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μ_2-Aqua-bis(μ_2-trifluoroaceto-κ^2O,O')bis[bis(pyridine-κN)(trifluoroacetato-κO)cobalt(II)]

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Key indicators

Single-crystal X-ray study
T = 180 K
Mean σ(C–C) = 0.010 Å
Disorder in main residue
R factor = 0.079
wR factor = 0.240
Data-to-parameter ratio = 17.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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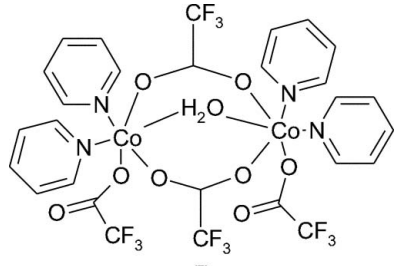
The title complex, $[Co_2(C_2F_3O_2)_4(C_5H_5N)_4(H_2O)]$, crystallizes as a neutral dinuclear molecule with two crystallographically distinct octahedrally coordinated Co^{II} ions in the asymmetric unit. The metal ions are connected by two μ_2-bridging trifluoroacetate ions and a single μ_2-bridging water molecule. Each cobalt(II) coordination sphere is completed by a further trifluoroacetate ion, which coordinates in a monodentate manner, and also by two pyridine molecules, resulting in local *cis*-CoN_2O_4 coordination. The water molecule H atoms participate in intramolecular O—H···O hydrogen bonds to the pendant O atoms of the monodentate trifluoroacetate ligands.

Comment

Complexes of divalent transition metals with mixed N-donor and acetate-related ligands have been studied widely due to their close structural analogy with reduced non-heme iron(II) proteins (Hagen *et al.*, 1993). During the course of investigations into possible complexes formed by cobalt(II), pyridine and acetate derivatives, the title compound, (I) (Fig. 1), was isolated. The red crystals consist of neutral dinuclear cobalt(II) molecules in which each cobalt ion is coordinated (Table 1) by two pyridine N atoms and one monodentate trifluoroacetate ion. Two further trifluoroacetate ions bridge the metal nuclei in a μ_2-manner, and the coordination shell is completed by a single μ_2-bridging water molecule. The water molecule H atoms make intramolecular hydrogen bonds (Table 2) to the uncoordinated O atoms of the non-bridging trifluoroacetate ions.



(I)

The overall molecular architecture of (I) is similar to that of related compounds (Corkery & Hockless, 1997; Turpeinen *et al.*, 1987; Hagen *et al.*, 1993). The Co1—O*W* and Co2—O*W* distances of 2.190 (3) and 2.196 (3) Å, respectively, are the same within experimental uncertainty. The Co—N distances for the pyridine molecules (weak π acceptors) *trans* to the water O atom (π neutral) are significantly shorter than those *trans* to the fluoroacetate O atoms (weak π donor) as a result

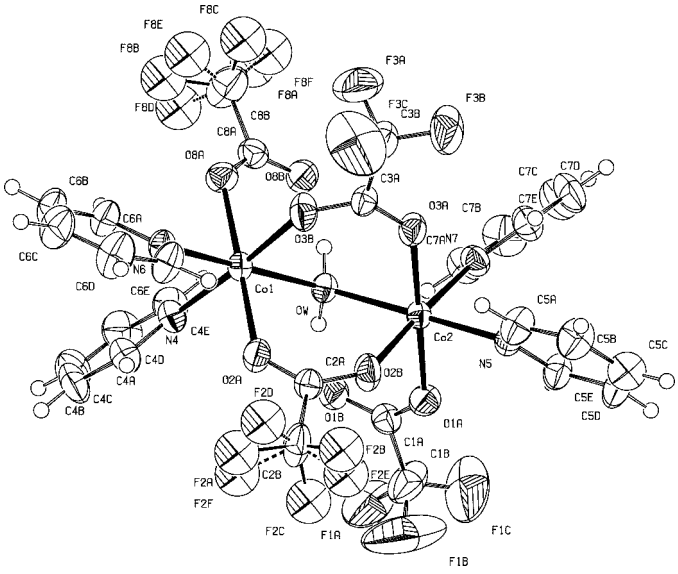


Figure 1
The molecular structure of (I), showing 50% displacement ellipsoids for the non-H atoms. The minor disorder components are indicated by dashed C—F bonds.

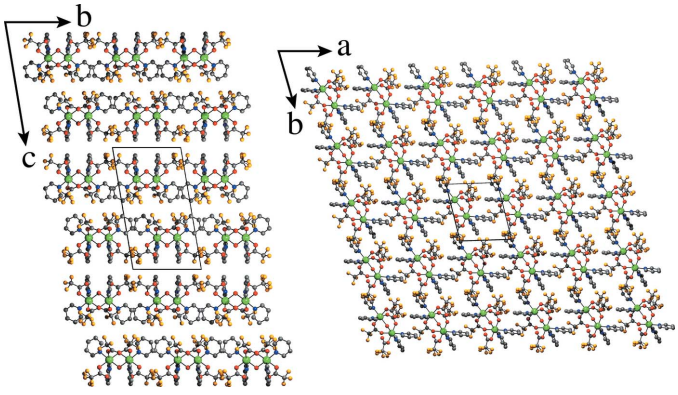


Figure 2
Packing diagrams for (I), showing the layered arrangement of molecules (left) and the plan of the layers (right).

of the well known *trans* influence [for example, Co1—N4 = 2.139 (4) Å *versus* Co1—N6 = 2.128 (4) Å]. The Co1—O*W*—Co2 angle is 116.86 (15)°, which is well within the expected range of values (*e.g.* Corkery & Hockless, 1997; Turpeinen *et al.*, 1997; Hagen *et al.*, 1993). There is no evidence of intermolecular hydrogen bonding or any other directional forces between the individual molecules. In terms of crystal packing, the molecules are arranged in layers in the *ab* plane (Fig. 2).

Experimental

$CoCl_2{\cdot}4H_2O$ (0.502 g) was mixed with Na_2CO_3 (0.154 g) and distilled water (approximately 10 ml) was added with stirring. Following this, trifluoroacetic acid (1 ml) was added dropwise. Pyridine (approximately 1 ml) was added and the mixture was reduced to dryness at 343 K on a rotary evaporator. Further pyridine (5 ml) was added and a pink precipitate was formed by addition of hexane (30 ml). The precipitate was dissolved in chloroform and mixed crystals (blue and red) were grown by vapour transport of diethyl ether. The blue crystals were shown to be pyridinium trichloropyridinecobalt(II) (Hahn *et al.*, 1997) by X-ray single-crystal analysis and the red crystals the title compound, (I).

Crystal data

$[Co_2(C_2F_3O_2)_4(C_5H_5N)_4(H_2O)]$
M_r = 903.86
Triclinic, $P\overline{1}$
a = 9.4211 (19) Å
b = 10.741 (2) Å
c = 19.185 (4) Å
α = 78.17 (3)°
β = 79.00 (3)°
γ = 76.00 (3)°
V = 1823.2 (6) Å^3
Z = 2
D_x = 1.647 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13594 reflections
θ = 1–27.5°
μ = 1.02 mm^{-1}
T = 180 (2) K
Block, red
0.28 × 0.10 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Thin–slice ω and φ scans
Absorption correction: multi-scan (SORTAV; Blessing 1995)
T_{min} = 0.775, T_{max} = 0.890
19699 measured reflections
8305 independent reflections
6603 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 27.5°
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -20 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.240
S = 1.05
8305 reflections
483 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.128P)^2 + 5.9158P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 1.69 e Å^{-3}
$\Delta\rho_{min}$ = −1.14 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O*W*	2.190 (3)	Co2—O*W*	2.196 (3)
Co1—O2*A*	2.070 (4)	Co2—O1*A*	2.095 (4)
Co1—O8*A*	2.092 (4)	Co2—O3*A*	2.074 (4)
Co1—O3*B*	2.098 (4)	Co2—O2*B*	2.095 (4)
Co1—N6	2.128 (4)	Co2—N5	2.124 (4)
Co1—N4	2.139 (4)	Co2—N7	2.138 (4)
Co1—O*W*—Co2	116.86 (15)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O*W*—H1···O8*B*	0.96 (5)	1.67 (5)	2.616 (5)	165 (5)
O*W*—H2···O1*B*	0.96 (5)	1.68 (5)	2.610 (5)	161 (4)

Difference maps indicated that the F atoms attached to C2*B* and C8*B* were disordered over two sets of positions. Refined occupancies (sum constrained to unity) of 0.667 (6):0.333 (6) and 0.601 (6):0.399 (6) resulted for the major and minor components of C2*B* and C8*B*, respectively. The disordered F atoms were modelled with isotropic displacement parameters. The F atoms around C1*B* and C3*B* may also be slightly disordered but this was not resolved in the present data. The water molecule H atoms were located in a difference map and refined with distance restraints (O—H = 0.96 Å). Pyridine H atoms were placed in idealized locations (C—H = 0.93 Å)

and refined as riding with the constraint $U_{iso}(H) = 1.2U_{eq}$(carrier) applied. The higest peak and depest hole in are located 1.51 Å from atom F1*C* and 0.49 Å from F2*A*, respectively.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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supporting information

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Crystal data

$[Co_2(C_2F_3O_2)_4(C_5H_5N)_4(H_2O)]$
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$V = 1823.2$ (6) Å^3
$Z = 2$
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Cell parameters from 13594 reflections
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$R_{int} = 0.044$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.1°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -20 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.079$
$wR(F^2) = 0.240$
$S = 1.05$
8305 reflections
483 parameters
16 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.128P)^2 + 5.9158P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.007$
$\Delta\rho_{max} = 1.69$ e Å^{-3}
$\Delta\rho_{min} = -1.14$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
OW	0.8111 (4)	0.5602 (3)	0.80300 (17)	0.0325 (7)	
H1	0.875 (5)	0.495 (4)	0.832 (3)	0.049*	
H2	0.731 (5)	0.602 (4)	0.835 (3)	0.049*	
Co1	0.75575 (7)	0.43208 (6)	0.74168 (3)	0.03078 (19)	
O1A	0.7439 (4)	0.8520 (4)	0.8004 (2)	0.0432 (8)	
O1B	0.6169 (4)	0.7176 (4)	0.8787 (2)	0.0449 (9)	
C1A	0.6472 (6)	0.8250 (5)	0.8512 (3)	0.0376 (10)	
F1A	0.4503 (6)	0.9173 (5)	0.9354 (3)	0.108 (2)	
F1C	0.6181 (9)	1.0246 (8)	0.8887 (6)	0.182 (5)	
C1B	0.5541 (10)	0.9408 (7)	0.8851 (5)	0.081 (3)	
F1B	0.4701 (11)	1.0206 (8)	0.8345 (5)	0.191 (5)	
Co2	0.90291 (7)	0.72589 (6)	0.74067 (3)	0.03106 (19)	
O2A	0.6358 (4)	0.5935 (3)	0.6830 (2)	0.0441 (9)	
O2B	0.7542 (5)	0.7579 (4)	0.6672 (2)	0.0480 (9)	
C2A	0.6589 (6)	0.7035 (5)	0.6582 (3)	0.0359 (10)	
C2B	0.5493 (8)	0.7866 (6)	0.6081 (4)	0.0609 (18)	
F2A	0.4625 (9)	0.7260 (8)	0.5897 (5)	0.0837 (11)*	0.667 (6)
F2B	0.6149 (9)	0.8563 (8)	0.5503 (4)	0.0837 (11)*	0.667 (6)
F2C	0.4552 (8)	0.8798 (7)	0.6448 (4)	0.0837 (11)*	0.667 (6)
F2D	0.5610 (18)	0.7183 (14)	0.5521 (8)	0.0837 (11)*	0.333 (6)
F2E	0.5702 (19)	0.8963 (14)	0.5738 (9)	0.0837 (11)*	0.333 (6)
F2F	0.4173 (16)	0.7542 (16)	0.6202 (9)	0.0837 (11)*	0.333 (6)
O3B	0.9538 (4)	0.4397 (4)	0.6707 (2)	0.0486 (9)	
O3A	1.0612 (4)	0.5987 (4)	0.6834 (2)	0.0435 (8)	
C3A	1.0552 (6)	0.4995 (5)	0.6616 (3)	0.0351 (10)	
F3B	1.3030 (5)	0.5039 (5)	0.6050 (4)	0.103 (2)	
F3A	1.2554 (6)	0.3208 (5)	0.6491 (4)	0.122 (3)	
C3B	1.1984 (7)	0.4383 (6)	0.6168 (4)	0.0582 (17)	
F3C	1.1738 (8)	0.4187 (9)	0.5557 (3)	0.137 (3)	
N4	0.5589 (5)	0.4119 (4)	0.8160 (2)	0.0401 (9)	
O8A	0.8737 (4)	0.2687 (3)	0.8022 (2)	0.0419 (8)	
O8B	0.9599 (5)	0.3560 (4)	0.8782 (2)	0.0475 (9)	
C8A	0.9430 (6)	0.2653 (5)	0.8516 (3)	0.0390 (11)	
C8B	1.0187 (10)	0.1290 (7)	0.8844 (4)	0.077 (2)	
C4A	0.4348 (6)	0.4159 (6)	0.7909 (3)	0.0486 (13)	

H4A	0.4332	0.4391	0.7405	0.058*	
C4B	0.3082 (7)	0.3877 (7)	0.8353 (4)	0.0615 (17)	
H4B	0.2223	0.3898	0.8157	0.074*	
C4E	0.5572 (7)	0.3835 (6)	0.8873 (3)	0.0507 (13)	
H4E	0.6440	0.3822	0.9060	0.061*	
C4C	0.3096 (8)	0.3570 (8)	0.9075 (5)	0.071 (2)	
H4C	0.2246	0.3363	0.9391	0.085*	
C4D	0.4353 (8)	0.3561 (8)	0.9346 (4)	0.0657 (18)	
H4D	0.4376	0.3368	0.9850	0.079*	
N5	0.9907 (5)	0.8835 (4)	0.6762 (2)	0.0359 (9)	
C5A	1.0482 (7)	0.8827 (6)	0.6064 (3)	0.0495 (13)	
H5A	1.0442	0.8112	0.5853	0.059*	
C5E	0.9932 (6)	0.9868 (5)	0.7033 (3)	0.0454 (12)	
H5E	0.9520	0.9902	0.7523	0.054*	
C5B	1.1123 (8)	0.9795 (7)	0.5641 (3)	0.0597 (16)	
H5B	1.1548	0.9737	0.5156	0.072*	
C5C	1.1137 (8)	1.0870 (7)	0.5942 (4)	0.0622 (16)*	
C5D	1.0530 (8)	1.0900 (6)	0.6637 (4)	0.0597 (17)	
H5D	1.0513	1.1625	0.6853	0.072*	
H5C	1.1556	1.1551	0.5658	0.072*	
N6	0.7082 (5)	0.3138 (4)	0.6763 (2)	0.0361 (9)	
C6A	0.6750 (7)	0.1987 (5)	0.7047 (3)	0.0457 (12)	
H6A	0.6788	0.1675	0.7545	0.055*	
C6E	0.7040 (8)	0.3553 (6)	0.6064 (3)	0.0515 (14)	
H6E	0.7312	0.4358	0.5851	0.062*	
C6B	0.6350 (8)	0.1223 (6)	0.6646 (4)	0.0558 (15)	
H6B	0.6141	0.0396	0.6863	0.067*	
C6C	0.6263 (9)	0.1681 (7)	0.5935 (4)	0.0636 (18)	
H6C	0.5961	0.1188	0.5653	0.076*	
C6D	0.6613 (9)	0.2861 (7)	0.5629 (4)	0.0653 (19)	
H6D	0.6566	0.3196	0.5134	0.078*	
N7	1.0523 (5)	0.7046 (4)	0.8154 (2)	0.0395 (9)	
C7A	1.0107 (7)	0.6884 (6)	0.8869 (3)	0.0491 (13)	
H7A	0.9130	0.6771	0.9056	0.059*	
C7E	1.1934 (6)	0.7171 (6)	0.7901 (4)	0.0492 (13)	
H7E	1.2260	0.7259	0.7397	0.059*	
C7D	1.2906 (7)	0.7176 (8)	0.8348 (5)	0.0659 (19)	
H7D	1.3885	0.7275	0.8153	0.079*	
C7B	1.1037 (9)	0.6876 (8)	0.9345 (4)	0.0683 (19)	
H7B	1.0708	0.6761	0.9849	0.082*	
C7C	1.2463 (9)	0.7039 (8)	0.9070 (5)	0.072 (2)	
H7C	1.3124	0.7055	0.9384	0.086*	
F8A	1.0761 (11)	0.1202 (10)	0.9415 (5)	0.0867 (12)*	0.601 (6)
F8B	0.9509 (11)	0.0371 (8)	0.8859 (5)	0.0867 (12)*	0.601 (6)
F8C	1.1380 (10)	0.0858 (9)	0.8306 (5)	0.0867 (12)*	0.601 (6)
F8D	0.9046 (14)	0.0914 (13)	0.9388 (7)	0.0867 (12)*	0.399 (6)
F8E	1.0324 (16)	0.0358 (12)	0.8542 (7)	0.0867 (12)*	0.399 (6)
F8F	1.1253 (15)	0.1243 (15)	0.9209 (8)	0.0867 (12)*	0.399 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
OW	0.0359 (17)	0.0322 (16)	0.0318 (16)	−0.0106 (13)	−0.0049 (13)	−0.0069 (13)
Co1	0.0328 (3)	0.0318 (3)	0.0303 (3)	−0.0115 (2)	−0.0053 (2)	−0.0046 (2)
O1A	0.042 (2)	0.0395 (19)	0.044 (2)	−0.0085 (15)	0.0040 (16)	−0.0087 (15)
O1B	0.041 (2)	0.044 (2)	0.050 (2)	−0.0133 (16)	0.0034 (16)	−0.0105 (16)
C1A	0.035 (2)	0.043 (3)	0.037 (2)	−0.009 (2)	−0.002 (2)	−0.012 (2)
F1A	0.110 (4)	0.076 (3)	0.109 (4)	−0.014 (3)	0.064 (3)	−0.032 (3)
F1C	0.132 (6)	0.155 (7)	0.292 (11)	−0.070 (5)	0.087 (7)	−0.176 (8)
C1B	0.087 (6)	0.048 (4)	0.095 (6)	−0.020 (4)	0.037 (5)	−0.026 (4)
F1B	0.178 (8)	0.113 (6)	0.184 (8)	0.073 (6)	0.044 (7)	0.003 (6)
Co2	0.0314 (3)	0.0319 (3)	0.0330 (3)	−0.0106 (2)	−0.0054 (2)	−0.0071 (2)
O2A	0.050 (2)	0.0360 (18)	0.051 (2)	−0.0164 (16)	−0.0219 (18)	0.0035 (15)
O2B	0.054 (2)	0.047 (2)	0.053 (2)	−0.0246 (18)	−0.0252 (19)	0.0020 (17)
C2A	0.039 (3)	0.038 (2)	0.034 (2)	−0.010 (2)	−0.0078 (19)	−0.0083 (19)
C2B	0.084 (5)	0.048 (3)	0.066 (4)	−0.036 (3)	−0.046 (4)	0.014 (3)
O3B	0.047 (2)	0.053 (2)	0.051 (2)	−0.0250 (18)	0.0100 (17)	−0.0207 (18)
O3A	0.0418 (19)	0.0413 (19)	0.052 (2)	−0.0151 (15)	0.0032 (16)	−0.0197 (16)
C3A	0.039 (2)	0.032 (2)	0.035 (2)	−0.0125 (19)	−0.0007 (19)	−0.0056 (18)
F3B	0.067 (3)	0.086 (3)	0.158 (5)	−0.044 (3)	0.055 (3)	−0.058 (3)
F3A	0.071 (3)	0.060 (3)	0.198 (7)	0.007 (2)	0.032 (4)	−0.009 (3)
C3B	0.053 (4)	0.051 (3)	0.072 (4)	−0.021 (3)	0.016 (3)	−0.026 (3)
F3C	0.117 (5)	0.216 (8)	0.094 (4)	−0.044 (5)	0.039 (4)	−0.099 (5)
N4	0.034 (2)	0.046 (2)	0.042 (2)	−0.0141 (18)	−0.0018 (17)	−0.0067 (18)
O8A	0.045 (2)	0.0383 (18)	0.044 (2)	−0.0053 (15)	−0.0149 (16)	−0.0056 (15)
O8B	0.051 (2)	0.042 (2)	0.054 (2)	−0.0095 (17)	−0.0211 (18)	−0.0057 (17)
C8A	0.035 (2)	0.041 (3)	0.039 (3)	−0.008 (2)	−0.007 (2)	−0.001 (2)
C8B	0.107 (6)	0.052 (4)	0.082 (5)	−0.013 (4)	−0.055 (5)	−0.003 (3)
C4A	0.038 (3)	0.058 (3)	0.053 (3)	−0.016 (2)	−0.005 (2)	−0.011 (3)
C4B	0.036 (3)	0.079 (5)	0.075 (5)	−0.026 (3)	−0.001 (3)	−0.018 (4)
C4E	0.051 (3)	0.056 (3)	0.040 (3)	−0.014 (3)	0.001 (2)	−0.002 (2)
C4C	0.050 (4)	0.076 (5)	0.082 (5)	−0.027 (3)	0.021 (4)	−0.015 (4)
C4D	0.059 (4)	0.077 (5)	0.051 (4)	−0.020 (3)	0.013 (3)	−0.002 (3)
N5	0.038 (2)	0.033 (2)	0.039 (2)	−0.0112 (16)	−0.0059 (17)	−0.0057 (16)
C5A	0.067 (4)	0.045 (3)	0.038 (3)	−0.018 (3)	−0.001 (3)	−0.010 (2)
C5E	0.051 (3)	0.042 (3)	0.047 (3)	−0.019 (2)	0.003 (2)	−0.015 (2)
C5B	0.075 (4)	0.058 (4)	0.043 (3)	−0.022 (3)	0.006 (3)	−0.007 (3)
C5D	0.071 (4)	0.041 (3)	0.071 (4)	−0.027 (3)	0.010 (3)	−0.019 (3)
N6	0.042 (2)	0.036 (2)	0.034 (2)	−0.0137 (17)	−0.0087 (17)	−0.0051 (16)
C6A	0.060 (3)	0.036 (3)	0.045 (3)	−0.018 (2)	−0.011 (3)	−0.002 (2)
C6E	0.078 (4)	0.044 (3)	0.039 (3)	−0.026 (3)	−0.010 (3)	−0.006 (2)
C6B	0.068 (4)	0.042 (3)	0.067 (4)	−0.023 (3)	−0.014 (3)	−0.013 (3)
C6C	0.085 (5)	0.059 (4)	0.063 (4)	−0.024 (3)	−0.022 (4)	−0.026 (3)
C6D	0.101 (6)	0.066 (4)	0.041 (3)	−0.030 (4)	−0.019 (3)	−0.014 (3)
N7	0.034 (2)	0.045 (2)	0.042 (2)	−0.0100 (18)	−0.0127 (18)	−0.0066 (18)
C7A	0.047 (3)	0.062 (4)	0.042 (3)	−0.013 (3)	−0.009 (2)	−0.014 (3)
C7E	0.040 (3)	0.056 (3)	0.055 (3)	−0.016 (2)	−0.011 (2)	−0.006 (3)

C7D	0.042 (3)	0.078 (5)	0.087 (5)	−0.023 (3)	−0.025 (3)	−0.010 (4)
C7B	0.075 (5)	0.086 (5)	0.051 (4)	−0.009 (4)	−0.029 (3)	−0.020 (3)
C7C	0.066 (4)	0.082 (5)	0.082 (5)	−0.015 (4)	−0.046 (4)	−0.015 (4)

Geometric parameters (Å, º)

Co1—OW	2.190 (3)	C8B—F8D	1.420 (13)
Co1—O2A	2.070 (4)	C8B—F8C	1.430 (11)
Co1—O8A	2.092 (4)	C4A—C4B	1.386 (8)
Co1—O3B	2.098 (4)	C4A—H4A	0.9500
Co1—N6	2.128 (4)	C4B—C4C	1.358 (11)
Co1—N4	2.139 (4)	C4B—H4B	0.9500
Co2—OW	2.196 (3)	C4E—C4D	1.373 (8)
Co2—O1A	2.095 (4)	C4E—H4E	0.9500
Co2—O3A	2.074 (4)	C4C—C4D	1.379 (11)
Co2—O2B	2.095 (4)	C4C—H4C	0.9500
Co2—N5	2.124 (4)	C4D—H4D	0.9500
Co2—N7	2.138 (4)	N5—C5E	1.325 (7)
OW—H1	0.962 (10)	N5—C5A	1.346 (7)
OW—H2	0.961 (10)	C5A—C5B	1.369 (9)
O1A—C1A	1.240 (6)	C5A—H5A	0.9500
O1B—C1A	1.241 (6)	C5E—C5D	1.384 (8)
C1A—C1B	1.526 (8)	C5E—H5E	0.9500
F1A—C1B	1.270 (9)	C5B—C5C	1.395 (10)
F1C—C1B	1.217 (10)	C5B—H5B	0.9500
C1B—F1B	1.388 (14)	C5C—C5D	1.351 (10)
O2A—C2A	1.235 (6)	C5C—H5C	0.9387
O2B—C2A	1.238 (6)	C5D—H5D	0.9500
C2A—C2B	1.538 (8)	N6—C6E	1.329 (7)
C2B—F2E	1.267 (13)	N6—C6A	1.330 (7)
C2B—F2A	1.295 (9)	C6A—C6B	1.388 (8)
C2B—F2F	1.338 (13)	C6A—H6A	0.9500
C2B—F2B	1.338 (9)	C6E—C6D	1.391 (8)
C2B—F2C	1.381 (9)	C6E—H6E	0.9500
C2B—F2D	1.392 (13)	C6B—C6C	1.362 (10)
F2D—F2F	1.72 (2)	C6B—H6B	0.9500
O3B—C3A	1.242 (6)	C6C—C6D	1.372 (10)
O3A—C3A	1.239 (6)	C6C—H6C	0.9500
C3A—C3B	1.533 (8)	C6D—H6D	0.9500
F3B—C3B	1.306 (7)	N7—C7A	1.339 (7)
F3A—C3B	1.320 (9)	N7—C7E	1.354 (7)
C3B—F3C	1.303 (9)	C7A—C7B	1.377 (8)
N4—C4A	1.335 (7)	C7A—H7A	0.9500
N4—C4E	1.337 (7)	C7E—C7D	1.371 (9)
O8A—C8A	1.239 (6)	C7E—H7E	0.9500
O8B—C8A	1.243 (7)	C7D—C7C	1.355 (11)
C8A—C8B	1.529 (9)	C7D—H7D	0.9500
C8B—F8E	1.226 (12)	C7B—C7C	1.386 (12)

C8B—F8A	1.287 (11)	C7B—H7B	0.9500
C8B—F8B	1.293 (10)	C7C—H7C	0.9500
C8B—F8F	1.315 (13)		

Co1—OW—Co2	116.86 (15)	O8B—C8A—C8B	115.5 (5)
Co1—OW—H1	98 (3)	F8E—C8B—F8A	122.6 (10)
Co2—OW—H1	117 (3)	F8E—C8B—F8B	41.0 (7)
Co1—OW—H2	116 (3)	F8A—C8B—F8B	114.4 (8)
Co2—OW—H2	102 (3)	F8E—C8B—F8F	115.8 (11)
H1—OW—H2	107 (5)	F8A—C8B—F8F	24.5 (7)
O2A—Co1—O8A	179.02 (16)	F8B—C8B—F8F	127.1 (10)
O2A—Co1—O3B	93.75 (17)	F8E—C8B—F8D	93.7 (10)
O8A—Co1—O3B	87.23 (17)	F8A—C8B—F8D	79.2 (8)
O2A—Co1—N6	88.85 (15)	F8B—C8B—F8D	53.6 (7)
O8A—Co1—N6	91.20 (15)	F8F—C8B—F8D	103.2 (10)
O3B—Co1—N6	87.56 (16)	F8E—C8B—F8C	53.6 (8)
O2A—Co1—N4	89.42 (17)	F8A—C8B—F8C	106.4 (8)
O8A—Co1—N4	89.59 (17)	F8B—C8B—F8C	94.6 (7)
O3B—Co1—N4	176.51 (17)	F8F—C8B—F8C	83.9 (9)
N6—Co1—N4	91.05 (17)	F8D—C8B—F8C	145.1 (8)
O2A—Co1—OW	89.35 (14)	F8E—C8B—C8A	120.7 (8)
O8A—Co1—OW	90.66 (13)	F8A—C8B—C8A	116.5 (7)
O3B—Co1—OW	89.57 (14)	F8B—C8B—C8A	115.6 (7)
N6—Co1—OW	176.51 (14)	F8F—C8B—C8A	115.5 (8)
N4—Co1—OW	91.92 (15)	F8D—C8B—C8A	101.7 (8)
C1A—O1A—Co2	128.6 (3)	F8C—C8B—C8A	105.8 (6)
O1B—C1A—O1A	129.4 (5)	N4—C4A—C4B	122.8 (6)
O1B—C1A—C1B	115.8 (5)	N4—C4A—H4A	118.6
O1A—C1A—C1B	114.8 (5)	C4B—C4A—H4A	118.6
F1C—C1B—F1A	118.0 (8)	C4C—C4B—C4A	118.7 (6)
F1C—C1B—F1B	93.7 (9)	C4C—C4B—H4B	120.7
F1A—C1B—F1B	99.2 (8)	C4A—C4B—H4B	120.7
F1C—C1B—C1A	116.5 (7)	N4—C4E—C4D	122.8 (6)
F1A—C1B—C1A	116.3 (6)	N4—C4E—H4E	118.6
F1B—C1B—C1A	107.6 (8)	C4D—C4E—H4E	118.6
O3A—Co2—O1A	178.90 (16)	C4B—C4C—C4D	119.4 (6)
O3A—Co2—O2B	92.81 (17)	C4B—C4C—H4C	120.3
O1A—Co2—O2B	88.01 (17)	C4D—C4C—H4C	120.3
O3A—Co2—N5	89.26 (16)	C4E—C4D—C4C	118.7 (7)
O1A—Co2—N5	91.51 (15)	C4E—C4D—H4D	120.6
O2B—Co2—N5	87.48 (16)	C4C—C4D—H4D	120.6
O3A—Co2—N7	89.36 (17)	C5E—N5—C5A	116.9 (5)
O1A—Co2—N7	89.85 (17)	C5E—N5—Co2	121.3 (4)
O2B—Co2—N7	176.81 (16)	C5A—N5—Co2	121.9 (4)
N5—Co2—N7	90.22 (17)	N5—C5A—C5B	123.5 (5)
O3A—Co2—OW	89.27 (14)	N5—C5A—H5A	118.3
O1A—Co2—OW	89.99 (14)	C5B—C5A—H5A	118.3
O2B—Co2—OW	90.54 (14)	N5—C5E—C5D	123.1 (5)

N5—Co2—OW	177.47 (14)	N5—C5E—H5E	118.4
N7—Co2—OW	91.82 (15)	C5D—C5E—H5E	118.4
C2A—O2A—Co1	132.4 (3)	C5A—C5B—C5C	118.4 (6)
C2A—O2B—Co2	136.1 (4)	C5A—C5B—H5B	120.8
O2A—C2A—O2B	130.9 (5)	C5C—C5B—H5B	120.8
O2A—C2A—C2B	114.1 (4)	C5D—C5C—C5B	118.5 (6)
O2B—C2A—C2B	115.0 (4)	C5D—C5C—H5C	121.8
F2E—C2B—F2A	122.0 (9)	C5B—C5C—H5C	119.7
F2E—C2B—F2F	122.6 (11)	C5C—C5D—C5E	119.6 (6)
F2A—C2B—F2F	32.1 (7)	C5C—C5D—H5D	120.2
F2E—C2B—F2B	30.8 (7)	C5E—C5D—H5D	120.2
F2A—C2B—F2B	111.0 (7)	C6E—N6—C6A	117.8 (5)
F2F—C2B—F2B	130.4 (9)	C6E—N6—Co1	121.0 (3)
F2E—C2B—F2C	73.1 (9)	C6A—N6—Co1	121.1 (4)
F2A—C2B—F2C	104.6 (7)	N6—C6A—C6B	122.7 (5)
F2F—C2B—F2C	74.8 (9)	N6—C6A—H6A	118.6
F2B—C2B—F2C	103.7 (6)	C6B—C6A—H6A	118.6
F2E—C2B—F2D	101.6 (11)	N6—C6E—C6D	122.9 (5)
F2A—C2B—F2D	46.2 (7)	N6—C6E—H6E	118.6
F2F—C2B—F2D	78.2 (10)	C6D—C6E—H6E	118.6
F2B—C2B—F2D	75.4 (8)	C6C—C6B—C6A	118.7 (6)
F2C—C2B—F2D	142.9 (9)	C6C—C6B—H6B	120.6
F2E—C2B—C2A	119.8 (9)	C6A—C6B—H6B	120.6
F2A—C2B—C2A	115.9 (6)	C6B—C6C—C6D	119.5 (6)
F2F—C2B—C2A	114.7 (8)	C6B—C6C—H6C	120.2
F2B—C2B—C2A	112.8 (6)	C6D—C6C—H6C	120.2
F2C—C2B—C2A	107.7 (5)	C6C—C6D—C6E	118.3 (6)
F2D—C2B—C2A	106.5 (8)	C6C—C6D—H6D	120.9
C2B—F2D—F2F	49.5 (7)	C6E—C6D—H6D	120.9
C2B—F2F—F2D	52.3 (7)	C7A—N7—C7E	117.6 (5)
C3A—O3B—Co1	136.5 (3)	C7A—N7—Co2	123.1 (4)
C3A—O3A—Co2	131.9 (3)	C7E—N7—Co2	119.1 (4)
O3A—C3A—O3B	131.1 (5)	N7—C7A—C7B	122.8 (6)
O3A—C3A—C3B	114.6 (5)	N7—C7A—H7A	118.6
O3B—C3A—C3B	114.3 (4)	C7B—C7A—H7A	118.6
F3C—C3B—F3B	109.6 (7)	N7—C7E—C7D	122.1 (6)
F3C—C3B—F3A	103.9 (7)	N7—C7E—H7E	118.9
F3B—C3B—F3A	105.8 (7)	C7D—C7E—H7E	118.9
F3C—C3B—C3A	111.5 (6)	C7C—C7D—C7E	119.7 (7)
F3B—C3B—C3A	114.2 (5)	C7C—C7D—H7D	120.1
F3A—C3B—C3A	111.3 (6)	C7E—C7D—H7D	120.1
C4A—N4—C4E	117.6 (5)	C7A—C7B—C7C	118.4 (7)
C4A—N4—Co1	119.4 (4)	C7A—C7B—H7B	120.8
C4E—N4—Co1	122.7 (4)	C7C—C7B—H7B	120.8
C8A—O8A—Co1	128.1 (3)	C7D—C7C—C7B	119.3 (6)
O8A—C8A—O8B	129.6 (5)	C7D—C7C—H7C	120.4
O8A—C8A—C8B	114.9 (5)	C7B—C7C—H7C	120.4

Co2—OW—Co1—O2A	−51.18 (18)	O8A—Co1—N4—C4E	42.2 (5)
Co2—OW—Co1—O8A	129.80 (18)	N6—Co1—N4—C4E	133.4 (5)
Co2—OW—Co1—O3B	42.57 (19)	OW—Co1—N4—C4E	−48.4 (5)
Co2—OW—Co1—N4	−140.58 (19)	O3B—Co1—O8A—C8A	88.9 (5)
Co2—O1A—C1A—O1B	−2.0 (9)	N6—Co1—O8A—C8A	176.4 (5)
Co2—O1A—C1A—C1B	177.1 (5)	N4—Co1—O8A—C8A	−92.5 (5)
O1B—C1A—C1B—F1C	142.9 (10)	OW—Co1—O8A—C8A	−0.6 (5)
O1A—C1A—C1B—F1C	−36.3 (13)	Co1—O8A—C8A—O8B	0.5 (9)
O1B—C1A—C1B—F1A	−3.5 (12)	Co1—O8A—C8A—C8B	−179.4 (4)
O1A—C1A—C1B—F1A	177.4 (8)	O8A—C8A—C8B—F8E	13.5 (13)
O1B—C1A—C1B—F1B	−113.5 (8)	O8B—C8A—C8B—F8E	−166.5 (11)
O1A—C1A—C1B—F1B	67.3 (9)	O8A—C8A—C8B—F8A	−171.7 (8)
C1A—O1A—Co2—O2B	92.7 (5)	O8B—C8A—C8B—F8A	8.3 (11)
C1A—O1A—Co2—N5	−179.9 (5)	O8A—C8A—C8B—F8B	−33.0 (10)
C1A—O1A—Co2—N7	−89.7 (5)	O8B—C8A—C8B—F8B	147.1 (8)
C1A—O1A—Co2—OW	2.1 (5)	O8A—C8A—C8B—F8F	161.0 (9)
Co1—OW—Co2—O3A	−52.61 (18)	O8B—C8A—C8B—F8F	−18.9 (12)
Co1—OW—Co2—O1A	128.20 (18)	O8A—C8A—C8B—F8D	−88.0 (8)
Co1—OW—Co2—O2B	40.19 (19)	O8B—C8A—C8B—F8D	92.0 (8)
Co1—OW—Co2—N7	−141.95 (19)	O8A—C8A—C8B—F8C	70.2 (7)
O3B—Co1—O2A—C2A	−49.6 (5)	O8B—C8A—C8B—F8C	−109.7 (6)
N6—Co1—O2A—C2A	−137.0 (5)	C4E—N4—C4A—C4B	−2.3 (9)
N4—Co1—O2A—C2A	131.9 (5)	Co1—N4—C4A—C4B	171.8 (5)
OW—Co1—O2A—C2A	40.0 (5)	N4—C4A—C4B—C4C	1.2 (11)
O3A—Co2—O2B—C2A	85.3 (6)	C4A—N4—C4E—C4D	1.4 (9)
O1A—Co2—O2B—C2A	−93.9 (6)	Co1—N4—C4E—C4D	−172.4 (5)
N5—Co2—O2B—C2A	174.5 (6)	C4A—C4B—C4C—C4D	0.7 (11)
OW—Co2—O2B—C2A	−4.0 (6)	N4—C4E—C4D—C4C	0.4 (11)
Co1—O2A—C2A—O2B	−9.2 (9)	C4B—C4C—C4D—C4E	−1.5 (12)
Co1—O2A—C2A—C2B	171.3 (4)	O3A—Co2—N5—C5E	−145.3 (4)
Co2—O2B—C2A—O2A	−15.6 (10)	O1A—Co2—N5—C5E	33.9 (4)
Co2—O2B—C2A—C2B	163.9 (5)	O2B—Co2—N5—C5E	121.9 (4)
O2A—C2A—C2B—F2E	−173.1 (11)	N7—Co2—N5—C5E	−55.9 (4)
O2B—C2A—C2B—F2E	7.3 (13)	O3A—Co2—N5—C5A	33.7 (5)
O2A—C2A—C2B—F2A	−10.0 (9)	O1A—Co2—N5—C5A	−147.1 (5)
O2B—C2A—C2B—F2A	170.5 (7)	O2B—Co2—N5—C5A	−59.1 (5)
O2A—C2A—C2B—F2F	25.6 (12)	N7—Co2—N5—C5A	123.1 (5)
O2B—C2A—C2B—F2F	−154.0 (10)	C5E—N5—C5A—C5B	2.4 (9)
O2A—C2A—C2B—F2B	−139.5 (6)	Co2—N5—C5A—C5B	−176.7 (5)
O2B—C2A—C2B—F2B	40.9 (8)	C5A—N5—C5E—C5D	−0.8 (9)
O2A—C2A—C2B—F2C	106.7 (6)	Co2—N5—C5E—C5D	178.2 (5)
O2B—C2A—C2B—F2C	−72.9 (7)	N5—C5A—C5B—C5C	−2.3 (11)
O2A—C2A—C2B—F2D	−58.8 (9)	C5A—C5B—C5C—C5D	0.6 (11)
O2B—C2A—C2B—F2D	121.6 (8)	C5B—C5C—C5D—C5E	0.8 (11)
F2E—C2B—F2D—F2F	−121.2 (12)	N5—C5E—C5D—C5C	−0.7 (11)
F2A—C2B—F2D—F2F	2.3 (11)	O2A—Co1—N6—C6E	37.2 (5)
F2B—C2B—F2D—F2F	−137.6 (9)	O8A—Co1—N6—C6E	−143.8 (5)
F2C—C2B—F2D—F2F	−44.0 (14)	O3B—Co1—N6—C6E	−56.6 (5)

C2A—C2B—F2D—F2F	112.6 (9)	N4—Co1—N6—C6E	126.6 (5)
F2E—C2B—F2F—F2D	96.4 (14)	O2A—Co1—N6—C6A	−139.6 (4)
F2A—C2B—F2F—F2D	−3.1 (15)	O8A—Co1—N6—C6A	39.4 (4)
F2B—C2B—F2F—F2D	59.0 (13)	O3B—Co1—N6—C6A	126.6 (4)
F2C—C2B—F2F—F2D	154.3 (9)	N4—Co1—N6—C6A	−50.2 (4)
C2A—C2B—F2F—F2D	−102.9 (9)	C6E—N6—C6A—C6B	−0.8 (9)
O2A—Co1—O3B—C3A	83.4 (6)	Co1—N6—C6A—C6B	176.1 (5)
O8A—Co1—O3B—C3A	−96.5 (6)	C6A—N6—C6E—C6D	2.4 (10)
N6—Co1—O3B—C3A	172.1 (6)	Co1—N6—C6E—C6D	−174.5 (6)
OW—Co1—O3B—C3A	−5.9 (6)	N6—C6A—C6B—C6C	−1.4 (10)
O2B—Co2—O3A—C3A	−53.4 (5)	C6A—C6B—C6C—C6D	2.0 (11)
N5—Co2—O3A—C3A	−140.9 (5)	C6B—C6C—C6D—C6E	−0.4 (12)
N7—Co2—O3A—C3A	128.9 (5)	N6—C6E—C6D—C6C	−1.9 (12)
OW—Co2—O3A—C3A	37.1 (5)	O3A—Co2—N7—C7A	−136.1 (5)
Co2—O3A—C3A—O3B	−4.9 (9)	O1A—Co2—N7—C7A	43.2 (5)
Co2—O3A—C3A—C3B	176.5 (4)	N5—Co2—N7—C7A	134.7 (5)
Co1—O3B—C3A—O3A	−16.9 (10)	OW—Co2—N7—C7A	−46.8 (5)
Co1—O3B—C3A—C3B	161.7 (5)	O3A—Co2—N7—C7E	48.8 (4)
O3A—C3A—C3B—F3C	−128.4 (7)	O1A—Co2—N7—C7E	−132.0 (4)
O3B—C3A—C3B—F3C	52.7 (8)	N5—Co2—N7—C7E	−40.5 (4)
O3A—C3A—C3B—F3B	−3.6 (9)	OW—Co2—N7—C7E	138.1 (4)
O3B—C3A—C3B—F3B	177.6 (6)	C7E—N7—C7A—C7B	1.8 (9)
O3A—C3A—C3B—F3A	116.1 (6)	Co2—N7—C7A—C7B	−173.4 (5)
O3B—C3A—C3B—F3A	−62.8 (8)	C7A—N7—C7E—C7D	−2.0 (9)
O2A—Co1—N4—C4A	48.5 (4)	Co2—N7—C7E—C7D	173.4 (5)
O8A—Co1—N4—C4A	−131.5 (4)	N7—C7E—C7D—C7C	0.7 (11)
N6—Co1—N4—C4A	−40.3 (4)	N7—C7A—C7B—C7C	−0.2 (11)
OW—Co1—N4—C4A	137.8 (4)	C7E—C7D—C7C—C7B	1.0 (12)
O2A—Co1—N4—C4E	−137.7 (5)	C7A—C7B—C7C—C7D	−1.2 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O*W*—H1···O8*B*	0.96 (5)	1.67 (5)	2.616 (5)	165 (5)
O*W*—H2···O1*B*	0.96 (5)	1.68 (5)	2.610 (5)	161 (4)