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Bis(dimethylglyoximato-*N*,*N*′)(ethanol-*O*)-nitrocobalt(III), $[Co(Hdmg)_2(NO_2)(EtOH)]$

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In the distorted octahedral title complex, $[Co(NO_2)(C_2H_6O)(C_4H_7N_2O_2)_2]$, the Co atom is coordinated to two chelating ligands in the equatorial plane, with nitro and ethanol groups occupying the axial positions. In addition to the asymmetric intramolecular hydrogen bridges between the equatorial ligands, strong intermolecular hydrogen bonds result in a pairwise arrangement of the molecules with respect to a crystallographic inversion center.

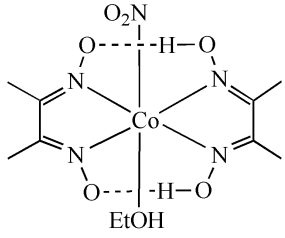
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.108
Data-to-parameter ratio = 18.1

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

Comment

We recently discussed the geometry of the intramolecular hydrogen bridges in bis(dimethylglyoximato) complexes (Englert *et al.*, 1999). We confirmed earlier X-ray diffraction results (Shkurpelo *et al.*, 1979) for the compound $[Co(Hdmg)_2(NO_2)(H_2O)]$ by neutron diffraction and showed that the intramolecular hydrogen bonds are correlated to the packing arrangement. Similar relationships between intra- and intermolecular hydrogen bridges were found for related compounds (Englert *et al.*, 2000).



(I)

Fig. 1 shows the geometry and the intramolecular hydrogen-bond pattern of the title complex, (I). The O1/N1/C1/C2/N2/O2 moiety may be considered as a formally dianionic ligand with slightly shorter bonds to the metal (Table 1). The abovementioned asymmetry in intramolecular hydrogen bridges is well related to strong intermolecular hydrogen bonds (Table 2) which occur between neighboring molecules by inversion. Each molecule provides an acceptor (O1 in the formally dianionic Hdmg moiety) and a donor (hydroxyl group of the ethanol ligand) to form the so-called $R_2^2(10)$-type hydrogen-bond pattern (Etter *et al.*, 1990) (Fig. 2).

Experimental

A small number of crystals of (I) were obtained from an ethanol solution of $[Co(Hdmg)_2(NO_2)(L)]$ (L is 3-methyl-5,6,7,8-tetrahydro-7,7-dimethyl-6*R*,8*R*-methanoisoquinoline) by ligand exchange.

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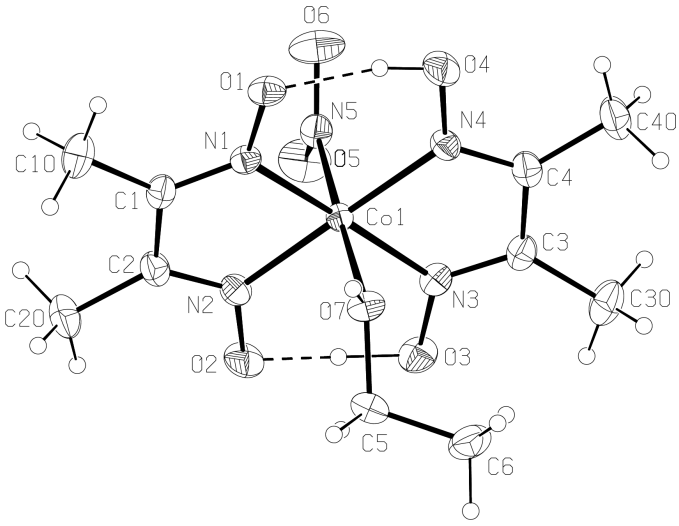

Figure 1
Displacement ellipsoid plot (30% probability) for (I).

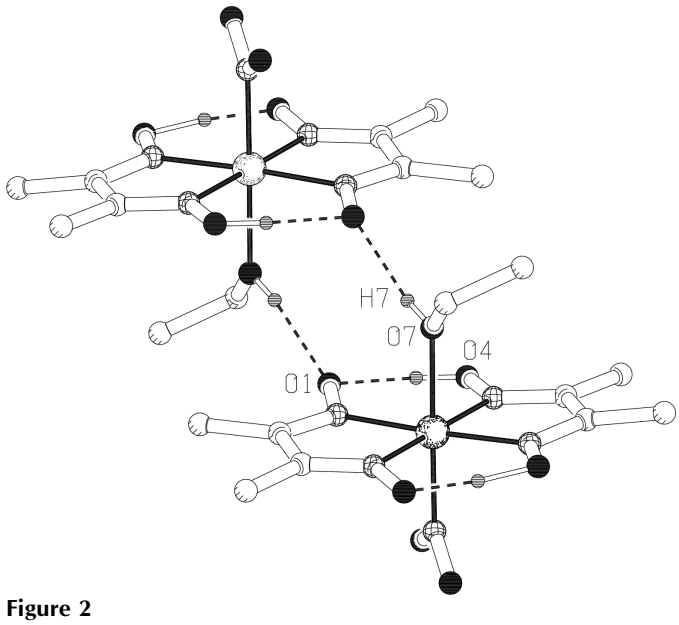

Figure 2
PLUTO representation of two neighboring molecules showing intra- and intermolecular hydrogen bonds. C-bonded H atoms have been omitted for clarity.

Crystal data

$[Co(NO_2)(C_2H_6O)(C_4H_7N_2O_2)_2]$
M_r = 381.24
Monoclinic, $P2_1/n$
a = 8.9591 (5) Å
b = 16.614 (1) Å
c = 10.7359 (6) Å
β = 91.83 (1)°
V = 1597.18 (16) Å^3
Z = 4
D_x = 1.585 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 14412 reflections
θ = 2.3–28.3°
μ = 1.12 mm^{-1}
T = 293 (2) K
Block, red
0.48 × 0.28 × 0.18 mm

Data collection

CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.694, T_{max} = 0.818
14 412 measured reflections
3973 independent reflections
3166 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 28.3°
$h = -11 \rightarrow 11$
$k = -22 \rightarrow 22$
$l = -14 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.108
S = 1.04
3973 reflections
220 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—N2	1.888 (2)	Co1—N4	1.904 (2)
Co1—N1	1.8918 (18)	Co1—N3	1.908 (2)
Co1—N5	1.900 (2)	Co1—O7	1.9856 (17)
N2—Co1—N5	89.61 (9)	N1—Co1—O7	89.34 (8)
N1—Co1—N5	90.99 (9)	N5—Co1—O7	179.05 (9)
N5—Co1—N4	90.43 (9)	N4—Co1—O7	88.65 (8)
N5—Co1—N3	92.08 (9)	N3—Co1—O7	87.59 (8)
N2—Co1—O7	91.31 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	1.13 (5)	1.36 (5)	2.486 (3)	175 (5)
O4—H4···O1	0.92 (4)	1.66 (4)	2.554 (3)	166 (3)
O7—H7···O1^{i}	0.75 (3)	1.85 (3)	2.572 (2)	163 (3)

Symmetry code: (i) $-x, -y, 2-z$.

All H atoms on C atoms were introduced in idealized positions (C—H = 0.98 Å) and included as riding with $U_{iso}(H) = 1.3U_{eq}$(non-H). H atoms on O atoms were located from difference Fourier syntheses and allowed to refine freely with isotropic displacement parameters.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT+* (Bruker, 1999); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 1990); software used to prepare material for publication: *SHELXTL*.

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