Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{6,6′-Diethoxy-2,2′-[2,2-dimethylpropane-1,3-diylbis(nitrilomethylidyne)]diphenolato}(2-ethoxy-6-formylphenolato)cobalt(III)–ethanol–water (1/1/1)

Reza Kia,[a]‡ Hadi Kargar,[b] Karim Zare[a] and Islam Ullah Khan[c]*

[a]Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran, [b]Department of Chemistry, School of Science, Payame Noor University (PNU), Ardakan, Yazd, Iran, and [c]Materials Chemistry Laboratory, Department of Chemistry, GC University, Lahore 54000, Pakistan
Correspondence e-mail: iuklodhi@yahoo.com

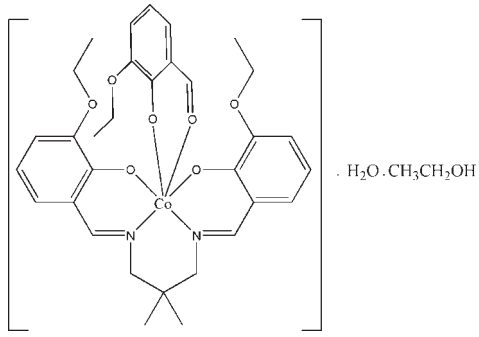
Received 28 February 2010; accepted 28 February 2010

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; disorder in solvent or counterion; R factor = 0.051; wR factor = 0.138; data-to-parameter ratio = 14.5.

The asymmetric unit of the title compound, $[Co(C_{23}H_{28}N_2O_4)(C_9H_9O_3)]\cdot C_2H_5OH\cdot H_2O$, comprises one complex molecule, a water molecule of crystallization and an ethanol molecule of crystallization, which is disordered over two positions with a ratio of refined site occupancies of 0.567 (10):0.433 (10). The Co^{III} ion is in a slightly distorted octahedral geometry involving an N_2O_2 atom set of the tetradenate Schiff base ligand and two O atoms of 2-ethoxy-6-formylphenolate. The H atoms of the water molecule act as donors in the formation of bifurcated intermolecular O—H···(O,O) hydrogen bonds with the O atoms of the hydroxy and ethoxy groups with $R_1^2(5)$ ring motifs, which may influence the molecular conformation. The crystal structure is further stabilized by intermolecular O—H···O and C—H···O interactions.

Related literature

For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For bond-length data, see: Allen *et al.* (1987). For background to Schiff base–metal complexes, see: Granovski *et al.* (1993); Blower *et al.* (1998); Elmali *et al.* (2000).



Experimental

Crystal data

$[Co(C_{23}H_{28}N_2O_4)(C_9H_9O_3)]\cdot C_2H_6O\cdot H_2O$
M_r = 684.65
Monoclinic, $P2_1/c$
a = 13.2827 (17) Å
b = 14.0158 (17) Å
c = 19.602 (2) Å
β = 106.491 (7)°
V = 3499.1 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.54 mm^{-1}
T = 298 K
0.42 × 0.21 × 0.15 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.804, T_{max} = 0.923
69893 measured reflections
6159 independent reflections
3652 reflections with $I > 2\sigma(I)$
R_{int} = 0.115

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.138
S = 1.05
6159 reflections
424 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O1	0.85	2.51	3.182 (5)	137
O1W—H1WA···O4	0.85	2.15	2.936 (5)	154
O1W—H1WB···O2	0.85	2.21	2.883 (5)	136
O1W—H1WB···O5	0.85	2.18	2.952 (5)	151
O7A—H7A···O1W	0.82	2.10	2.899 (19)	164
C8—H8C···O3	0.97	2.31	2.829 (5)	113

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

HK and RK thank PNU for the financial support. RK and KZ also thank the Science and Research Branch, Islamic Azad University. IUK thanks GC University of Lahore, for the research facilities.

‡ Additional correspondence author, e-mail: zsrkk@yahoo.com. Thomson Reuters Researcher ID: A-5471-2009.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2132).

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Blower, P. J. (1998). *Transition Met. Chem.* **23**, 109–112.

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Elmali, A., Elerman, Y. & Svoboda, I. (2000). *Acta Cryst.* C**56**, 423–424.

Granovski, A. D., Nivorozhkin, A. L. & Minkin, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2010). E**66**, m366-m367 [**doi:10.1107/S1600536810007622**]

{6,6'-Diethoxy-2,2'-[2,2-dimethylpropane-1,3-diylbis(nitrilomethylidyne)]diphenolato}(2-ethoxy-6-formylphenolato)cobalt(III)-ethanol-water (1/1/1)

R. Kia, H. Kargar, K. Zare and I. U. Khan

Comment

Schiff base complexes are one of the most important stereochemical models in transition metal coordination chemistry, with the ease of preparation and structural variations (Granovski *et al.,* 1993). Metal derivatives of the Schiff bases have been studied extensively, and they play a major role in both synthetic and structurel research (Elmali *et al.,* 2000; Blower *et al.,* 1998). The structure of the title compound was determined to clarify the identity of the synthesis product.

The asymmetric unit of the title compound, Fig. 1, $[Co(C_{32}H_{37}N_2O_7)]$. C_2H_6O. H_2O, comprises a unit of the complex, a water molecule of crystallization and an ethanol of crystallization. The H atoms of the water molecule act as donors in the formation of bifurcated O—H···(O,O) intermolecular hydrogen bonds with the O atoms of the hydroxy and ethoxy groups with $R^2_1(5)$ ring motifs (Bernstein *et al.,* 1995) which may influence the molecular conformation. The crystal structure is further stabilized by the intermolecular C—H···O and O—H···O interactions (Table 1).

Experimental

The title compound was synthesized by adding 6,6'-Diethoxy-2,2'- [2,3-dimethyl-propylenebis(nitrilomethylidyne)]-diphenol (2 mmol) to a solution of $CoCl_2$. 6 H_2O (2 mmol) in ethanol (30 ml). The mixture was refluxed with stirring for half an hour. The resultant red solution was filtered. Brown single crystals of the title compound suitable for *X*-ray structure determination were recrystallized from ethanol by slow evaporation of the solvents at room temperature over several days.

Refinement

The H atoms of the water molecule were located in a difference Fourier map and constrained to refine with the parent atom with $U_{iso}(H) = 1.5\ U_{eq}(O)$. The H atoms of the ethanol molecules were positioned geometrically and constrained to refine with the parent atoms with $U_{iso}(H) = 1.5\ U_{eq}(O)$. The rest of the H atoms were positioned geometrically and refined using a riding model with $U_{iso}(H) = 1.2$ or $1.5\ U_{eq}(C)$. Distant restraints were applied to the ethanol molecules.

Figures

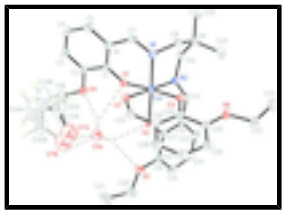


Fig. 1. The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids and the atomic numbering. All H atoms except those of water and ethanol molecules were omitted for clarity. Intramolecular hydrogen bonds are drawn as dashed lines.

{6,6'-Diethoxy-2,2'-[2,2-dimethylpropane-1,3- diylbis(nitrilomethylidyne)]diphenolato}(2-ethoxy-6-formylphenolato)cobalt(III)–ethanol–water (1/1/1

Crystal data

$[Co(C_{23}H_{28}N_2O_4)(C_9H_9O_3)]\cdot C_2H_6O\cdot H_2O$	$F(000) = 1448$
$M_r = 684.65$	$D_x = 1.300$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 6054 reflections
$a = 13.2827$ (17) Å	$\theta = 2.6$–$18.8°$
$b = 14.0158$ (17) Å	$\mu = 0.54$ mm^{-1}
$c = 19.602$ (2) Å	$T = 298$ K
$\beta = 106.491$ (7)°	Block, brown
$V = 3499.1$ (8) Å^3	0.42 × 0.21 × 0.15 mm
$Z = 4$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	6159 independent reflections
Radiation source: fine-focus sealed tube	3652 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.115$
φ and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.2°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$h = -15\rightarrow15$
$T_{min} = 0.804$, $T_{max} = 0.923$	$k = -16\rightarrow16$
69893 measured reflections	$l = -23\rightarrow23$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.051$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.138$	H-atom parameters constrained
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 2.3725P]$ where $P = (F_o^2 + 2F_c^2)/3$
6159 reflections	$(\Delta/\sigma)_{max} = 0.001$
424 parameters	$\Delta\rho_{max} = 0.35$ e Å^{-3}
6 restraints	$\Delta\rho_{min} = -0.38$ 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.

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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Co1	0.08603 (4)	0.66689 (3)	0.10882 (3)	0.03716 (18)	
O1	0.16611 (19)	0.55376 (17)	0.11696 (13)	0.0400 (6)	
O2	0.1630 (2)	0.71434 (17)	0.04880 (13)	0.0420 (7)	
O3	0.0100 (2)	0.78205 (17)	0.09545 (13)	0.0440 (7)	
O4	0.3340 (2)	0.4494 (2)	0.13168 (16)	0.0633 (8)	
O5	0.2931 (2)	0.7862 (2)	−0.01411 (17)	0.0634 (9)	
O6	−0.1080 (2)	0.92553 (19)	0.04635 (16)	0.0558 (8)	
N1	0.0146 (3)	0.6214 (2)	0.17440 (16)	0.0411 (8)	
N2	−0.0255 (2)	0.6182 (2)	0.03404 (16)	0.0360 (7)	
O7	0.1986 (2)	0.71601 (19)	0.18559 (13)	0.0471 (7)	
C1	0.1982 (3)	0.5046 (3)	0.1762 (2)	0.0401 (9)	
C17	0.1290 (3)	0.7202 (2)	−0.0207 (2)	0.0390 (10)	
C30	0.0521 (3)	0.8646 (3)	0.1149 (2)	0.0409 (10)	
C10	−0.1038 (3)	0.5570 (3)	0.0523 (2)	0.0441 (10)	
H10A	−0.0682	0.5028	0.0794	0.053*	
H10B	−0.1517	0.5328	0.0087	0.053*	
C12	0.0297 (3)	0.6901 (2)	−0.0623 (2)	0.0400 (10)	
C6	0.1477 (3)	0.5041 (3)	0.2303 (2)	0.0463 (10)	
C11	−0.0402 (3)	0.6393 (2)	−0.0321 (2)	0.0399 (10)	
H11	−0.1032	0.6192	−0.0634	0.048*	
C32	−0.1803 (4)	1.0022 (3)	0.0196 (3)	0.0634 (13)	
H32A	−0.1557	1.0412	−0.0132	0.076*	
H32B	−0.1870	1.0422	0.0585	0.076*	
C16	0.1978 (4)	0.7582 (3)	−0.0578 (2)	0.0477 (11)	
C25	−0.0104 (4)	0.9476 (3)	0.0882 (2)	0.0450 (10)	
C8	−0.0929 (3)	0.6532 (3)	0.1644 (2)	0.0487 (11)	
H8C	−0.0960	0.7222	0.1607	0.058*	
H8B	−0.1159	0.6348	0.2053	0.058*	
C7	0.0531 (3)	0.5571 (3)	0.2221 (2)	0.0492 (11)	
H7	0.0154	0.5441	0.2544	0.059*	
C29	0.1529 (3)	0.8801 (3)	0.1619 (2)	0.0471 (10)	
C2	0.2861 (3)	0.4432 (3)	0.1853 (2)	0.0527 (11)	
C13	0.0010 (4)	0.6986 (3)	−0.1375 (2)	0.0547 (12)	
H13	−0.0654	0.6791	−0.1642	0.066*	
C28	0.1908 (4)	0.9753 (3)	0.1800 (2)	0.0575 (12)	
H28	0.2571	0.9853	0.2114	0.069*	
C14	0.0689 (4)	0.7348 (3)	−0.1707 (2)	0.0604 (13)	
H14	0.0494	0.7397	−0.2201	0.073*	

C9	−0.1676 (3)	0.6083 (3)	0.0956 (2)	0.0484 (11)	
C31	0.2158 (3)	0.8032 (3)	0.1952 (2)	0.0521 (11)	
H31	0.2784	0.8194	0.2288	0.063*	
C5	0.1836 (4)	0.4445 (4)	0.2893 (2)	0.0670 (14)	
H5	0.1493	0.4444	0.3246	0.080*	
C3	0.3193 (4)	0.3866 (3)	0.2438 (3)	0.0720 (14)	
H3A	0.3773	0.3473	0.2489	0.086*	
C27	0.1302 (4)	1.0495 (3)	0.1514 (3)	0.0645 (14)	
H27	0.1558	1.1110	0.1623	0.077*	
C15	0.1682 (4)	0.7648 (3)	−0.1310 (2)	0.0622 (13)	
H15	0.2148	0.7895	−0.1540	0.075*	
C22	−0.2350 (4)	0.5316 (4)	0.1163 (3)	0.0779 (16)	
H22D	−0.2805	0.5035	0.0741	0.117*	
H22E	−0.2764	0.5598	0.1439	0.117*	
H22C	−0.1904	0.4833	0.1440	0.117*	
C4	0.2673 (5)	0.3872 (4)	0.2957 (3)	0.0826 (17)	
H4	0.2902	0.3478	0.3353	0.099*	
C26	0.0291 (4)	1.0369 (3)	0.1054 (2)	0.0570 (12)	
H26	−0.0113	1.0899	0.0864	0.068*	
C23	−0.2355 (4)	0.6871 (4)	0.0513 (3)	0.0736 (15)	
H23A	−0.2814	0.6600	0.0088	0.110*	
H23B	−0.1911	0.7339	0.0388	0.110*	
H23C	−0.2765	0.7169	0.0786	0.110*	
C18	0.4309 (4)	0.3987 (4)	0.1404 (3)	0.0895 (17)	
H18A	0.4171	0.3309	0.1336	0.107*	
H18B	0.4767	0.4085	0.1881	0.107*	
C33	−0.2833 (4)	0.9583 (4)	−0.0174 (3)	0.0921 (18)	
H33E	−0.3325	1.0074	−0.0388	0.138*	
H33D	−0.3091	0.9234	0.0163	0.138*	
H33C	−0.2747	0.9156	−0.0537	0.138*	
C19	0.4820 (5)	0.4348 (5)	0.0872 (4)	0.1229 (17)	
H19D	0.5439	0.3980	0.0899	0.184*	
H19E	0.5010	0.5006	0.0970	0.184*	
H19C	0.4342	0.4293	0.0404	0.184*	
C20	0.3736 (4)	0.8077 (4)	−0.0458 (3)	0.099 (2)	
H20C	0.3576	0.8665	−0.0730	0.119*	
H20B	0.3805	0.7568	−0.0777	0.119*	
C21	0.4742 (5)	0.8185 (5)	0.0139 (4)	0.1229 (17)	
H21D	0.5327	0.8221	−0.0056	0.184*	
H21B	0.4828	0.7644	0.0451	0.184*	
H21E	0.4710	0.8757	0.0401	0.184*	
O1W	0.3766 (3)	0.6483 (3)	0.1020 (2)	0.1109 (15)	
H1WA	0.3438	0.5975	0.1061	0.166*	
H1WB	0.3331	0.6857	0.0744	0.166*	
O7B	0.500 (3)	0.7112 (17)	0.2156 (14)	0.187 (8)	0.433 (10)
H7B	0.5110	0.7029	0.1769	0.281*	0.433 (10)
C34B	0.483 (2)	0.614 (2)	0.3126 (16)	0.226 (9)	0.433 (10)
H34H	0.5100	0.6487	0.3561	0.338*	0.433 (10)
H34G	0.4872	0.5466	0.3226	0.338*	0.433 (10)

H34C	0.4105	0.6310	0.2916	0.338*	0.433 (10)
C35B	0.5463 (16)	0.6375 (16)	0.2612 (12)	0.138 (5)	0.433 (10)
H35E	0.6168	0.6560	0.2880	0.166*	0.433 (10)
H35B	0.5515	0.5813	0.2335	0.166*	0.433 (10)
O7A	0.4612 (19)	0.7350 (11)	0.2408 (10)	0.187 (8)	0.567 (10)
H7A	0.4379	0.7212	0.1986	0.281*	0.567 (10)
C34A	0.5407 (18)	0.5896 (16)	0.2956 (15)	0.226 (9)	0.567 (10)
H34B	0.5435	0.5513	0.3367	0.338*	0.567 (10)
H34D	0.6049	0.6249	0.3035	0.338*	0.567 (10)
H34A	0.5317	0.5491	0.2549	0.338*	0.567 (10)
C35A	0.4496 (10)	0.6580 (10)	0.2828 (9)	0.138 (5)	0.567 (10)
H35A	0.3852	0.6245	0.2596	0.166*	0.567 (10)
H35C	0.4440	0.6815	0.3282	0.166*	0.567 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0447 (3)	0.0301 (3)	0.0365 (3)	−0.0004 (3)	0.0113 (2)	−0.0034 (2)
O1	0.0476 (17)	0.0347 (14)	0.0375 (15)	0.0035 (12)	0.0118 (13)	−0.0009 (12)
O2	0.0439 (17)	0.0405 (15)	0.0408 (16)	−0.0030 (13)	0.0109 (13)	0.0034 (12)
O3	0.0494 (18)	0.0260 (14)	0.0538 (17)	−0.0013 (12)	0.0101 (14)	−0.0069 (12)
O4	0.056 (2)	0.066 (2)	0.071 (2)	0.0214 (16)	0.0230 (18)	0.0092 (17)
O5	0.054 (2)	0.067 (2)	0.077 (2)	−0.0061 (17)	0.0308 (19)	0.0121 (17)
O6	0.059 (2)	0.0381 (16)	0.070 (2)	0.0076 (15)	0.0171 (17)	0.0010 (14)
N1	0.046 (2)	0.0384 (18)	0.0389 (19)	0.0002 (16)	0.0124 (16)	−0.0070 (16)
N2	0.044 (2)	0.0275 (16)	0.0386 (19)	0.0012 (15)	0.0144 (16)	−0.0034 (14)
O7	0.0524 (18)	0.0415 (17)	0.0427 (16)	−0.0020 (14)	0.0058 (14)	−0.0032 (13)
C1	0.045 (3)	0.035 (2)	0.037 (2)	−0.0011 (19)	0.006 (2)	0.0004 (18)
C17	0.055 (3)	0.025 (2)	0.040 (2)	0.0093 (18)	0.017 (2)	0.0008 (17)
C30	0.051 (3)	0.034 (2)	0.044 (2)	−0.0012 (19)	0.024 (2)	−0.0052 (18)
C10	0.049 (3)	0.037 (2)	0.045 (2)	−0.0064 (19)	0.011 (2)	−0.0042 (19)
C12	0.058 (3)	0.024 (2)	0.038 (2)	0.0021 (18)	0.014 (2)	0.0007 (16)
C6	0.054 (3)	0.044 (2)	0.041 (2)	0.005 (2)	0.015 (2)	0.005 (2)
C11	0.047 (3)	0.028 (2)	0.039 (2)	0.0034 (18)	0.003 (2)	−0.0072 (17)
C32	0.077 (4)	0.047 (3)	0.074 (3)	0.021 (3)	0.034 (3)	0.015 (2)
C16	0.054 (3)	0.036 (2)	0.057 (3)	0.005 (2)	0.022 (2)	0.004 (2)
C25	0.056 (3)	0.035 (2)	0.051 (3)	0.002 (2)	0.027 (2)	−0.0046 (19)
C8	0.048 (3)	0.052 (3)	0.051 (2)	0.001 (2)	0.022 (2)	−0.006 (2)
C7	0.061 (3)	0.053 (3)	0.038 (2)	−0.008 (2)	0.021 (2)	−0.005 (2)
C29	0.061 (3)	0.042 (2)	0.041 (2)	−0.005 (2)	0.019 (2)	−0.007 (2)
C2	0.053 (3)	0.047 (3)	0.058 (3)	0.002 (2)	0.013 (2)	0.006 (2)
C13	0.080 (3)	0.038 (2)	0.044 (3)	0.005 (2)	0.014 (2)	0.002 (2)
C28	0.065 (3)	0.043 (3)	0.068 (3)	−0.018 (2)	0.026 (3)	−0.014 (2)
C14	0.090 (4)	0.048 (3)	0.044 (3)	0.006 (3)	0.020 (3)	0.005 (2)
C9	0.040 (3)	0.048 (3)	0.059 (3)	−0.002 (2)	0.017 (2)	−0.007 (2)
C31	0.055 (3)	0.055 (3)	0.042 (2)	−0.012 (2)	0.007 (2)	−0.010 (2)
C5	0.076 (4)	0.076 (3)	0.050 (3)	0.006 (3)	0.019 (3)	0.020 (3)
C3	0.072 (4)	0.066 (3)	0.074 (3)	0.022 (3)	0.013 (3)	0.024 (3)

C27	0.087 (4)	0.037 (3)	0.075 (3)	−0.018 (3)	0.033 (3)	−0.020 (2)
C15	0.089 (4)	0.052 (3)	0.057 (3)	0.008 (3)	0.039 (3)	0.013 (2)
C22	0.067 (4)	0.089 (4)	0.089 (4)	−0.028 (3)	0.042 (3)	−0.018 (3)
C4	0.089 (4)	0.086 (4)	0.067 (4)	0.020 (3)	0.013 (3)	0.044 (3)
C26	0.075 (4)	0.031 (2)	0.075 (3)	−0.002 (2)	0.037 (3)	−0.003 (2)
C23	0.064 (3)	0.078 (4)	0.071 (3)	0.014 (3)	0.007 (3)	−0.014 (3)
C18	0.073 (4)	0.087 (4)	0.111 (5)	0.029 (3)	0.030 (4)	0.005 (4)
C33	0.064 (4)	0.086 (4)	0.112 (5)	0.017 (3)	0.001 (3)	0.011 (4)
C19	0.069 (3)	0.137 (4)	0.172 (5)	−0.002 (3)	0.050 (3)	−0.001 (4)
C20	0.079 (4)	0.098 (5)	0.134 (5)	0.000 (4)	0.055 (4)	0.016 (4)
C21	0.069 (3)	0.137 (4)	0.172 (5)	−0.002 (3)	0.050 (3)	−0.001 (4)
O1W	0.074 (3)	0.105 (3)	0.148 (4)	0.000 (2)	0.022 (3)	0.045 (3)
O7B	0.201 (19)	0.138 (10)	0.179 (14)	−0.046 (8)	−0.017 (10)	−0.026 (10)
C34B	0.20 (3)	0.23 (2)	0.21 (2)	0.105 (17)	−0.010 (18)	−0.023 (16)
C35B	0.119 (10)	0.118 (11)	0.142 (12)	0.006 (9)	−0.021 (9)	−0.004 (8)
O7A	0.201 (19)	0.138 (10)	0.179 (14)	−0.046 (8)	−0.017 (10)	−0.026 (10)
C34A	0.20 (3)	0.23 (2)	0.21 (2)	0.105 (17)	−0.010 (18)	−0.023 (16)
C35A	0.119 (10)	0.118 (11)	0.142 (12)	0.006 (9)	−0.021 (9)	−0.004 (8)

Geometric parameters (Å, °)

Co1—O3	1.882 (2)	C9—C22	1.525 (6)
Co1—O2	1.885 (3)	C9—C23	1.531 (6)
Co1—O1	1.891 (2)	C31—H31	0.9300
Co1—N2	1.891 (3)	C5—C4	1.348 (6)
Co1—N1	1.910 (3)	C5—H5	0.9300
Co1—O7	1.923 (3)	C3—C4	1.382 (7)
O1—C1	1.313 (4)	C3—H3A	0.9300
O2—C17	1.311 (4)	C27—C26	1.400 (6)
O3—C30	1.294 (4)	C27—H27	0.9300
O4—C2	1.378 (5)	C15—H15	0.9300
O4—C18	1.436 (5)	C22—H22D	0.9600
O5—C16	1.369 (5)	C22—H22E	0.9600
O5—C20	1.414 (6)	C22—H22C	0.9600
O6—C25	1.358 (5)	C4—H4	0.9300
O6—C32	1.437 (5)	C26—H26	0.9300
N1—C7	1.295 (5)	C23—H23A	0.9600
N1—C8	1.456 (5)	C23—H23B	0.9600
N2—C11	1.288 (4)	C23—H23C	0.9600
N2—C10	1.468 (5)	C18—C19	1.486 (8)
O7—C31	1.247 (5)	C18—H18A	0.9700
C1—C6	1.405 (5)	C18—H18B	0.9700
C1—C2	1.421 (5)	C33—H33E	0.9600
C17—C12	1.404 (5)	C33—H33D	0.9600
C17—C16	1.423 (5)	C33—H33C	0.9600
C30—C29	1.410 (6)	C19—H19D	0.9600
C30—C25	1.440 (5)	C19—H19E	0.9600
C10—C9	1.538 (5)	C19—H19C	0.9600
C10—H10A	0.9700	C20—C21	1.514 (8)

C10—H10B	0.9700	C20—H20C	0.9700
C12—C13	1.418 (5)	C20—H20B	0.9700
C12—C11	1.427 (5)	C21—H21D	0.9600
C6—C5	1.397 (6)	C21—H21B	0.9600
C6—C7	1.429 (6)	C21—H21E	0.9600
C11—H11	0.9300	O1W—H1WA	0.8508
C32—C33	1.487 (6)	O1W—H1WB	0.8508
C32—H32A	0.9700	O7B—C35B	1.390 (10)
C32—H32B	0.9700	O7B—H7B	0.8202
C16—C15	1.379 (6)	O7B—H7A	0.8084
C25—C26	1.361 (5)	C34B—C35B	1.526 (10)
C8—C9	1.561 (5)	C34B—H34H	0.9600
C8—H8C	0.9700	C34B—H34G	0.9600
C8—H8B	0.9700	C34B—H34C	0.9600
C7—H7	0.9300	C35B—H35E	0.9700
C29—C31	1.407 (6)	C35B—H35B	0.9700
C29—C28	1.434 (5)	O7A—C35A	1.392 (9)
C2—C3	1.360 (6)	O7A—H7A	0.8200
C13—C14	1.353 (6)	C34A—C35A	1.508 (9)
C13—H13	0.9300	C34A—H34B	0.9600
C28—C27	1.338 (6)	C34A—H34D	0.9600
C28—H28	0.9300	C34A—H34A	0.9600
C14—C15	1.392 (6)	C35A—H35A	0.9700
C14—H14	0.9300	C35A—H35C	0.9700
O3—Co1—O2	88.56 (11)	C23—C9—C10	110.6 (3)
O3—Co1—O1	175.99 (11)	C22—C9—C8	109.4 (4)
O2—Co1—O1	87.52 (11)	C23—C9—C8	109.1 (3)
O3—Co1—N2	86.00 (12)	C10—C9—C8	110.5 (3)
O2—Co1—N2	95.04 (12)	O7—C31—C29	128.4 (4)
O1—Co1—N2	93.50 (11)	O7—C31—H31	115.8
O3—Co1—N1	91.77 (13)	C29—C31—H31	115.8
O2—Co1—N1	176.57 (12)	C4—C5—C6	120.8 (5)
O1—Co1—N1	92.20 (12)	C4—C5—H5	119.6
N2—Co1—N1	88.39 (13)	C6—C5—H5	119.6
O3—Co1—O7	93.96 (11)	C2—C3—C4	120.5 (5)
O2—Co1—O7	85.60 (11)	C2—C3—H3A	119.8
O1—Co1—O7	86.58 (11)	C4—C3—H3A	119.8
N2—Co1—O7	179.36 (13)	C28—C27—C26	121.7 (4)
N1—Co1—O7	90.97 (12)	C28—C27—H27	119.2
C1—O1—Co1	123.2 (2)	C26—C27—H27	119.2
C17—O2—Co1	125.7 (2)	C16—C15—C14	120.4 (4)
C30—O3—Co1	123.8 (2)	C16—C15—H15	119.8
C2—O4—C18	118.0 (4)	C14—C15—H15	119.8
C16—O5—C20	117.8 (4)	C9—C22—H22D	109.5
C25—O6—C32	118.3 (3)	C9—C22—H22E	109.5
C7—N1—C8	118.8 (4)	H22D—C22—H22E	109.5
C7—N1—Co1	123.3 (3)	C9—C22—H22C	109.5
C8—N1—Co1	117.6 (3)	H22D—C22—H22C	109.5
C11—N2—C10	117.6 (3)	H22E—C22—H22C	109.5

C11—N2—Co1	123.9 (3)	C5—C4—C3	120.4 (4)
C10—N2—Co1	118.4 (2)	C5—C4—H4	119.8
C31—O7—Co1	122.5 (3)	C3—C4—H4	119.8
O1—C1—C6	124.4 (4)	C25—C26—C27	120.5 (4)
O1—C1—C2	118.5 (4)	C25—C26—H26	119.8
C6—C1—C2	116.9 (4)	C27—C26—H26	119.8
O2—C17—C12	125.1 (4)	C9—C23—H23A	109.5
O2—C17—C16	118.3 (4)	C9—C23—H23B	109.5
C12—C17—C16	116.6 (4)	H23A—C23—H23B	109.5
O3—C30—C29	125.5 (4)	C9—C23—H23C	109.5
O3—C30—C25	117.4 (4)	H23A—C23—H23C	109.5
C29—C30—C25	117.1 (4)	H23B—C23—H23C	109.5
N2—C10—C9	113.7 (3)	O4—C18—C19	108.7 (5)
N2—C10—H10A	108.8	O4—C18—H18A	110.0
C9—C10—H10A	108.8	C19—C18—H18A	110.0
N2—C10—H10B	108.8	O4—C18—H18B	110.0
C9—C10—H10B	108.8	C19—C18—H18B	110.0
H10A—C10—H10B	107.7	H18A—C18—H18B	108.3
C17—C12—C13	120.6 (4)	C32—C33—H33E	109.5
C17—C12—C11	121.6 (3)	C32—C33—H33D	109.5
C13—C12—C11	117.3 (4)	H33E—C33—H33D	109.5
C5—C6—C1	120.3 (4)	C32—C33—H33C	109.5
C5—C6—C7	119.0 (4)	H33E—C33—H33C	109.5
C1—C6—C7	120.4 (4)	H33D—C33—H33C	109.5
N2—C11—C12	127.0 (4)	C18—C19—H19D	109.5
N2—C11—H11	116.5	C18—C19—H19E	109.5
C12—C11—H11	116.5	H19D—C19—H19E	109.5
O6—C32—C33	107.2 (4)	C18—C19—H19C	109.5
O6—C32—H32A	110.3	H19D—C19—H19C	109.5
C33—C32—H32A	110.3	H19E—C19—H19C	109.5
O6—C32—H32B	110.3	O5—C20—C21	107.0 (5)
C33—C32—H32B	110.3	O5—C20—H20C	110.3
H32A—C32—H32B	108.5	C21—C20—H20C	110.3
O5—C16—C15	124.9 (4)	O5—C20—H20B	110.3
O5—C16—C17	113.6 (4)	C21—C20—H20B	110.3
C15—C16—C17	121.5 (4)	H20C—C20—H20B	108.6
O6—C25—C26	126.4 (4)	C20—C21—H21D	109.5
O6—C25—C30	112.8 (3)	C20—C21—H21B	109.5
C26—C25—C30	120.7 (4)	H21D—C21—H21B	109.5
N1—C8—C9	110.7 (3)	C20—C21—H21E	109.5
N1—C8—H8C	109.5	H21D—C21—H21E	109.5
C9—C8—H8C	109.5	H21B—C21—H21E	109.5
N1—C8—H8B	109.5	H1WA—O1W—H1WB	107.5
C9—C8—H8B	109.5	C35B—O7B—H7B	109.1
H8C—C8—H8B	108.1	C35B—O7B—H7A	127.3
N1—C7—C6	126.6 (4)	H7B—O7B—H7A	94.1
N1—C7—H7	116.7	C35B—C34B—H34H	109.5
C6—C7—H7	116.7	C35B—C34B—H34G	109.5
C31—C29—C30	120.9 (4)	H34H—C34B—H34G	109.5

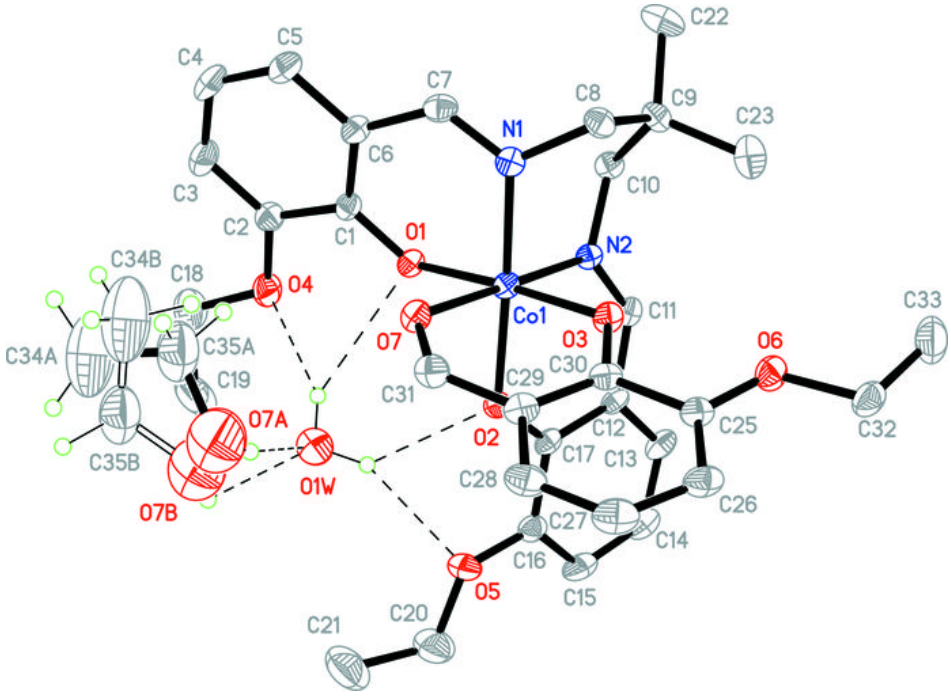
C31—C29—C28	118.5 (4)	C35B—C34B—H34C	109.5
C30—C29—C28	120.5 (4)	H34H—C34B—H34C	109.5
C3—C2—O4	124.8 (4)	H34G—C34B—H34C	109.5
C3—C2—C1	121.1 (4)	O7B—C35B—C34B	111.1 (10)
O4—C2—C1	114.0 (4)	O7B—C35B—H35E	109.4
C14—C13—C12	120.8 (4)	C34B—C35B—H35E	109.4
C14—C13—H13	119.6	O7B—C35B—H35B	109.4
C12—C13—H13	119.6	C34B—C35B—H35B	109.4
C27—C28—C29	119.5 (4)	H35E—C35B—H35B	108.0
C27—C28—H28	120.3	C35A—O7A—H7A	109.9
C29—C28—H28	120.3	O7A—C35A—C34A	111.9 (10)
C13—C14—C15	119.9 (4)	O7A—C35A—H35A	109.2
C13—C14—H14	120.0	C34A—C35A—H35A	109.2
C15—C14—H14	120.0	O7A—C35A—H35C	109.2
C22—C9—C23	111.4 (4)	C34A—C35A—H35C	109.2
C22—C9—C10	105.9 (3)	H35A—C35A—H35C	107.9
O2—Co1—O1—C1	142.6 (3)	O2—C17—C16—O5	−1.2 (5)
N2—Co1—O1—C1	−122.5 (3)	C12—C17—C16—O5	179.9 (3)
N1—Co1—O1—C1	−34.0 (3)	O2—C17—C16—C15	178.8 (4)
O7—Co1—O1—C1	56.8 (3)	C12—C17—C16—C15	−0.1 (5)
O3—Co1—O2—C17	−76.0 (3)	C32—O6—C25—C26	−3.4 (6)
O1—Co1—O2—C17	103.2 (3)	C32—O6—C25—C30	176.5 (3)
N2—Co1—O2—C17	9.9 (3)	O3—C30—C25—O6	1.2 (5)
O7—Co1—O2—C17	−170.1 (3)	C29—C30—C25—O6	−176.7 (3)
O2—Co1—O3—C30	−62.5 (3)	O3—C30—C25—C26	−178.9 (4)
N2—Co1—O3—C30	−157.7 (3)	C29—C30—C25—C26	3.2 (6)
N1—Co1—O3—C30	114.0 (3)	C7—N1—C8—C9	−103.9 (4)
O7—Co1—O3—C30	22.9 (3)	Co1—N1—C8—C9	69.2 (4)
O3—Co1—N1—C7	−156.5 (3)	C8—N1—C7—C6	166.9 (4)
O1—Co1—N1—C7	24.1 (3)	Co1—N1—C7—C6	−5.8 (6)
N2—Co1—N1—C7	117.5 (3)	C5—C6—C7—N1	173.3 (4)
O7—Co1—N1—C7	−62.6 (3)	C1—C6—C7—N1	−12.9 (6)
O3—Co1—N1—C8	30.7 (3)	O3—C30—C29—C31	−3.1 (6)
O1—Co1—N1—C8	−148.7 (3)	C25—C30—C29—C31	174.6 (4)
N2—Co1—N1—C8	−55.3 (3)	O3—C30—C29—C28	−179.5 (4)
O7—Co1—N1—C8	124.7 (3)	C25—C30—C29—C28	−1.8 (6)
O3—Co1—N2—C11	74.6 (3)	C18—O4—C2—C3	−5.3 (7)
O2—Co1—N2—C11	−13.6 (3)	C18—O4—C2—C1	172.6 (4)
O1—Co1—N2—C11	−101.4 (3)	O1—C1—C2—C3	−176.3 (4)
N1—Co1—N2—C11	166.5 (3)	C6—C1—C2—C3	0.1 (6)
O3—Co1—N2—C10	−101.8 (3)	O1—C1—C2—O4	5.6 (5)
O2—Co1—N2—C10	170.0 (2)	C6—C1—C2—O4	−178.0 (4)
O1—Co1—N2—C10	82.2 (3)	C17—C12—C13—C14	0.8 (6)
N1—Co1—N2—C10	−9.9 (3)	C11—C12—C13—C14	−171.5 (4)
O3—Co1—O7—C31	−20.5 (3)	C31—C29—C28—C27	−177.0 (4)
O2—Co1—O7—C31	67.8 (3)	C30—C29—C28—C27	−0.6 (6)
O1—Co1—O7—C31	155.5 (3)	C12—C13—C14—C15	−0.4 (6)
N1—Co1—O7—C31	−112.3 (3)	N2—C10—C9—C22	−173.8 (3)
Co1—O1—C1—C6	26.2 (5)	N2—C10—C9—C23	65.4 (4)

Co1—O1—C1—C2	−157.7 (3)	N2—C10—C9—C8	−55.5 (4)
Co1—O2—C17—C12	−1.3 (5)	N1—C8—C9—C22	107.1 (4)
Co1—O2—C17—C16	179.9 (2)	N1—C8—C9—C23	−130.9 (4)
Co1—O3—C30—C29	−15.0 (5)	N1—C8—C9—C10	−9.2 (5)
Co1—O3—C30—C25	167.2 (2)	Co1—O7—C31—C29	10.0 (6)
C11—N2—C10—C9	−112.7 (4)	C30—C29—C31—O7	5.7 (7)
Co1—N2—C10—C9	64.0 (4)	C28—C29—C31—O7	−177.9 (4)
O2—C17—C12—C13	−179.3 (3)	C1—C6—C5—C4	0.5 (7)
C16—C17—C12—C13	−0.5 (5)	C7—C6—C5—C4	174.2 (5)
O2—C17—C12—C11	−7.4 (6)	O4—C2—C3—C4	178.3 (5)
C16—C17—C12—C11	171.4 (3)	C1—C2—C3—C4	0.5 (7)
O1—C1—C6—C5	175.6 (4)	C29—C28—C27—C26	1.6 (7)
C2—C1—C6—C5	−0.5 (6)	O5—C16—C15—C14	−179.6 (4)
O1—C1—C6—C7	2.0 (6)	C17—C16—C15—C14	0.5 (6)
C2—C1—C6—C7	−174.2 (4)	C13—C14—C15—C16	−0.2 (7)
C10—N2—C11—C12	−174.1 (3)	C6—C5—C4—C3	0.1 (8)
Co1—N2—C11—C12	9.5 (5)	C2—C3—C4—C5	−0.6 (8)
C17—C12—C11—N2	2.9 (6)	O6—C25—C26—C27	177.6 (4)
C13—C12—C11—N2	175.1 (4)	C30—C25—C26—C27	−2.3 (6)
C25—O6—C32—C33	−174.0 (4)	C28—C27—C26—C25	−0.2 (7)
C20—O5—C16—C15	−11.7 (6)	C2—O4—C18—C19	−165.4 (4)
C20—O5—C16—C17	168.2 (4)	C16—O5—C20—C21	−169.8 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O1	0.85	2.51	3.182 (5)	137
O1W—H1WA···O4	0.85	2.15	2.936 (5)	154
O1W—H1WB···O2	0.85	2.21	2.883 (5)	136
O1W—H1WB···O5	0.85	2.18	2.952 (5)	151
O7A—H7A···O1W	0.82	2.10	2.899 (19)	164
C8—H8C···O3	0.97	2.31	2.829 (5)	113

Fig. 1


C22
C5
C4
C7
C8
C9
C23
N1
C6
C10
C3
C2
C1
O1
N2
C34B
C18
O4
Co1
C11
C33
O7
O3
O6
C34A
C35A
C30
C19
C29
C31
C12
C25
O7A
O2
C32
C35B
C17
C13
O1W
C28
C26
C27
C14
O7B
C16
O5
C15
C20
C21