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Di-μ-aqua-bis[aqua(2,2′-bipyridine-κ^2N,N')(4-formylbenzoato-κO)cobalt(II)] bis(4-formylbenzoate)

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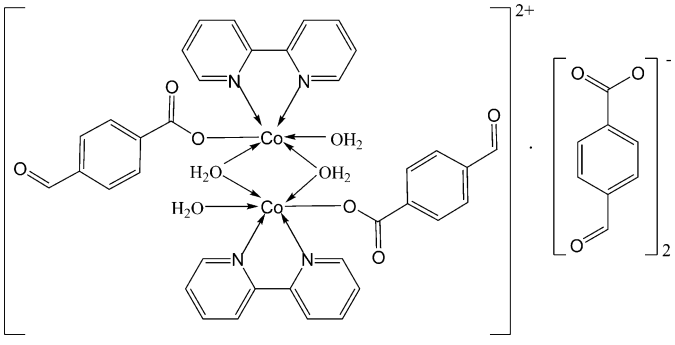
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.044; wR factor = 0.147; data-to-parameter ratio = 15.5.

The cation of the title salt, $[Co_2(C_8H_5O_3)_2(C_{10}H_8N_2)_2(H_2O)_4](C_8H_5O_3)_2$, or $[Co_2(4\text{-FBA})_2(2,2'\text{-bipy})_2(H_2O)_4]\cdot(4\text{-FBA})_2$ [where 4-FBA$^-$ is the 4-formylbenzoate monoanion and 2,2′-bipy is 2,2′-bipyridine], is a dinuclear Co^{II} complex which is located on an inversion centre. The Co atom is six-coordinated by one O atom of a 4-FBA$^-$ ligand, one 2,2′-bipy ligand and three water molecules in an octahedral geometry. The two Co atoms are bridged by two water molecules into a four-membered Co_2O_2 ring, with a Co···Co distance of 3.344 (4) Å. A linear chain running along the a axis is formed through hydrogen-bonding interactions between cations and anions. Two O atoms are disordered equally over two sites.

Related literature

For the metal compounds of 4-formylbenzoic acid, see Deng, Gao, Huo *et al.* (2006*a*,*b*), Deng *et al.* (2006, 2007*a*,*b*).



Experimental

Crystal data

$[Co_2(C_8H_5O_3)_2(C_{10}H_8N_2)_2(H_2O)_4](C_8H_5O_3)_2$
M_r = 1098.77
Triclinic, $P\overline{1}$
a = 7.3813 (15) Å
b = 10.654 (2) Å
c = 16.385 (3) Å
α = 98.77 (3)°
β = 101.17 (3)°
γ = 104.11 (3)°
V = 1198.7 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 295 (2) K
0.34 × 0.28 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.780, T_{max} = 0.849
11854 measured reflections
5451 independent reflections
4776 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.147
S = 1.08
5451 reflections
352 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.29 e Å^{-3}
$\Delta\rho_{min}$ = −1.21 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co1—O1	2.0494 (17)	Co1—N1	2.110 (2)
Co1—O2*W*	2.0841 (18)	Co1—O1*W*	2.1464 (18)
Co1—N2	2.108 (2)	Co1—O1*W*^{i}	2.1756 (17)

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

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 (3)	1.83 (3)	2.639 (2)	159 (3)
O1*W*—H1*W*2···O5^{ii}	0.85 (3)	1.67 (3)	2.517 (3)	177 (3)
O2*W*—H2*W*1···O2^{ii}	0.85 (3)	2.04 (4)	2.857 (3)	160 (4)
O2*W*—H2*W*2···O4	0.85 (2)	1.85 (3)	2.676 (3)	164 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2376).

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supplementary materials

Acta Cryst. (2007). E**63**, m3124-m3125 [**doi:10.1107/S160053680705979X**]

Di-μ-aqua-bis[aqua(2,2'-bipyridine-κ^2N,N')(4-formylbenzoato-κO)cobalt(II)] bis(4-formylbenzoate)

Z.-P. Deng, S. Gao, L.-H. Huo and H. Zhao

Comment

Many metal compounds base on 4-formylbenzoic acid (4-FBAH) ligand have been reported up to date (Deng, Gao, Huo *et al.*, 2006*a*,b; Deng *et al.*, 2007*a*,b). Thereinto, we have showing the mononuclear cobalt complex, $[Co(H_2O)_6](4\text{-}FBA)_2{\cdot}2H_2O$, which obtained by the reaction of 4-FBAH and cobalt diacetate (Deng *et al.*, 2006*c*). Herein, we introduced 2,2'-bipy to the above system leading to the formation of title dinuclear complex, $[Co_2(4\text{-}FBA)_2(2,2'\text{-}bipy)_2(H_2O)_4].(4\text{-}FBA)_2$, (I), in which the Co^{II} atom is six-coordinated by one O atoms of $4\text{-}FBA^-$ ligand, one 2,2'-bipy ligand and three coordinated water molecules, giving rise to a distorted octahedral geometry. The two Co^{II} atom are bridged by two water molecules to generate a four-memberd ring, Co_2O_2, with the Co···Co distance being 3.344 (4) Å. A one-dimensional supramolecular chain is constructed by hydrogen-bonding interactions between the water molecules and O atoms of $4\text{-}FBA^-$ ligands along the *a* axis.

Experimental

Cobalt(II) sulfate (1.55 g, 10 mmol) was added to an H_2O/EtOH solution (1:1 *v*/*v*) of 4-formylbenzoic acid (3.00 g, 20 mmol) and 2,2'-bipydine (1.56 g 10 mmol). Sodium hydroxide (0.1 *M*) was added dropwise until the solution registered a pH of 5. Orange single crystals separated from the filtered solution after several days. CH&N analysis. Calc. for $C_{52}H_{44}N_4O_{16}Co$: C 56.84, H 4.04, N 5.10. Found: C 56.85, H 4.01, N 5.11.

Refinement

Carbon-bound H atoms were placed in calculated positions, with C—H = 0.93 and $U_{iso}(H) = 1.2U_{eq}$ (C), and were included in the refinement in the riding model approximation. The H atoms of water molecules were located in difference Fourier maps and refined with the O—H and H···H distance restraints to 0.85 (1) and 1.39 (1) Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$.

Figures

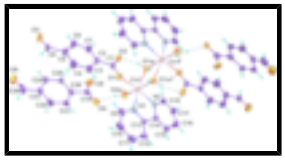


Fig. 1. Molecular structure of the title compound with 50% probability ellipsoid for the non-H atoms. Dashed lines indicate O—H···O hydrogen bonds.

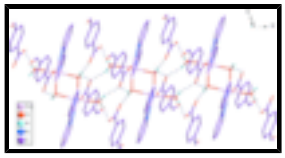


Fig. 2. Chain structure of the title complex along the *a* axis formed by hydrogen-bonding interactions, with the O—H···O hydrogen bonds denoted by dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

Di-μ-aqua-κ^2*O*:*O*-di-4-formylbenzoato-κ*O*-bis[aqua(2,2'-bipyridine- κ^2*N*,*N*')cobalt(II)] bis(4-formylbenzoate)

Crystal data

$[Co_2(C_8H_5O_3)_2(C_{10}H_8N_2)_2(H_2O)_4](2C_8H_5O_3)_2$	$Z = 1$
$M_r = 1098.77$	$F_{000} = 566$
Triclinic, $P\overline{1}$	$D_x = 1.522$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.3813$ (15) Å	Cell parameters from 10238 reflections
$b = 10.654$ (2) Å	$\theta = 3.1$–27.5º
$c = 16.385$ (3) Å	$\mu = 0.77$ mm^{-1}
$\alpha = 98.77$ (3)º	$T = 295$ (2) K
$\beta = 101.17$ (3)º	Block, orange
$\gamma = 104.11$ (3)º	0.34 × 0.28 × 0.22 mm
$V = 1198.7$ (5) Å^3	

Data collection

Rigaku RAXIS-RAPID diffractometer	5451 independent reflections
Radiation source: fine-focus sealed tube	4776 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.018$
Detector resolution: 10.000 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 295$(2) K	$\theta_{min} = 3.1$º
ω scan	$h = -9 \rightarrow 9$
Absorption correction: multi-scan ABSCOR (Higashi, 1995)	$k = -13 \rightarrow 13$
$T_{min} = 0.780$, $T_{max} = 0.849$	$l = -21 \rightarrow 21$
11854 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.147$	$w = 1/[\sigma^2(F_o^2) + (0.0987P)^2 + 0.4736P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
5451 reflections	$\Delta\rho_{max} = 1.29$ e Å^{-3}

352 parameters
8 restraints
Primary atom site location: structure-invariant direct methods

$\Delta\rho_{min} = -1.21$ e Å^{-3}
Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	0.56663 (4)	0.36254 (3)	0.475623 (17)	0.02743 (13)	
O1W	0.6901 (2)	0.57079 (16)	0.52683 (10)	0.0283 (3)	
H1W1	0.742 (4)	0.597 (3)	0.4882 (11)	0.043*	
H1W2	0.768 (3)	0.600 (3)	0.5753 (8)	0.043*	
O2W	0.8315 (3)	0.3225 (2)	0.48421 (12)	0.0443 (4)	
H2W1	0.935 (3)	0.367 (3)	0.5202 (16)	0.066*	
H2W2	0.857 (4)	0.290 (3)	0.4386 (12)	0.066*	
O1	0.5747 (3)	0.40142 (18)	0.35747 (10)	0.0364 (4)	
O2	0.8156 (3)	0.58935 (18)	0.38767 (11)	0.0394 (4)	
O3	0.7988 (10)	0.4816 (6)	−0.0513 (3)	0.0890 (14)	0.50
O3'	0.5967 (10)	0.3087 (6)	−0.0686 (3)	0.0890 (14)	0.50
O4	0.8548 (3)	0.1796 (2)	0.33943 (13)	0.0534 (5)	
O5	1.0836 (3)	0.3501 (2)	0.32778 (12)	0.0545 (6)	
O6	0.8590 (13)	0.1155 (9)	−0.1128 (4)	0.1135 (19)	0.50
O6'	0.7076 (13)	−0.0190 (8)	−0.1110 (4)	0.1135 (19)	0.50
N1	0.3885 (3)	0.1664 (2)	0.43106 (13)	0.0327 (4)	
N2	0.5494 (3)	0.29679 (19)	0.58964 (12)	0.0303 (4)	
C1	0.6972 (3)	0.4893 (2)	0.33741 (14)	0.0320 (5)	
C2	0.6931 (3)	0.4728 (2)	0.24375 (14)	0.0329 (5)	
C3	0.5606 (4)	0.3659 (3)	0.18631 (17)	0.0467 (7)	
H3	0.4728	0.3056	0.2052	0.056*	
C4	0.5587 (5)	0.3488 (3)	0.10092 (17)	0.0546 (8)	
H4	0.4696	0.2766	0.0626	0.066*	
C5	0.6881 (5)	0.4382 (3)	0.07181 (16)	0.0460 (6)	
C6	0.8183 (5)	0.5456 (3)	0.12839 (18)	0.0536 (8)	
H6	0.9043	0.6068	0.1092	0.064*	
C7	0.8209 (4)	0.5624 (3)	0.21457 (17)	0.0465 (6)	
H7	0.9096	0.6348	0.2529	0.056*	
C8	0.6896 (6)	0.4134 (4)	−0.01888 (18)	0.0621 (9)	
H8	0.5987	0.3388	−0.0542	0.074*	0.50
H8'	0.5958	0.3398	−0.0537	0.074*	0.50
C9	0.3118 (4)	0.1067 (3)	0.34934 (16)	0.0423 (6)	
H9	0.3480	0.1500	0.3074	0.051*	
C10	0.1795 (5)	−0.0182 (3)	0.32517 (19)	0.0499 (7)	
H10	0.1285	−0.0580	0.2679	0.060*	
C11	0.1256 (4)	−0.0818 (3)	0.3872 (2)	0.0505 (7)	
H11	0.0363	−0.1649	0.3724	0.061*	
C12	0.2049 (4)	−0.0216 (3)	0.47170 (18)	0.0408 (6)	
H12	0.1710	−0.0637	0.5145	0.049*	
C13	0.3362 (3)	0.1033 (2)	0.49165 (15)	0.0308 (5)	

C14	0.4292 (3)	0.1755 (2)	0.58092 (14)	0.0303 (4)	
C15	0.3981 (4)	0.1224 (3)	0.65135 (18)	0.0446 (6)	
H15	0.3129	0.0392	0.6446	0.054*	
C16	0.4968 (5)	0.1964 (3)	0.73143 (18)	0.0541 (8)	
H16	0.4782	0.1631	0.7794	0.065*	
C17	0.6216 (5)	0.3183 (3)	0.74036 (17)	0.0476 (7)	
H17	0.6900	0.3683	0.7940	0.057*	
C18	0.6440 (4)	0.3656 (3)	0.66786 (15)	0.0376 (5)	
H18	0.7285	0.4488	0.6738	0.045*	
C19	0.9535 (4)	0.2432 (2)	0.29810 (16)	0.0360 (5)	
C20	0.9171 (4)	0.1921 (3)	0.20316 (16)	0.0377 (5)	
C21	0.7775 (5)	0.0744 (3)	0.1627 (2)	0.0604 (9)	
H21	0.7066	0.0252	0.1940	0.072*	
C22	0.7436 (6)	0.0300 (4)	0.0754 (2)	0.0698 (10)	
H22	0.6509	−0.0495	0.0488	0.084*	
C23	0.8439 (5)	0.1012 (4)	0.02857 (19)	0.0582 (8)	
C24	0.9863 (6)	0.2189 (4)	0.0682 (2)	0.0607 (8)	
H24	1.0568	0.2672	0.0363	0.073*	
C25	1.0221 (5)	0.2634 (3)	0.15529 (18)	0.0508 (7)	
H25	1.1174	0.3417	0.1819	0.061*	
C26	0.8069 (8)	0.0632 (5)	−0.0654 (2)	0.0907 (16)	
H26	0.7237	−0.0211	−0.0886	0.109*	0.50
H26'	0.7222	−0.0202	−0.0898	0.109*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.03158 (19)	0.02631 (19)	0.02254 (18)	0.00316 (12)	0.00900 (13)	0.00451 (12)
O1W	0.0281 (7)	0.0302 (8)	0.0221 (7)	0.0013 (6)	0.0069 (6)	0.0020 (6)
O2W	0.0354 (9)	0.0580 (12)	0.0382 (9)	0.0162 (9)	0.0088 (8)	0.0017 (9)
O1	0.0425 (9)	0.0401 (9)	0.0244 (7)	0.0037 (7)	0.0127 (7)	0.0070 (7)
O2	0.0409 (9)	0.0437 (10)	0.0276 (8)	0.0005 (8)	0.0124 (7)	0.0034 (7)
O3	0.128 (4)	0.096 (3)	0.0314 (15)	0.010 (3)	0.027 (2)	0.0037 (18)
O3'	0.128 (4)	0.096 (3)	0.0314 (15)	0.010 (3)	0.027 (2)	0.0037 (18)
O4	0.0667 (13)	0.0418 (11)	0.0453 (11)	−0.0003 (9)	0.0255 (10)	−0.0004 (9)
O5	0.0613 (13)	0.0474 (12)	0.0320 (9)	−0.0136 (10)	−0.0040 (9)	0.0065 (8)
O6	0.166 (6)	0.133 (5)	0.043 (2)	0.052 (4)	0.021 (3)	0.012 (3)
O6'	0.166 (6)	0.133 (5)	0.043 (2)	0.052 (4)	0.021 (3)	0.012 (3)
N1	0.0369 (10)	0.0276 (9)	0.0303 (9)	0.0061 (8)	0.0071 (8)	0.0022 (7)
N2	0.0347 (10)	0.0291 (9)	0.0254 (9)	0.0048 (8)	0.0076 (8)	0.0064 (7)
C1	0.0354 (11)	0.0378 (12)	0.0246 (10)	0.0099 (9)	0.0109 (9)	0.0076 (9)
C2	0.0364 (12)	0.0385 (12)	0.0238 (10)	0.0099 (10)	0.0092 (9)	0.0054 (9)
C3	0.0510 (15)	0.0475 (16)	0.0317 (12)	−0.0046 (12)	0.0123 (12)	0.0063 (11)
C4	0.068 (2)	0.0530 (18)	0.0273 (12)	−0.0005 (15)	0.0045 (13)	−0.0014 (11)
C5	0.0600 (17)	0.0561 (17)	0.0255 (11)	0.0194 (14)	0.0149 (12)	0.0085 (11)
C6	0.0648 (19)	0.0587 (18)	0.0353 (13)	0.0020 (14)	0.0241 (13)	0.0137 (12)
C7	0.0521 (16)	0.0486 (16)	0.0302 (12)	−0.0021 (12)	0.0142 (12)	0.0042 (11)
C8	0.083 (2)	0.076 (2)	0.0277 (13)	0.0208 (19)	0.0188 (15)	0.0084 (14)

C9	0.0523 (15)	0.0366 (13)	0.0324 (12)	0.0099 (11)	0.0066 (11)	−0.0006 (10)
C10	0.0561 (17)	0.0404 (15)	0.0403 (14)	0.0089 (13)	0.0006 (13)	−0.0081 (11)
C11	0.0495 (15)	0.0322 (13)	0.0568 (17)	0.0025 (11)	0.0048 (14)	−0.0039 (12)
C12	0.0423 (13)	0.0285 (12)	0.0481 (14)	0.0029 (10)	0.0129 (11)	0.0060 (10)
C13	0.0308 (10)	0.0260 (10)	0.0344 (11)	0.0067 (8)	0.0086 (9)	0.0038 (9)
C14	0.0321 (11)	0.0287 (11)	0.0309 (11)	0.0066 (9)	0.0107 (9)	0.0083 (9)
C15	0.0501 (15)	0.0383 (14)	0.0437 (14)	0.0003 (11)	0.0173 (12)	0.0158 (11)
C16	0.071 (2)	0.0561 (18)	0.0342 (13)	0.0055 (15)	0.0169 (14)	0.0216 (13)
C17	0.0594 (17)	0.0486 (16)	0.0288 (12)	0.0045 (13)	0.0095 (12)	0.0089 (11)
C18	0.0455 (13)	0.0340 (12)	0.0276 (11)	0.0020 (10)	0.0076 (10)	0.0063 (9)
C19	0.0363 (12)	0.0335 (12)	0.0339 (12)	0.0057 (10)	0.0058 (10)	0.0041 (9)
C20	0.0381 (12)	0.0353 (12)	0.0341 (12)	0.0067 (10)	0.0054 (10)	0.0005 (10)
C21	0.069 (2)	0.0480 (17)	0.0457 (16)	−0.0127 (15)	0.0164 (15)	−0.0017 (13)
C22	0.077 (2)	0.059 (2)	0.0454 (17)	−0.0072 (18)	0.0027 (17)	−0.0146 (15)
C23	0.069 (2)	0.065 (2)	0.0359 (14)	0.0255 (17)	0.0049 (14)	−0.0027 (13)
C24	0.079 (2)	0.063 (2)	0.0424 (15)	0.0147 (18)	0.0231 (16)	0.0143 (14)
C25	0.0597 (18)	0.0458 (16)	0.0384 (14)	0.0030 (13)	0.0097 (13)	0.0059 (12)
C26	0.111 (4)	0.104 (4)	0.042 (2)	0.047 (3)	−0.008 (2)	−0.022 (2)

Geometric parameters (Å, °)

Co1—O1	2.0494 (17)	C6—H6	0.9300
Co1—O2W	2.0841 (18)	C7—H7	0.9300
Co1—N2	2.108 (2)	C8—H8	0.9300
Co1—N1	2.110 (2)	C8—H8'	0.9301
Co1—O1W	2.1464 (18)	C9—C10	1.391 (4)
Co1—O1W^{i}	2.1756 (17)	C9—H9	0.9300
O1W—Co1^{i}	2.1756 (17)	C10—C11	1.373 (5)
O1W—H1W1	0.85 (3)	C10—H10	0.9300
O1W—H1W2	0.85 (3)	C11—C12	1.380 (4)
O2W—H2W1	0.85 (3)	C11—H11	0.9300
O2W—H2W2	0.85 (2)	C12—C13	1.390 (3)
O1—C1	1.264 (3)	C12—H12	0.9300
O2—C1	1.256 (3)	C13—C14	1.487 (3)
O3—C8	1.208 (6)	C14—C15	1.394 (3)
O3'—C8	1.229 (6)	C15—C16	1.382 (4)
O3'—H8'	0.3824	C15—H15	0.9300
O4—C19	1.240 (3)	C16—C17	1.365 (4)
O5—C19	1.255 (3)	C16—H16	0.9300
O6—C26	1.096 (7)	C17—C18	1.382 (4)
O6'—C26	1.067 (7)	C17—H17	0.9300
O6'—H26'	0.3457	C18—H18	0.9300
N1—C9	1.338 (3)	C19—C20	1.516 (3)
N1—C13	1.346 (3)	C20—C25	1.387 (4)
N2—C18	1.336 (3)	C20—C21	1.388 (4)
N2—C14	1.347 (3)	C21—C22	1.388 (4)
C1—C2	1.511 (3)	C21—H21	0.9300
C2—C7	1.380 (4)	C22—C23	1.355 (6)
C2—C3	1.383 (4)	C22—H22	0.9300

C3—C4	1.380 (4)	C23—C24	1.394 (5)
C3—H3	0.9300	C23—C26	1.485 (5)
C4—C5	1.385 (5)	C24—C25	1.385 (4)
C4—H4	0.9300	C24—H24	0.9300
C5—C6	1.374 (4)	C25—H25	0.9300
C5—C8	1.472 (4)	C26—H26	0.9300
C6—C7	1.392 (4)	C26—H26'	0.9300
O1—Co1—O2W	89.03 (8)	C5—C8—H8'	116.3
O1—Co1—N2	172.67 (7)	N1—C9—C10	122.1 (3)
O2W—Co1—N2	89.14 (8)	N1—C9—H9	119.0
O1—Co1—N1	95.60 (8)	C10—C9—H9	119.0
O2W—Co1—N1	98.01 (9)	C11—C10—C9	118.9 (3)
N2—Co1—N1	77.64 (8)	C11—C10—H10	120.5
O1—Co1—O1W	87.94 (7)	C9—C10—H10	120.5
O2W—Co1—O1W	94.42 (8)	C10—C11—C12	119.5 (3)
N2—Co1—O1W	99.28 (7)	C10—C11—H11	120.2
N1—Co1—O1W	167.12 (7)	C12—C11—H11	120.2
O1—Co1—O1W^{i}	90.74 (7)	C11—C12—C13	118.7 (3)
O2W—Co1—O1W^{i}	173.06 (7)	C11—C12—H12	120.6
N2—Co1—O1W^{i}	91.94 (7)	C13—C12—H12	120.6
N1—Co1—O1W^{i}	88.92 (8)	N1—C13—C12	121.9 (2)
O1W—Co1—O1W^{i}	78.64 (7)	N1—C13—C14	115.6 (2)
Co1—O1W—Co1^{i}	101.36 (7)	C12—C13—C14	122.4 (2)
Co1—O1W—H1W1	102 (2)	N2—C14—C15	121.6 (2)
Co1^{i}—O1W—H1W1	109 (2)	N2—C14—C13	115.2 (2)
Co1—O1W—H1W2	122 (2)	C15—C14—C13	123.2 (2)
Co1^{i}—O1W—H1W2	110 (2)	C16—C15—C14	118.4 (2)
H1W1—O1W—H1W2	110.9 (16)	C16—C15—H15	120.8
Co1—O2W—H2W1	125 (2)	C14—C15—H15	120.8
Co1—O2W—H2W2	118 (2)	C17—C16—C15	120.2 (3)
H2W1—O2W—H2W2	109.8 (17)	C17—C16—H16	119.9
C1—O1—Co1	128.49 (16)	C15—C16—H16	119.9
C26—O6'—H26'	57.9	C16—C17—C18	118.5 (3)
C9—N1—C13	118.8 (2)	C16—C17—H17	120.8
C9—N1—Co1	125.57 (18)	C18—C17—H17	120.8
C13—N1—Co1	115.33 (15)	N2—C18—C17	122.7 (2)
C18—N2—C14	118.7 (2)	N2—C18—H18	118.6
C18—N2—Co1	125.63 (17)	C17—C18—H18	118.6
C14—N2—Co1	115.67 (15)	O4—C19—O5	125.6 (2)
O2—C1—O1	125.9 (2)	O4—C19—C20	119.3 (2)
O2—C1—C2	118.2 (2)	O5—C19—C20	115.1 (2)
O1—C1—C2	115.9 (2)	C25—C20—C21	119.0 (3)
C7—C2—C3	119.3 (2)	C25—C20—C19	120.3 (2)
C7—C2—C1	121.0 (2)	C21—C20—C19	120.7 (3)
C3—C2—C1	119.7 (2)	C20—C21—C22	120.1 (3)
C4—C3—C2	120.0 (3)	C20—C21—H21	120.0
C4—C3—H3	120.0	C22—C21—H21	120.0

C2—C3—H3	120.0	C23—C22—C21	120.8 (3)
C3—C4—C5	120.6 (3)	C23—C22—H22	119.6
C3—C4—H4	119.7	C21—C22—H22	119.6
C5—C4—H4	119.7	C22—C23—C24	120.0 (3)
C6—C5—C4	119.7 (2)	C22—C23—C26	123.4 (4)
C6—C5—C8	120.9 (3)	C24—C23—C26	116.5 (4)
C4—C5—C8	119.4 (3)	C25—C24—C23	119.6 (3)
C5—C6—C7	119.7 (3)	C25—C24—H24	120.2
C5—C6—H6	120.2	C23—C24—H24	120.2
C7—C6—H6	120.2	C24—C25—C20	120.5 (3)
C2—C7—C6	120.7 (3)	C24—C25—H25	119.7
C2—C7—H7	119.7	C20—C25—H25	119.7
C6—C7—H7	119.7	O6'—C26—O6	95.1 (6)
O3—C8—O3'	111.1 (4)	O6'—C26—C23	132.2 (7)
O3—C8—C5	125.5 (4)	O6—C26—C23	132.3 (6)
O3'—C8—C5	122.6 (4)	O6—C26—H26	113.8
O3—C8—H8	117.2	C23—C26—H26	113.8
C5—C8—H8	117.2	O6—C26—H26'	112.7
O3—C8—H8'	118.1	C23—C26—H26'	115.0
O1—Co1—O1W—Co1^{i}	91.17 (8)	C4—C5—C8—O3'	−9.0 (7)
O2W—Co1—O1W—Co1^{i}	−179.97 (7)	C13—N1—C9—C10	0.2 (4)
N2—Co1—O1W—Co1^{i}	−90.12 (8)	Co1—N1—C9—C10	−173.1 (2)
N1—Co1—O1W—Co1^{i}	−15.1 (3)	N1—C9—C10—C11	0.3 (5)
O1W^{i}—Co1—O1W—Co1^{i}	0.0	C9—C10—C11—C12	−0.7 (5)
O2W—Co1—O1—C1	−60.9 (2)	C10—C11—C12—C13	0.7 (4)
N1—Co1—O1—C1	−158.9 (2)	C9—N1—C13—C12	−0.1 (4)
O1W—Co1—O1—C1	33.5 (2)	Co1—N1—C13—C12	173.83 (19)
O1W^{i}—Co1—O1—C1	112.1 (2)	C9—N1—C13—C14	179.4 (2)
O1—Co1—N1—C9	−2.9 (2)	Co1—N1—C13—C14	−6.7 (3)
O2W—Co1—N1—C9	−92.7 (2)	C11—C12—C13—N1	−0.3 (4)
N2—Co1—N1—C9	180.0 (2)	C11—C12—C13—C14	−179.8 (2)
O1W—Co1—N1—C9	102.6 (3)	C18—N2—C14—C15	1.8 (4)
O1W^{i}—Co1—N1—C9	87.8 (2)	Co1—N2—C14—C15	−177.2 (2)
O1—Co1—N1—C13	−176.36 (16)	C18—N2—C14—C13	−177.5 (2)
O2W—Co1—N1—C13	93.83 (17)	Co1—N2—C14—C13	3.6 (3)
N2—Co1—N1—C13	6.49 (16)	N1—C13—C14—N2	2.1 (3)
O1W—Co1—N1—C13	−70.9 (4)	C12—C13—C14—N2	−178.4 (2)
O1W^{i}—Co1—N1—C13	−85.73 (17)	N1—C13—C14—C15	−177.1 (2)
O2W—Co1—N2—C18	77.4 (2)	C12—C13—C14—C15	2.4 (4)
N1—Co1—N2—C18	175.7 (2)	N2—C14—C15—C16	−1.2 (4)
O1W—Co1—N2—C18	−17.0 (2)	C13—C14—C15—C16	177.9 (3)
O1W^{i}—Co1—N2—C18	−95.8 (2)	C14—C15—C16—C17	−0.1 (5)
O2W—Co1—N2—C14	−103.74 (18)	C15—C16—C17—C18	0.8 (5)
N1—Co1—N2—C14	−5.35 (16)	C14—N2—C18—C17	−1.0 (4)
O1W—Co1—N2—C14	161.92 (17)	Co1—N2—C18—C17	177.9 (2)
O1W^{i}—Co1—N2—C14	83.12 (17)	C16—C17—C18—N2	−0.3 (5)
Co1—O1—C1—O2	−16.9 (4)	O4—C19—C20—C25	178.3 (3)

Co1—O1—C1—C2	165.47 (16)	O5—C19—C20—C25	−1.0 (4)
O2—C1—C2—C7	2.5 (4)	O4—C19—C20—C21	−1.1 (4)
O1—C1—C2—C7	−179.7 (2)	O5—C19—C20—C21	179.7 (3)
O2—C1—C2—C3	−178.0 (3)	C25—C20—C21—C22	−0.5 (5)
O1—C1—C2—C3	−0.2 (4)	C19—C20—C21—C22	178.9 (3)
C7—C2—C3—C4	0.8 (5)	C20—C21—C22—C23	−0.8 (6)
C1—C2—C3—C4	−178.7 (3)	C21—C22—C23—C24	1.6 (6)
C2—C3—C4—C5	−0.2 (5)	C21—C22—C23—C26	−176.4 (4)
C3—C4—C5—C6	−0.7 (5)	C22—C23—C24—C25	−1.0 (6)
C3—C4—C5—C8	176.7 (3)	C26—C23—C24—C25	177.1 (4)
C4—C5—C6—C7	1.0 (5)	C23—C24—C25—C20	−0.2 (5)
C8—C5—C6—C7	−176.3 (3)	C21—C20—C25—C24	1.0 (5)
C3—C2—C7—C6	−0.5 (5)	C19—C20—C25—C24	−178.4 (3)
C1—C2—C7—C6	179.0 (3)	C22—C23—C26—O6'	−1.2 (11)
C5—C6—C7—C2	−0.4 (5)	C24—C23—C26—O6'	−179.2 (8)
C6—C5—C8—O3	−0.4 (7)	C22—C23—C26—O6	169.9 (8)
C4—C5—C8—O3	−177.8 (6)	C24—C23—C26—O6	−8.1 (10)
C6—C5—C8—O3'	168.4 (5)		

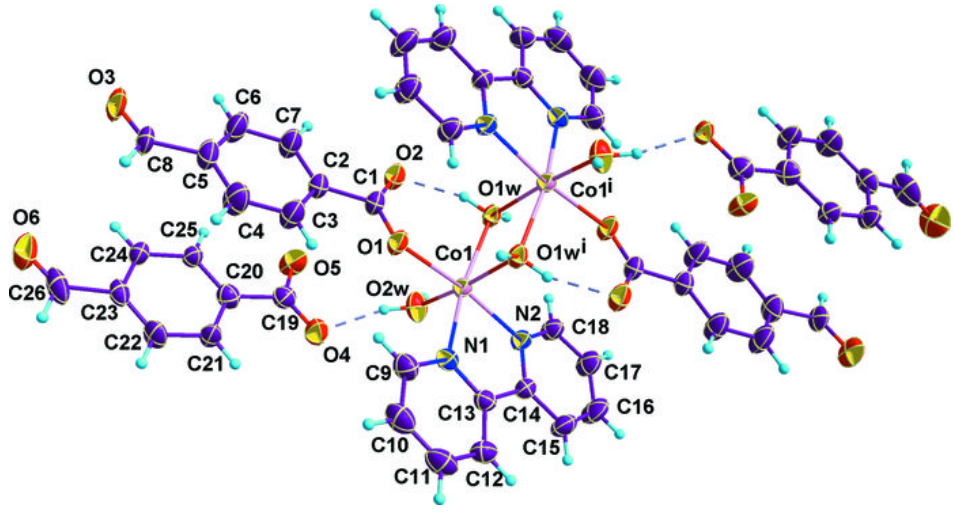
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1W1···O2	0.85 (3)	1.83 (3)	2.639 (2)	159 (3)
O1W—H1W2···O5^{ii}	0.85 (3)	1.67 (3)	2.517 (3)	177 (3)
O2W—H2W1···O2^{ii}	0.85 (3)	2.04 (4)	2.857 (3)	160 (4)
O2W—H2W2···O4	0.85 (2)	1.85 (3)	2.676 (3)	164 (3)

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

Fig. 1


O3
C6
C7
C8
C5
C2
C1
O2
O1w
Co1i
O6
C25
C4
C3
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Co1
O1wi
C24
C20
O5
C26
O2w
C23
C19
N2
C18
C22
O4
N1
C9
C17
C21
C13
C14
C16
C10
C15
C11
C12

Fig. 2