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Tetrakis(μ-2-phenylacetato-κ^2O:O')bis{[4-(dimethylamino)pyridine-κN^1]cobalt(II)}

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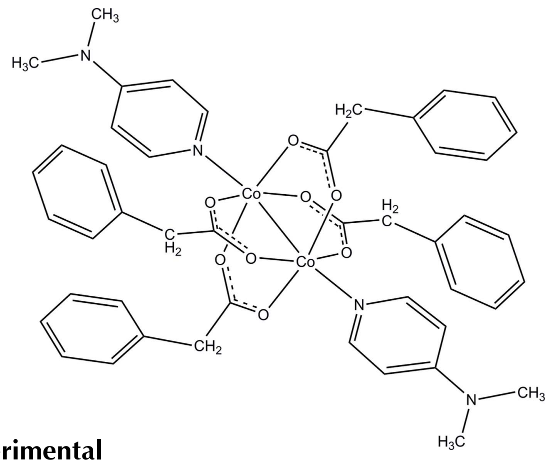
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.025; wR factor = 0.060; data-to-parameter ratio = 13.5.

The title compound, $[Co_2(C_8H_7O_2)_4(C_7H_{10}N_2)_2]$, crystallizes as a centrosymmetric dimer containing two Co^{II} atoms bridged by four bidentate phenylacetate ligands in *syn–syn* bridging modes. Each Co^{II} atom is five-coordinated by four O atoms from four different carboxylate ligands and the ring N atom of a 4-(dimethylamino)pyridine unit, generating a distorted square-pyramidal geometry in which the four O atoms form the basal plane and the N atom occupies the axial position. In the crystal, C—H$\cdots$O interactions link the dinuclear complex molecules into a three-dimensional network.

Related literature

For properties of the 4-(dimethylamino)pyridine ligand as a homogeneous catalyst, see: Satgé *et al.* (2004). For transition metal complexes of 4-(dimethylamino)pyridine which exhibit luminescence properties, see: Araki *et al.* (2005). For biological and magnetic properties of carboxylic acid complexes of cobalt(II), see: Cotton *et al.* (1999). For related centrosymmetric dinuclear cobalt(II) complexes bridged by carboxylates, see: Cui *et al.* (1999); Catterick & Thornton (1977).



Experimental

Crystal data

$[Co_2(C_8H_7O_2)_4(C_7H_{10}N_2)_2]$
M_r = 902.74
Triclinic, $P\bar{1}$
a = 8.107 (5) Å
b = 11.043 (5) Å
c = 12.573 (5) Å
α = 99.766 (5)°
β = 101.878 (5)°
γ = 105.335 (5)°
V = 1031.9 (9) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.86 mm^{-1}
T = 150 K
0.15 × 0.10 × 0.01 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.902, T_{max} = 0.991
9238 measured reflections
3645 independent reflections
3352 reflections with $I > 2\sigma(I)$)
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.060
S = 1.05
3645 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D$$\cdots$$A$	D—H$\cdots$$A$
C6—H6$A$$\cdots$O2^{i}	0.96	2.53	3.337 (3)	142
C23—H23$\cdots$O3^{ii}	0.93	2.58	3.469 (3)	159

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

Data collection: *APEX2* (Bruker, 2012); cell refinement: *SAINT* (Bruker, 2012); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97*.

This work was supported by the University of Constantine 1.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LR2113).

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supporting information

Acta Cryst. (2013). E**69**, m517–m518   [doi:10.1107/S1600536813023258]

Tetrakis(*μ*-2-phenylacetato-*κ*²*O*:*O*′)bis{[4-(dimethylamino)pyridine-*κN*¹]cobalt(II)}

Meriem Benslimane, Yasmine Kheira Redjel, Georges Dénès and Hocine Merazig

S1. Comment

The N-heteroaromatic ligand 4-(dimethylamino)pyridine (DMAP) finds use as a homogeneous catalyst in cellulose acylation in 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). Our interest in cobalt(II) carboxylates with DMAP evolves from their catalytic activity. Moreover, carboxylic acid complexes of cobalt(II) have properties of special interest in the fields of biology and magnetism (Cotton *et al.*, 1999). The coordination chemistry of centrosymmetric dinuclear Co^{2+} complexes bridged by carboxylates has been investigated (Cui *et al.*, 1999, Catterick *et al.*, 1977). In order to explore further the coordination behaviour of the Co^{2+} ion, the title complex, incorporating phenylacetate and DMAP as co-ligand has been prepared and its crystal structure is reported here.

The title molecule is a centrosymmetric dimer with four bidentate phenylacetate groups as bridging ligands between two Co^{II} centres, to each of which a DMAP group is also coordinated, as shown in Fig. 1. The coordination geometry about each Co atom is distorted square pyramidal, with four O atoms from four different carboxylate ligands forming the basal plane and a pyridine N atom occupying the axial position, where the most distorted angle is 101.39 (5)° for $O2^{i}$—Co—N2 [symmetry code: (i) -*x* + 1,-*y*,-*z*]. The interatomic distances of Co—O [2.0224 (12)–2.0628 (16) Å], Co—N2 [2.0460 (16) Å] and Co···Co [2.8019 (12) Å] agree well with the related values recorded for the structures of the analogous pivalate (Cui *et al.*, 1999) and benzoate (Catterick *et al.*, 1977). The Co(II) atom is 0.2286 (2) Å from the mean plane formed by the four equatorial O atoms. On the other hand, the coordinated N2 atom also lies in the same direction, at a distance of 2.2643 (13) Å from the plane. The dihedral angles between the mean planes through the C10—C15 and C18—C23 benzene rings and the DMPA plane are 7.46 (9)° and 72.08 (9)°, respectively. The dihedral angle between the planes trough $Co1/O3/O4/C16/Co1^{i}/O3^{i}/O4^{i}/C16^{i}$ and $Co1/O1/O2/C8/Co1^{i}/O1^{i}/O2^{i}/C8^{i}$ [symmetry code:(i) 1 - *x*, -*y*, -*z*] is 87.22 (4)°, which is close to the ideal value of 90°. Nonclassical C—H···O hydrogen bonds (Table 1) occur in the structure, which link adjacent complex molecule into a three-dimensional network , Fig. 2 and Fig. 3.

S2. Experimental

$CoCl_2.2H_2O$ (0.116 g,1 mmol) was dissolved in methanol (10 ml). To this solution, phenyacetic acid ($C_6H_5CH_2COOH$; 0.136 g, 1 mmol) was added and the mixture was stirred for *ca* 10 min to obtain a bleu solution. 4-(Dimethylamino)-pyridine (0.122 g, 1 mmol) was added and the mixture was stirred for an additional 2 h. Single crystals suitable for X-ray diffraction were obtained from a methanol solution of the title complex by slow evaporation.

S3. Refinement

The C-bound H atoms were included in calculated positions, with C—H = 0.93 Å (aromatic), 0.96 Å (methyl), 0.97 Å(aliphatic) and refined using a riding model, with $U_{iso}(H) = 1.5U_{eq}(C)$ for the methyl groups and $1.2U_{eq}(C)$ for the remainder.

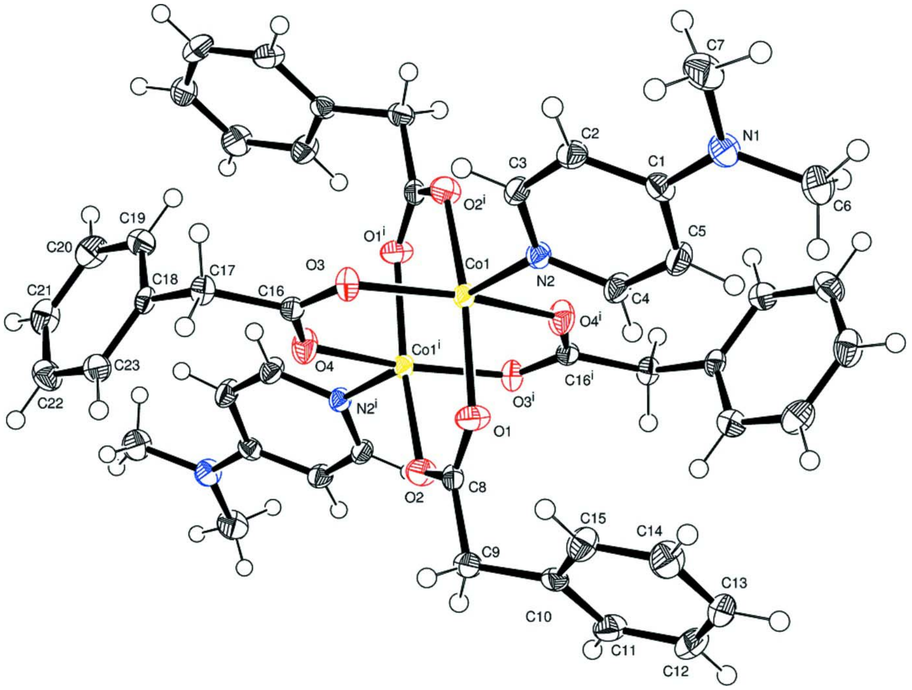

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Symmetry code, (i):1 - *x*, -*y*, -*z*.

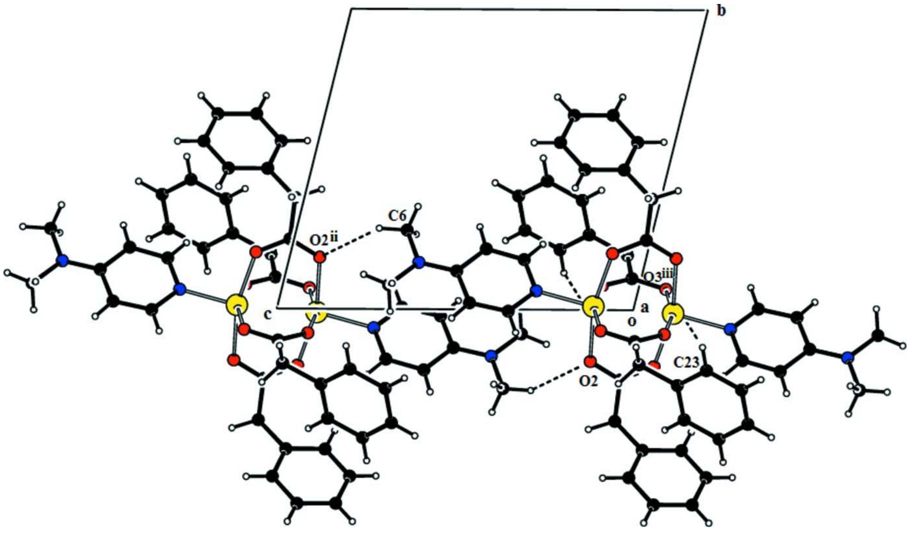

Figure 2

The crystal packing of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines. Symmetry code, (ii): *x*, *y*, 1 + *z*.

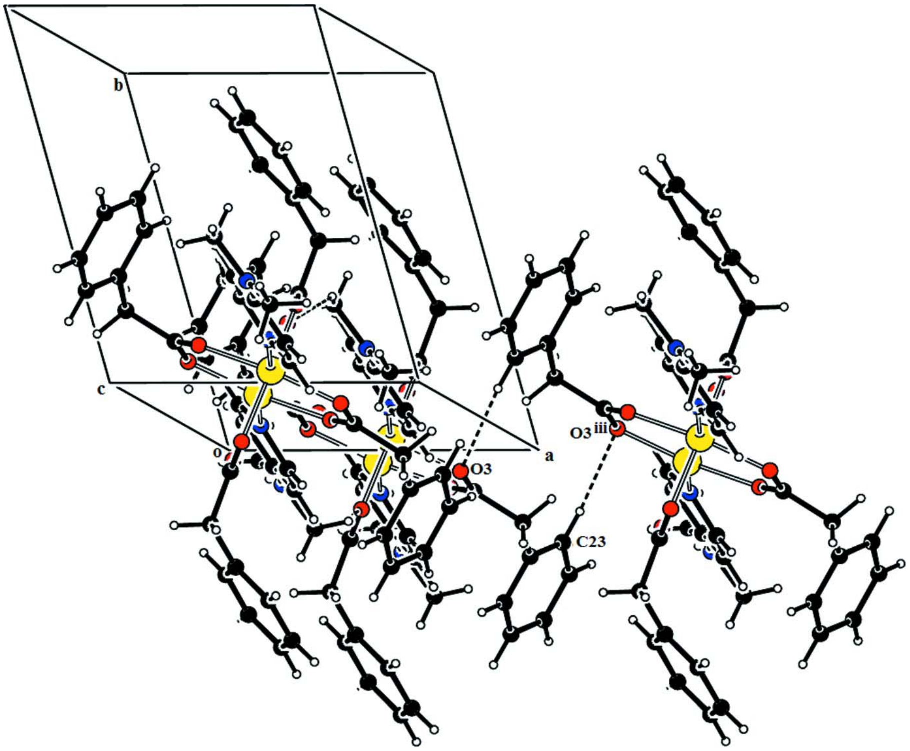

Figure 3

The crystal packing of the title compound, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.Symmetry code, (iii):2 - *x*, -*y*, -*z*.

Tetrakis(*μ*-2-phenylacetato-*κ*²*O*:*O′*)bis{[4-(dimethylamino)pyridine-*κN*¹]cobalt(II)}

Crystal data

$[Co_2(C_8H_7O_2)_4(C_7H_{10}N_2)_2]$
M_r = 902.74
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.107 (5) Å
b = 11.043 (5) Å
c = 12.573 (5) Å
α = 99.766 (5)°
β = 101.878 (5)°
γ = 105.335 (5)°
V = 1031.9 (9) Å^3
Z = 1
F(000) = 470
D_x = 1.453 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4872 reflections
θ = 2.3–25°
µ = 0.86 mm^{-1}
T = 150 K
Box, blue
0.15 × 0.1 × 0.01 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and *φ* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.902, T_{max} = 0.991
9238 measured reflections
3645 independent reflections
3352 reflections with $I > 2\sigma(I)$)
R_{int} = 0.019
θ_{max} = 25.0°, θ_{min} = 2.7°
$h = -9 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.060$
$S = 1.05$
3645 reflections
271 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0206P)^2 + 0.6871P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Co1	0.56888 (3)	0.01135 (2)	0.114253 (18)	0.01603 (8)
O1	0.70384 (17)	0.18802 (11)	0.09742 (10)	0.0256 (3)
O3	0.75242 (16)	−0.06983 (12)	0.07678 (10)	0.0241 (3)
O2	0.59969 (17)	0.17191 (12)	−0.08452 (10)	0.0248 (3)
O4	0.64516 (17)	−0.08060 (13)	−0.10383 (10)	0.0277 (3)
N1	0.7414 (2)	0.15583 (15)	0.63408 (12)	0.0259 (3)
N2	0.64381 (19)	0.06270 (13)	0.28539 (11)	0.0178 (3)
C10	0.7997 (2)	0.46694 (16)	0.12315 (14)	0.0192 (4)
C3	0.7158 (2)	−0.00546 (16)	0.34964 (14)	0.0197 (4)
H3	0.7415	−0.0764	0.3139	0.024*
C11	0.7164 (3)	0.55861 (17)	0.10444 (16)	0.0256 (4)
H11	0.6661	0.5599	0.0313	0.031*
C1	0.7158 (2)	0.12779 (17)	0.52207 (14)	0.0195 (4)
C18	0.8183 (2)	−0.25048 (16)	−0.17600 (14)	0.0181 (4)
C13	0.7818 (3)	0.64805 (18)	0.30092 (16)	0.0302 (4)
H13	0.7766	0.7085	0.3603	0.036*
C17	0.8651 (2)	−0.18185 (17)	−0.05447 (14)	0.0205 (4)
H17A	0.9855	−0.1236	−0.0338	0.025*
H17B	0.8624	−0.2454	−0.0097	0.025*
C23	0.9124 (2)	−0.20046 (17)	−0.24739 (15)	0.0222 (4)
H23	1.0052	−0.1233	−0.2202	0.027*
C2	0.7540 (2)	0.02208 (17)	0.46401 (14)	0.0216 (4)
H2	0.8051	−0.0289	0.5033	0.026*
C19	0.6790 (2)	−0.36483 (17)	−0.21909 (15)	0.0245 (4)
H19	0.6135	−0.399	−0.1724	0.029*
C9	0.8102 (3)	0.37074 (16)	0.02588 (15)	0.0236 (4)
H9A	0.9324	0.3717	0.0358	0.028*
H9B	0.7754	0.3982	−0.0424	0.028*

C14	0.8655 (3)	0.55707 (19)	0.32101 (16)	0.0311 (4)
H14	0.9163	0.5563	0.3942	0.037*
C4	0.6139 (2)	0.16674 (17)	0.34079 (14)	0.0228 (4)
H4	0.568	0.2179	0.299	0.027*
C15	0.8741 (2)	0.46726 (18)	0.23306 (15)	0.0267 (4)
H15	0.9303	0.4063	0.2476	0.032*
C5	0.6466 (2)	0.20198 (17)	0.45452 (15)	0.0246 (4)
H5	0.6231	0.2753	0.4876	0.029*
C22	0.8696 (3)	−0.26441 (19)	−0.35918 (15)	0.0274 (4)
H22	0.934	−0.23	−0.4062	0.033*
C16	0.7435 (2)	−0.10501 (16)	−0.02568 (14)	0.0180 (4)
C20	0.6361 (3)	−0.42857 (18)	−0.33028 (16)	0.0291 (4)
H20	0.5425	−0.5053	−0.3579	0.035*
C12	0.7061 (3)	0.64871 (18)	0.19226 (17)	0.0322 (5)
H12	0.6487	0.7091	0.178	0.039*
C8	0.6943 (2)	0.23260 (16)	0.01192 (14)	0.0186 (4)
C7	0.8177 (3)	0.0810 (2)	0.70317 (16)	0.0328 (5)
H7A	0.8256	0.1152	0.7802	0.049*
H7B	0.9341	0.0858	0.6946	0.049*
H7C	0.7438	−0.0076	0.6804	0.049*
C21	0.7319 (3)	−0.37875 (19)	−0.40079 (15)	0.0292 (4)
H21	0.7037	−0.4219	−0.4756	0.035*
C6	0.6940 (3)	0.2633 (2)	0.68950 (16)	0.0353 (5)
H6A	0.721	0.2693	0.7686	0.053*
H6B	0.5694	0.2493	0.6611	0.053*
H6C	0.7601	0.3421	0.6754	0.053*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.02007 (13)	0.01633 (13)	0.01213 (12)	0.00678 (9)	0.00475 (9)	0.00211 (9)
O1	0.0329 (7)	0.0188 (6)	0.0213 (7)	0.0030 (5)	0.0044 (6)	0.0066 (5)
O3	0.0262 (7)	0.0258 (7)	0.0218 (7)	0.0115 (5)	0.0093 (5)	0.0010 (5)
O2	0.0293 (7)	0.0213 (6)	0.0190 (6)	0.0020 (5)	0.0056 (6)	0.0022 (5)
O4	0.0278 (7)	0.0354 (8)	0.0261 (7)	0.0202 (6)	0.0074 (6)	0.0073 (6)
N1	0.0366 (9)	0.0275 (8)	0.0140 (7)	0.0111 (7)	0.0067 (7)	0.0044 (6)
N2	0.0212 (7)	0.0178 (7)	0.0146 (7)	0.0072 (6)	0.0048 (6)	0.0029 (6)
C10	0.0187 (9)	0.0152 (8)	0.0212 (9)	0.0001 (7)	0.0075 (7)	0.0034 (7)
C3	0.0234 (9)	0.0163 (8)	0.0209 (9)	0.0086 (7)	0.0065 (7)	0.0030 (7)
C11	0.0319 (10)	0.0201 (9)	0.0238 (9)	0.0060 (8)	0.0054 (8)	0.0080 (8)
C1	0.0196 (9)	0.0213 (9)	0.0160 (8)	0.0035 (7)	0.0054 (7)	0.0040 (7)
C18	0.0181 (8)	0.0187 (9)	0.0209 (9)	0.0111 (7)	0.0059 (7)	0.0041 (7)
C13	0.0418 (12)	0.0204 (9)	0.0283 (10)	0.0084 (9)	0.0156 (9)	0.0003 (8)
C17	0.0190 (9)	0.0212 (9)	0.0213 (9)	0.0081 (7)	0.0052 (7)	0.0023 (7)
C23	0.0182 (9)	0.0231 (9)	0.0252 (9)	0.0068 (7)	0.0047 (7)	0.0066 (8)
C2	0.0265 (10)	0.0217 (9)	0.0196 (9)	0.0109 (8)	0.0055 (7)	0.0085 (7)
C19	0.0248 (10)	0.0238 (9)	0.0256 (10)	0.0062 (8)	0.0090 (8)	0.0068 (8)
C9	0.0301 (10)	0.0185 (9)	0.0221 (9)	0.0041 (8)	0.0114 (8)	0.0047 (7)

C14	0.0390 (12)	0.0316 (11)	0.0200 (9)	0.0107 (9)	0.0046 (9)	0.0034 (8)
C4	0.0330 (10)	0.0216 (9)	0.0180 (9)	0.0151 (8)	0.0061 (8)	0.0057 (7)
C15	0.0289 (10)	0.0255 (10)	0.0270 (10)	0.0132 (8)	0.0043 (8)	0.0059 (8)
C5	0.0346 (11)	0.0213 (9)	0.0199 (9)	0.0144 (8)	0.0069 (8)	0.0016 (7)
C22	0.0283 (10)	0.0366 (11)	0.0224 (10)	0.0131 (9)	0.0097 (8)	0.0117 (8)
C16	0.0165 (8)	0.0139 (8)	0.0234 (9)	0.0029 (7)	0.0081 (7)	0.0030 (7)
C20	0.0277 (10)	0.0222 (9)	0.0285 (10)	0.0035 (8)	0.0000 (8)	−0.0017 (8)
C12	0.0420 (12)	0.0205 (10)	0.0393 (12)	0.0154 (9)	0.0124 (10)	0.0098 (9)
C8	0.0189 (9)	0.0179 (9)	0.0208 (9)	0.0070 (7)	0.0089 (7)	0.0026 (7)
C7	0.0410 (12)	0.0410 (12)	0.0191 (10)	0.0146 (10)	0.0071 (9)	0.0124 (9)
C21	0.0347 (11)	0.0350 (11)	0.0169 (9)	0.0160 (9)	0.0022 (8)	0.0006 (8)
C6	0.0547 (14)	0.0327 (11)	0.0196 (10)	0.0140 (10)	0.0148 (9)	0.0022 (8)

Geometric parameters (Å, º)

Co1—O3	2.0224 (15)	C13—H13	0.93
Co1—O1	2.0382 (14)	C17—C16	1.519 (2)
Co1—O2^{i}	2.0429 (15)	C17—H17A	0.97
Co1—N2	2.0460 (16)	C17—H17B	0.97
Co1—O4^{i}	2.0628 (16)	C23—C22	1.388 (3)
Co1—Co1^{i}	2.8020 (12)	C23—H23	0.93
O1—C8	1.253 (2)	C2—H2	0.93
O3—C16	1.262 (2)	C19—C20	1.381 (3)
O2—C8	1.256 (2)	C19—H19	0.93
O2—Co1^{i}	2.0429 (15)	C9—C8	1.524 (2)
O4—C16	1.247 (2)	C9—H9A	0.97
O4—Co1^{i}	2.0628 (16)	C9—H9B	0.97
N1—C1	1.349 (2)	C14—C15	1.381 (3)
N1—C6	1.453 (2)	C14—H14	0.93
N1—C7	1.454 (2)	C4—C5	1.366 (2)
N2—C3	1.343 (2)	C4—H4	0.93
N2—C4	1.345 (2)	C15—H15	0.93
C10—C11	1.383 (3)	C5—H5	0.93
C10—C15	1.388 (3)	C22—C21	1.380 (3)
C10—C9	1.510 (2)	C22—H22	0.93
C3—C2	1.369 (2)	C20—C21	1.384 (3)
C3—H3	0.93	C20—H20	0.93
C11—C12	1.387 (3)	C12—H12	0.93
C11—H11	0.93	C7—H7A	0.96
C1—C2	1.410 (2)	C7—H7B	0.96
C1—C5	1.411 (2)	C7—H7C	0.96
C18—C23	1.386 (2)	C21—H21	0.93
C18—C19	1.388 (3)	C6—H6A	0.96
C18—C17	1.506 (2)	C6—H6B	0.96
C13—C12	1.380 (3)	C6—H6C	0.96
C13—C14	1.382 (3)		

O3—Co1—O1	93.27 (6)	C3—C2—H2	120.1

O3—Co1—O2$^{\rm i}$	87.33 (6)	C1—C2—H2	120.1
O1—Co1—O2$^{\rm i}$	163.77 (5)	C20—C19—C18	120.91 (17)
O3—Co1—N2	102.92 (6)	C20—C19—H19	119.5
O1—Co1—N2	94.29 (5)	C18—C19—H19	119.5
O2$^{\rm i}$—Co1—N2	101.39 (5)	C10—C9—C8	114.21 (14)
O3—Co1—O4$^{\rm i}$	163.73 (5)	C10—C9—H9A	108.7
O1—Co1—O4$^{\rm i}$	85.64 (6)	C8—C9—H9A	108.7
O2$^{\rm i}$—Co1—O4$^{\rm i}$	89.27 (7)	C10—C9—H9B	108.7
N2—Co1—O4$^{\rm i}$	93.35 (5)	C8—C9—H9B	108.7
O3—Co1—Co1$^{\rm i}$	89.34 (4)	H9A—C9—H9B	107.6
O1—Co1—Co1$^{\rm i}$	79.04 (4)	C15—C14—C13	120.40 (18)
O2$^{\rm i}$—Co1—Co1$^{\rm i}$	84.75 (4)	C15—C14—H14	119.8
N2—Co1—Co1$^{\rm i}$	166.44 (4)	C13—C14—H14	119.8
O4$^{\rm i}$—Co1—Co1$^{\rm i}$	74.50 (4)	N2—C4—C5	124.16 (16)
C8—O1—Co1	129.17 (11)	N2—C4—H4	117.9
C16—O3—Co1	116.62 (11)	C5—C4—H4	117.9
C8—O2—Co1$^{\rm i}$	121.65 (11)	C14—C15—C10	120.78 (17)
C16—O4—Co1$^{\rm i}$	133.30 (12)	C14—C15—H15	119.6
C1—N1—C6	120.56 (16)	C10—C15—H15	119.6
C1—N1—C7	121.55 (16)	C4—C5—C1	120.39 (16)
C6—N1—C7	117.89 (15)	C4—C5—H5	119.8
C3—N2—C4	115.61 (15)	C1—C5—H5	119.8
C3—N2—Co1	124.00 (11)	C21—C22—C23	120.28 (18)
C4—N2—Co1	120.31 (11)	C21—C22—H22	119.9
C11—C10—C15	118.12 (17)	C23—C22—H22	119.9
C11—C10—C9	120.35 (16)	O4—C16—O3	125.35 (16)
C15—C10—C9	121.52 (16)	O4—C16—C17	118.12 (15)
N2—C3—C2	124.67 (16)	O3—C16—C17	116.52 (15)
N2—C3—H3	117.7	C19—C20—C21	120.23 (18)
C2—C3—H3	117.7	C19—C20—H20	119.9
C10—C11—C12	121.52 (18)	C21—C20—H20	119.9
C10—C11—H11	119.2	C13—C12—C11	119.52 (18)
C12—C11—H11	119.2	C13—C12—H12	120.2
N1—C1—C2	122.71 (16)	C11—C12—H12	120.2
N1—C1—C5	122.05 (16)	O1—C8—O2	125.30 (16)
C2—C1—C5	115.23 (16)	O1—C8—C9	117.19 (15)
C23—C18—C19	118.53 (16)	O2—C8—C9	117.50 (15)
C23—C18—C17	120.81 (16)	N1—C7—H7A	109.5
C19—C18—C17	120.66 (16)	N1—C7—H7B	109.5
C12—C13—C14	119.66 (18)	H7A—C7—H7B	109.5
C12—C13—H13	120.2	N1—C7—H7C	109.5
C14—C13—H13	120.2	H7A—C7—H7C	109.5
C18—C17—C16	114.52 (14)	H7B—C7—H7C	109.5
C18—C17—H17A	108.6	C22—C21—C20	119.40 (17)
C16—C17—H17A	108.6	C22—C21—H21	120.3
C18—C17—H17B	108.6	C20—C21—H21	120.3
C16—C17—H17B	108.6	N1—C6—H6A	109.5
H17A—C17—H17B	107.6	N1—C6—H6B	109.5

C18—C23—C22	120.65 (17)	H6A—C6—H6B	109.5
C18—C23—H23	119.7	N1—C6—H6C	109.5
C22—C23—H23	119.7	H6A—C6—H6C	109.5
C3—C2—C1	119.85 (16)	H6B—C6—H6C	109.5

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6*A*···O2^{ii}	0.96	2.53	3.337 (3)	142
C23—H23···O3^{iii}	0.93	2.58	3.469 (3)	159

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