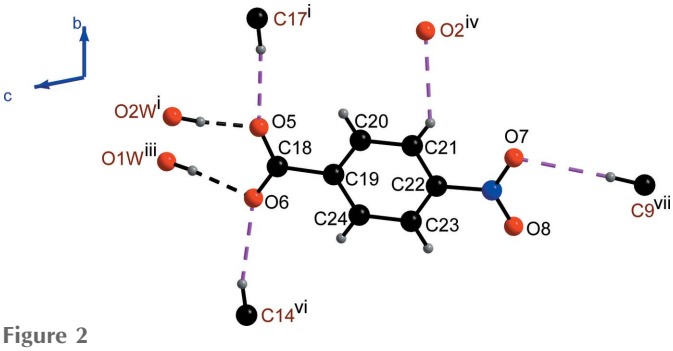


Figure 2
The hydrogen-bonding scheme around the 4-nitrobenzoate anion showing the O—H···O and C—H···O hydrogen bonds as dashed lines. For symmetry codes see Table 1.

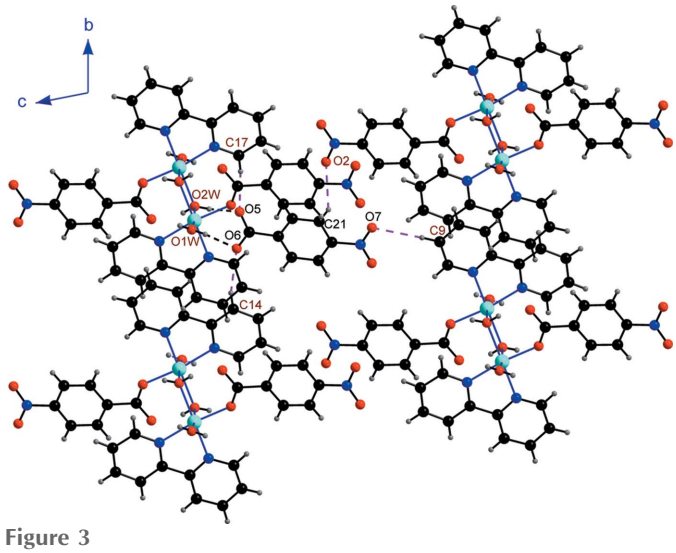


Figure 3
Environment of the anion, showing its hydrogen bonds to four symmetrically related dications *via* O—H···O and C—H···O bonds.

and completes the hexa-coordination around the metal ions resulting in a Co···Co($1-x$, $1-y$, $1-z$) separation of 3.326 (2) Å. It is interesting to note that in three of the four known dinuclear cobalt compounds (Singh *et al.*, 2007; Yang *et al.*, 2011; Wang & Qi, 2014), the 4-nitrobenzoate anion functions as a monodentate ligand as in the title compound. One example each of a dinuclear (Jung *et al.*, 2009) and a tetranuclear cobalt compound (Dimitrou *et al.*, 2001) is known where the 4-nitrobenzoate ion functions as a symmetric bridging ligand.

The geometric parameters of **1** are in their normal ranges and are in agreement with reported data (Srinivasan *et al.*, 2020). The Co—O$_w$ (w = water) bonds [2.0743 (10) and 2.1617 (9) Å] are elongated as compared to the Co—O$_c$ (c = carboxylate) distance, which is the shortest at 2.0494 (9) Å. The *cis*-O—Co—O and N—Co—N bond angles range between 77.97 (4) and 100.02 (4)°, while the *trans* bond angles deviate from ideal values, indicating a distortion of the {CoN$_2$O$_4$} octahedron.

All of the H atoms attached to the aqua ligands, and five of the other H atoms *viz.* H9, H14, H16, H17 and H21 bonded to C9, C14, C16, C17 and C21, respectively, function as hydrogen-bond donors, while the oxygen atoms O2, O3, O5, O6 and O7 of the 4-nitrobenzoate ions function as acceptors, resulting in a

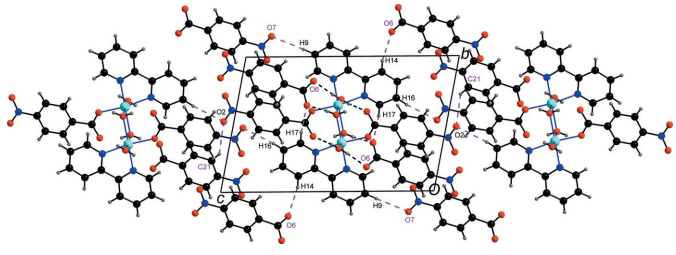


Figure 4
The hydrogen-bonding scheme around the dication showing its linking with eight anions and two cations *via* O—H···O and C—H···O hydrogen bonds.

total of four O—H···O and five C—H···O hydrogen bonds (Table 1). Each free 4-nitrobenzoate anion is linked with four symmetry-related dications with the aid of two O—H···O hydrogen bonds and four C—H···O hydrogen bonds (Figs. 2 and 3). Each of the dinuclear dicobalt dicationic species is linked with two symmetry-related dications and eight symmetry-generated anions (Fig. 4), resulting in a three-dimensional supramolecular network.

Synthesis and crystallization

Crystals of **2** (0.0292 g, 0.05 mmol) were taken in DMSO (3 ml) to obtain a purple solution. 2,2′-Bipyridine (0.0078 g, 0.05 mmol) was dissolved in DMSO (3 ml) in a separate beaker and then was added dropwise to the cobalt solution with continuous swirling. The pale-orange solution thus obtained was left undisturbed at room temperature. After to days, dark-orange blocks of **1** started forming in the solution, which were isolated by filtration and air dried. Yield 60%.

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co_2(C_7H_4NO_4)_2(C_{10}H_8N_2)_2(H_2O)_4](C_7H_4NO_4)_2$
M_r	1166.74
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	7.2747 (5), 10.4927 (8), 16.3560 (12)
α, β, γ (°)	97.735 (2), 102.840 (2), 102.607 (2)
V (Å^3)	1165.70 (15)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.81
Crystal size (mm)	0.45 × 0.32 × 0.21
Data collection	
Diffractometer	Bruker D8 Quest eco
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	26747, 5763, 5312
R_{int}	0.025
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.064, 1.05
No. of reflections	5763
No. of parameters	368
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.36, −0.31

Computer programs: *APEX3* and *SAINT* (Bruker, 2019), *SHELXT2014/5* (Sheldrick, 20015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg, 1999) and *shelXle* (Hübschle *et al.*, 2011).

Funding information

We thank Council of Scientific and Industrial Research (CSIR) New Delhi, for financial support.

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full crystallographic data

IUCrData (2020). **5**, x200796 [https://doi.org/10.1107/S2414314620007968]

Di-μ-aqua-bis[aqua(2,2′-bipyridine)(4-nitrobenzoato)cobalt(II)] bis(4-nitrobenzoate)

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Crystal data

$[Co_2(C_7H_4NO_4)_2(C_{10}H_8N_2)_2(H_2O)_4](C_7H_4NO_4)_2$
M_r = 1166.74
Triclinic, $P\overline{1}$
a = 7.2747 (5) Å
b = 10.4927 (8) Å
c = 16.3560 (12) Å
α = 97.735 (2)°
β = 102.840 (2)°
γ = 102.607 (2)°
V = 1165.70 (15) Å^3
Z = 1
$F(000)$ = 598
D_x = 1.662 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9978 reflections
θ = 2.9–28.2°
μ = 0.81 mm^{-1}
T = 296 K
Block, orange
0.45 × 0.32 × 0.21 mm

Data collection

Bruker D8 Quest eco diffractometer
Radiation source: Sealed Tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
26747 measured reflections
5763 independent reflections
5312 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 28.3°, θ_{min} = 2.6°
h = −9→9
k = −13→13
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.064
S = 1.05
5763 reflections
368 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0255P)^2 + 0.6838P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.43361 (2)	0.63922 (2)	0.52457 (2)	0.01063 (5)
O1	0.43137 (17)	0.71403 (11)	1.06326 (6)	0.0261 (2)
N1	0.32901 (17)	0.60682 (12)	1.01984 (7)	0.0180 (2)
C1	0.32850 (19)	0.57702 (13)	0.92928 (8)	0.0147 (2)
O2	0.22558 (18)	0.52407 (11)	1.04780 (7)	0.0289 (2)
N2	0.61203 (16)	0.83416 (10)	0.57038 (7)	0.0131 (2)
C2	0.45366 (19)	0.66787 (13)	0.89966 (8)	0.0168 (3)
H2	0.539777	0.742960	0.936466	0.020*
O3	0.19021 (13)	0.40968 (9)	0.61539 (6)	0.01502 (18)
N3	0.44762 (16)	0.70799 (11)	0.41050 (7)	0.0130 (2)
C3	0.44682 (19)	0.64358 (13)	0.81350 (8)	0.0161 (2)
H3	0.529735	0.703100	0.792083	0.019*
O4	0.43133 (13)	0.59742 (9)	0.64323 (6)	0.01478 (18)
N4	0.82411 (18)	0.08005 (12)	−0.06413 (8)	0.0207 (2)
C4	0.31743 (18)	0.53122 (12)	0.75861 (8)	0.0129 (2)
C5	0.1950 (2)	0.44082 (13)	0.79086 (8)	0.0169 (3)
H5	0.109775	0.365050	0.754405	0.020*
O5	1.07575 (15)	0.36007 (10)	0.32867 (6)	0.0211 (2)
C6	0.1994 (2)	0.46313 (13)	0.87707 (8)	0.0180 (3)
H6	0.118041	0.403405	0.899036	0.022*
O6	0.85644 (15)	0.18061 (9)	0.33776 (6)	0.0203 (2)
C7	0.31025 (18)	0.51044 (12)	0.66454 (8)	0.0127 (2)
O7	0.91826 (18)	0.15271 (12)	−0.10126 (7)	0.0317 (3)
C8	0.6889 (2)	0.89288 (13)	0.65249 (8)	0.0167 (3)
H8	0.650756	0.848993	0.694104	0.020*
O8	0.70001 (17)	−0.02340 (11)	−0.10076 (7)	0.0297 (2)
C9	0.8231 (2)	1.01652 (13)	0.67843 (9)	0.0188 (3)
H9	0.874547	1.054302	0.736112	0.023*
C10	0.8785 (2)	1.08205 (13)	0.61629 (9)	0.0191 (3)
H10	0.967902	1.164988	0.631700	0.023*
C11	0.79935 (19)	1.02285 (13)	0.53093 (9)	0.0165 (2)
H11	0.834491	1.065696	0.488378	0.020*
C12	0.66666 (18)	0.89850 (12)	0.50973 (8)	0.0131 (2)
C13	0.57188 (18)	0.82847 (12)	0.41994 (8)	0.0130 (2)
C14	0.6047 (2)	0.88285 (13)	0.34951 (9)	0.0176 (3)
H14	0.691802	0.965414	0.356946	0.021*
C15	0.5048 (2)	0.81138 (14)	0.26838 (9)	0.0206 (3)
H15	0.525861	0.845041	0.220521	0.025*
C16	0.3734 (2)	0.68944 (14)	0.25880 (9)	0.0188 (3)
H16	0.302949	0.641070	0.204804	0.023*
C17	0.34957 (19)	0.64140 (13)	0.33163 (8)	0.0155 (2)
H17	0.261827	0.559500	0.325489	0.019*
C18	0.95292 (19)	0.24975 (13)	0.29757 (8)	0.0146 (2)
C19	0.92261 (19)	0.20072 (13)	0.20274 (8)	0.0149 (2)
C20	1.03275 (19)	0.27527 (13)	0.15766 (9)	0.0173 (3)

H20	1.127507	0.352694	0.186407	0.021*
O1W	0.16527 (15)	0.68171 (11)	0.51582 (7)	0.0186 (2)
C21	1.0024 (2)	0.23507 (14)	0.07020 (9)	0.0189 (3)
H21	1.075168	0.284846	0.039878	0.023*
C22	0.8611 (2)	0.11911 (13)	0.02938 (9)	0.0178 (3)
C23	0.7511 (2)	0.04133 (14)	0.07225 (9)	0.0218 (3)
H23	0.658049	−0.036827	0.043395	0.026*
C24	0.7839 (2)	0.08360 (14)	0.15973 (9)	0.0203 (3)
H24	0.712092	0.032818	0.189930	0.024*
O2W	0.30828 (13)	0.43132 (9)	0.47476 (6)	0.01185 (17)
H1A	0.148 (3)	0.718 (2)	0.5594 (15)	0.042 (6)*
H1B	0.066 (3)	0.650 (2)	0.4773 (14)	0.039 (6)*
H2A	0.264 (3)	0.410 (2)	0.5123 (15)	0.045 (6)*
H2B	0.223 (3)	0.404 (2)	0.4276 (14)	0.039 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.01158 (9)	0.01116 (8)	0.00889 (8)	0.00091 (6)	0.00424 (6)	0.00170 (6)
O1	0.0363 (6)	0.0240 (5)	0.0128 (5)	0.0000 (5)	0.0064 (4)	−0.0016 (4)
N1	0.0228 (6)	0.0209 (6)	0.0115 (5)	0.0064 (5)	0.0061 (4)	0.0034 (4)
C1	0.0187 (6)	0.0180 (6)	0.0092 (6)	0.0061 (5)	0.0056 (5)	0.0031 (5)
O2	0.0405 (6)	0.0285 (6)	0.0170 (5)	−0.0013 (5)	0.0154 (5)	0.0056 (4)
N2	0.0144 (5)	0.0128 (5)	0.0126 (5)	0.0034 (4)	0.0045 (4)	0.0024 (4)
C2	0.0173 (6)	0.0177 (6)	0.0128 (6)	0.0004 (5)	0.0037 (5)	0.0011 (5)
O3	0.0163 (4)	0.0161 (4)	0.0111 (4)	0.0010 (3)	0.0048 (3)	0.0008 (3)
N3	0.0136 (5)	0.0141 (5)	0.0118 (5)	0.0033 (4)	0.0047 (4)	0.0025 (4)
C3	0.0166 (6)	0.0180 (6)	0.0130 (6)	0.0003 (5)	0.0061 (5)	0.0032 (5)
O4	0.0174 (4)	0.0162 (4)	0.0112 (4)	0.0019 (4)	0.0065 (3)	0.0032 (3)
N4	0.0239 (6)	0.0204 (6)	0.0168 (6)	0.0057 (5)	0.0054 (5)	0.0002 (5)
C4	0.0139 (6)	0.0156 (6)	0.0108 (6)	0.0051 (5)	0.0049 (4)	0.0028 (5)
C5	0.0200 (6)	0.0154 (6)	0.0135 (6)	0.0003 (5)	0.0063 (5)	0.0008 (5)
O5	0.0234 (5)	0.0185 (5)	0.0136 (5)	−0.0051 (4)	−0.0005 (4)	0.0027 (4)
C6	0.0230 (7)	0.0176 (6)	0.0141 (6)	0.0014 (5)	0.0092 (5)	0.0041 (5)
O6	0.0241 (5)	0.0161 (4)	0.0205 (5)	−0.0001 (4)	0.0116 (4)	0.0012 (4)
C7	0.0139 (6)	0.0154 (6)	0.0109 (6)	0.0056 (5)	0.0053 (4)	0.0037 (5)
O7	0.0416 (7)	0.0307 (6)	0.0202 (5)	−0.0008 (5)	0.0134 (5)	0.0028 (5)
C8	0.0194 (6)	0.0161 (6)	0.0143 (6)	0.0047 (5)	0.0046 (5)	0.0016 (5)
O8	0.0345 (6)	0.0258 (5)	0.0202 (5)	−0.0017 (5)	0.0046 (5)	−0.0046 (4)
C9	0.0200 (6)	0.0174 (6)	0.0156 (6)	0.0047 (5)	0.0011 (5)	−0.0023 (5)
C10	0.0165 (6)	0.0137 (6)	0.0240 (7)	0.0017 (5)	0.0038 (5)	−0.0003 (5)
C11	0.0163 (6)	0.0135 (6)	0.0199 (6)	0.0024 (5)	0.0065 (5)	0.0036 (5)
C12	0.0126 (6)	0.0133 (6)	0.0141 (6)	0.0038 (5)	0.0042 (5)	0.0026 (5)
C13	0.0125 (6)	0.0130 (5)	0.0134 (6)	0.0027 (4)	0.0041 (5)	0.0022 (5)
C14	0.0194 (6)	0.0159 (6)	0.0173 (6)	0.0008 (5)	0.0069 (5)	0.0047 (5)
C15	0.0271 (7)	0.0216 (7)	0.0138 (6)	0.0032 (6)	0.0079 (5)	0.0064 (5)
C16	0.0234 (7)	0.0194 (6)	0.0125 (6)	0.0036 (5)	0.0050 (5)	0.0025 (5)
C17	0.0174 (6)	0.0138 (6)	0.0135 (6)	0.0009 (5)	0.0045 (5)	0.0014 (5)

C18	0.0140 (6)	0.0137 (6)	0.0155 (6)	0.0039 (5)	0.0030 (5)	0.0024 (5)
C19	0.0137 (6)	0.0146 (6)	0.0161 (6)	0.0037 (5)	0.0033 (5)	0.0024 (5)
C20	0.0149 (6)	0.0162 (6)	0.0178 (6)	−0.0001 (5)	0.0036 (5)	0.0013 (5)
O1W	0.0149 (5)	0.0254 (5)	0.0154 (5)	0.0058 (4)	0.0049 (4)	0.0004 (4)
C21	0.0190 (6)	0.0185 (6)	0.0188 (7)	0.0015 (5)	0.0071 (5)	0.0039 (5)
C22	0.0199 (6)	0.0178 (6)	0.0153 (6)	0.0055 (5)	0.0047 (5)	0.0003 (5)
C23	0.0242 (7)	0.0156 (6)	0.0194 (7)	−0.0032 (5)	0.0044 (5)	−0.0018 (5)
C24	0.0235 (7)	0.0159 (6)	0.0183 (7)	−0.0019 (5)	0.0068 (5)	0.0013 (5)
O2W	0.0120 (4)	0.0137 (4)	0.0085 (4)	0.0000 (3)	0.0036 (3)	0.0012 (3)

Geometric parameters (Å, º)

Co1—O4	2.0494 (9)	C8—H8	0.9300
Co1—O1W	2.0743 (10)	C9—C10	1.385 (2)
Co1—N2	2.1038 (11)	C9—H9	0.9300
Co1—N3	2.1039 (11)	C10—C11	1.386 (2)
Co1—O2W	2.1394 (9)	C10—H10	0.9300
Co1—O2W^{i}	2.1617 (9)	C11—C12	1.3908 (17)
O1—N1	1.2282 (16)	C11—H11	0.9300
N1—O2	1.2262 (15)	C12—C13	1.4868 (18)
N1—C1	1.4712 (16)	C13—C14	1.3960 (18)
C1—C2	1.3833 (18)	C14—C15	1.3845 (19)
C1—C6	1.3851 (19)	C14—H14	0.9300
N2—C8	1.3376 (17)	C15—C16	1.3861 (19)
N2—C12	1.3550 (16)	C15—H15	0.9300
C2—C3	1.3857 (18)	C16—C17	1.3851 (18)
C2—H2	0.9300	C16—H16	0.9300
O3—C7	1.2581 (16)	C17—H17	0.9300
N3—C17	1.3386 (16)	C18—C19	1.5176 (18)
N3—C13	1.3511 (16)	C19—C24	1.3906 (18)
C3—C4	1.3918 (18)	C19—C20	1.3934 (18)
C3—H3	0.9300	C20—C21	1.3890 (19)
O4—C7	1.2655 (15)	C20—H20	0.9300
N4—O7	1.2251 (16)	O1W—H1A	0.81 (2)
N4—O8	1.2284 (16)	O1W—H1B	0.82 (2)
N4—C22	1.4763 (17)	C21—C22	1.3831 (19)
C4—C5	1.3951 (17)	C21—H21	0.9300
C4—C7	1.5121 (17)	C22—C23	1.3844 (19)
C5—C6	1.3900 (18)	C23—C24	1.390 (2)
C5—H5	0.9300	C23—H23	0.9300
O5—C18	1.2590 (16)	C24—H24	0.9300
C6—H6	0.9300	O2W—H2A	0.79 (2)
O6—C18	1.2499 (16)	O2W—H2B	0.84 (2)
C8—C9	1.3897 (19)		

O4—Co1—O1W	88.78 (4)	C9—C10—C11	119.35 (12)
O4—Co1—N2	95.06 (4)	C9—C10—H10	120.3
O1W—Co1—N2	98.21 (4)	C11—C10—H10	120.3

O4—Co1—N3	172.65 (4)	C10—C11—C12	119.11 (12)
O1W—Co1—N3	89.91 (4)	C10—C11—H11	120.4
N2—Co1—N3	77.97 (4)	C12—C11—H11	120.4
O4—Co1—O2W	87.29 (4)	N2—C12—C11	121.70 (12)
O1W—Co1—O2W	93.78 (4)	N2—C12—C13	115.43 (11)
N2—Co1—O2W	167.83 (4)	C11—C12—C13	122.86 (12)
N3—Co1—O2W	100.02 (4)	N3—C13—C14	121.59 (12)
O4—Co1—O2W^{i}	91.60 (4)	N3—C13—C12	115.34 (11)
O1W—Co1—O2W^{i}	172.46 (4)	C14—C13—C12	123.07 (11)
N2—Co1—O2W^{i}	89.26 (4)	C15—C14—C13	118.67 (12)
N3—Co1—O2W^{i}	90.64 (4)	C15—C14—H14	120.7
O2W—Co1—O2W^{i}	78.72 (4)	C13—C14—H14	120.7
O2—N1—O1	123.42 (12)	C14—C15—C16	119.70 (12)
O2—N1—C1	118.33 (11)	C14—C15—H15	120.2
O1—N1—C1	118.23 (11)	C16—C15—H15	120.2
C2—C1—C6	123.04 (12)	C17—C16—C15	118.36 (13)
C2—C1—N1	117.76 (12)	C17—C16—H16	120.8
C6—C1—N1	119.15 (11)	C15—C16—H16	120.8
C8—N2—C12	118.50 (11)	N3—C17—C16	122.72 (12)
C8—N2—Co1	126.05 (9)	N3—C17—H17	118.6
C12—N2—Co1	115.11 (8)	C16—C17—H17	118.6
C1—C2—C3	117.98 (12)	O6—C18—O5	125.68 (12)
C1—C2—H2	121.0	O6—C18—C19	119.05 (12)
C3—C2—H2	121.0	O5—C18—C19	115.27 (11)
C17—N3—C13	118.93 (11)	C24—C19—C20	119.42 (12)
C17—N3—Co1	125.64 (9)	C24—C19—C18	120.96 (12)
C13—N3—Co1	115.41 (8)	C20—C19—C18	119.60 (12)
C2—C3—C4	120.82 (12)	C21—C20—C19	120.64 (12)
C2—C3—H3	119.6	C21—C20—H20	119.7
C4—C3—H3	119.6	C19—C20—H20	119.7
C7—O4—Co1	129.34 (8)	Co1—O1W—H1A	116.9 (15)
O7—N4—O8	123.35 (12)	Co1—O1W—H1B	127.0 (15)
O7—N4—C22	118.32 (12)	H1A—O1W—H1B	114 (2)
O8—N4—C22	118.33 (12)	C22—C21—C20	118.29 (13)
C3—C4—C5	119.66 (12)	C22—C21—H21	120.9
C3—C4—C7	119.19 (11)	C20—C21—H21	120.9
C5—C4—C7	121.15 (11)	C21—C22—C23	122.70 (13)
C6—C5—C4	120.51 (12)	C21—C22—N4	117.93 (12)
C6—C5—H5	119.7	C23—C22—N4	119.34 (12)
C4—C5—H5	119.7	C22—C23—C24	117.98 (13)
C1—C6—C5	117.98 (12)	C22—C23—H23	121.0
C1—C6—H6	121.0	C24—C23—H23	121.0
C5—C6—H6	121.0	C23—C24—C19	120.94 (13)
O3—C7—O4	126.09 (11)	C23—C24—H24	119.5
O3—C7—C4	118.54 (11)	C19—C24—H24	119.5
O4—C7—C4	115.36 (11)	Co1—O2W—Co1^{i}	101.28 (4)
N2—C8—C9	122.98 (12)	Co1—O2W—H2A	100.6 (16)
N2—C8—H8	118.5	Co1^{i}—O2W—H2A	110.0 (16)

C9—C8—H8	118.5	Co1—O2W—H2B	121.6 (14)
C10—C9—C8	118.37 (13)	Co1^{i}—O2W—H2B	112.2 (14)
C10—C9—H9	120.8	H2A—O2W—H2B	110 (2)
C8—C9—H9	120.8		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2*W*—H2*B*···O5^{ii}	0.84 (2)	1.67 (2)	2.5101 (13)	173 (2)
O2*W*—H2*A*···O3	0.79 (2)	1.88 (2)	2.6483 (13)	164 (2)
O1*W*—H1*B*···O3^{iii}	0.82 (2)	2.04 (2)	2.8477 (14)	174 (2)
O1*W*—H1*A*···O6^{i}	0.81 (2)	1.88 (2)	2.6803 (14)	171 (2)
C21—H21···O2^{iv}	0.93	2.48	3.2219 (17)	137
C17—H17···O5^{ii}	0.93	2.24	3.1679 (16)	172
C16—H16···O2^{v}	0.93	2.57	3.4644 (17)	160
C14—H14···O6^{vi}	0.93	2.41	3.3126 (16)	164
C9—H9···O7^{vii}	0.93	2.64	3.5467 (18)	164

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