Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(1-Benzyl-1*H*-imidazole)chlorobis(dimethylglyoximato)cobalt(**III**)

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Received 29 March 2005
Accepted 12 April 2005
Online 23 April 2005

In the title compound, $[Co(C_4H_7N_2O_2)_2Cl(C_{10}H_{10}N_2)]$, the Co^{III} atom has a distorted octahedral geometry defined by five N atoms from two dimethylglyoximate ligands and one 1-benzylimidazole group, and one chloro anion. The two dimethylglyoximate ligands lie *trans* to each other.

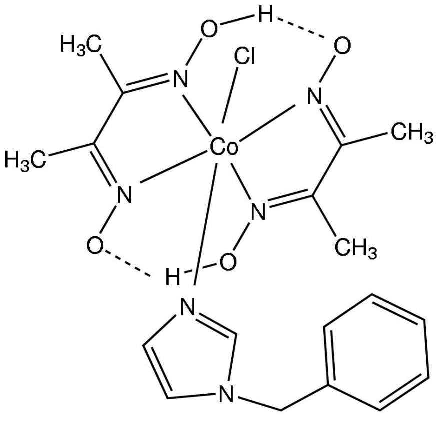
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.045
wR factor = 0.112
Data-to-parameter ratio = 15.6

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

Comment

The dimethylglyoximate anion is an excellent ligand for the preparation of mono-, bi- or trinuclear compounds, which are commonly used as precursors to supramolecular systems (Birkelbach *et al.*, 1998; Liu *et al.*, 2002; Zhan *et al.*, 1999). This property is seen in the work over the years on the dimethylglyoximate–cobalt complexes that mimic the vitamin B12 coenzyme (Bresciani-Pahor *et al.*, 1985; Randaccio *et al.*, 1989). The title cobalt compound, (I) (Fig. 1), forms part of our systematic studies on metal dimethylglyoximates.



(I)

The Co atom has a slightly distorted octahedral geometry, being coordinated by four N atoms from two dimethylglyoximate ligands, a chloro anion and an N atom from the 1-benzylimidazole ligand. The Co atom and four N atoms of the dimethylglyoximate groups are coplanar, and the Co—N bond lengths are similar to those observed previously in the corresponding cobalt(III)–azide complex (Dong *et al.*, 2003). Intramolecular O—H···O hydrogen bonds between the two dimethylglyoximate ligands enhance the stability of the structure.

Experimental

Dimethylglyoxime (0.232 g, 2 mmol) was added to a solution of cobaltous chloride hexahydrate (0.238 g, 1 mmol) in methanol (40 ml). After the mixture had been stirred for 4 h, 1-benzylimidazole (0.158 g, 1 mmol) was added, followed by the addition of sodium hydroxide (1 *M*). The resulting dark red–brown solution was filtered. After 2 d, dark red crystals were obtained. Analysis calculated for $C_{18}H_{24}ClCoN_6O_4$: C 44.78, H 5.01, N 17.41%; found: C 44.68, H 4.96, N 17.40%.

Crystal data

$[Co(C_4H_7N_2O_2)_2Cl(C_{10}H_{10}N_2)]$
$M_r = 482.81$
Monoclinic, $P2_1/n$
$a = 8.1038$ (7) Å
$b = 21.6750$ (10) Å
$c = 12.6164$ (9) Å
$\beta = 94.126$ (6)°
$V = 2210.3$ (3) Å^3
$Z = 4$
$D_x = 1.451$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2951 reflections
$\theta = 1.9$–28.4°
$\mu = 0.93$ mm^{-1}
$T = 295$ (2) K
Prism, dark red
0.37 × 0.24 × 0.15 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.753$, $T_{max} = 0.871$
13 220 measured reflections
4332 independent reflections
2676 reflections with $I > 2\sigma(I)$
$R_{int} = 0.078$
$\theta_{max} = 26.0°$
$h = -9 \rightarrow 9$
$k = -26 \rightarrow 18$
$l = -15 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.112$
$S = 0.92$
4332 reflections
277 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—Cl1	2.2373 (9)	Co1—N3	1.907 (3)
Co1—N1	1.901 (3)	Co1—N4	1.899 (3)
Co1—N2	1.894 (3)	Co1—N5	1.939 (2)
N1—Co1—N3	179.63 (13)	N3—Co1—N5	89.66 (10)
N1—Co1—N5	90.22 (11)	N3—Co1—Cl1	90.26 (8)
N1—Co1—Cl1	89.87 (8)	N4—Co1—N1	98.96 (12)
N2—Co1—N1	81.43 (13)	N4—Co1—N3	81.39 (12)
N2—Co1—N3	98.22 (12)	N4—Co1—N5	88.88 (11)
N2—Co1—N4	179.61 (13)	N4—Co1—Cl1	89.35 (8)
N2—Co1—N5	91.15 (11)	N5—Co1—Cl1	178.22 (8)
N2—Co1—Cl1	90.63 (8)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O4	0.86 (1)	1.66 (1)	2.512 (4)	168 (4)
O3—H3···O2	0.87 (3)	1.62 (3)	2.482 (4)	170 (5)

The hydroxy H atoms were located in difference Fourier maps and refined isotropically, with O—H distances restrained to 0.85 (1) Å and with fixed isotropic displacement parameters of 0.08 Å^2. The other H atoms were positioned geometrically and were treated as riding on their parent C atoms, with aromatic C—H distances of 0.93 Å, methyl C—H distances of 0.96 Å and methylene C—H distances of 0.97 Å, with fixed isotropic displacement parameters of 0.08 Å^2. As a resuly of the atomic vibration of the terminal methyl groups and phenyl ring, the displacement parameters of those C atoms are relatively large.

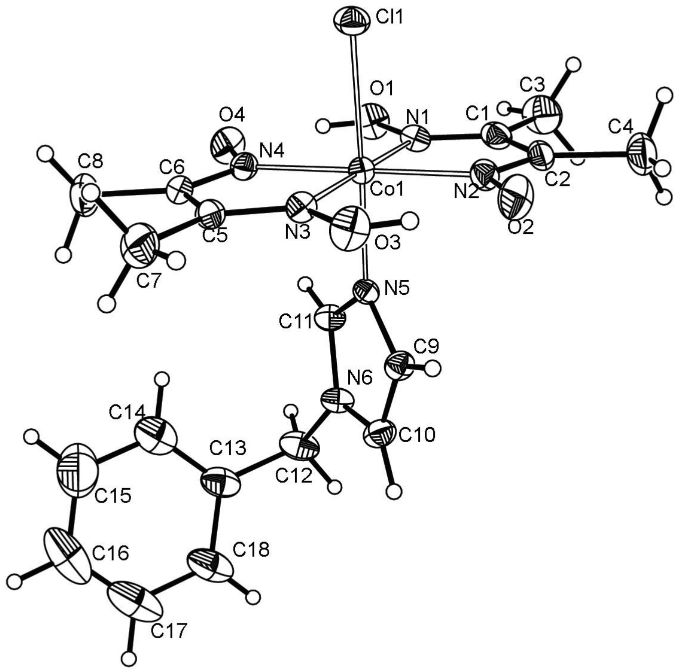


Figure 1
A view of the title compound. Displacement ellipsoids are drawn at the 40% probability level.

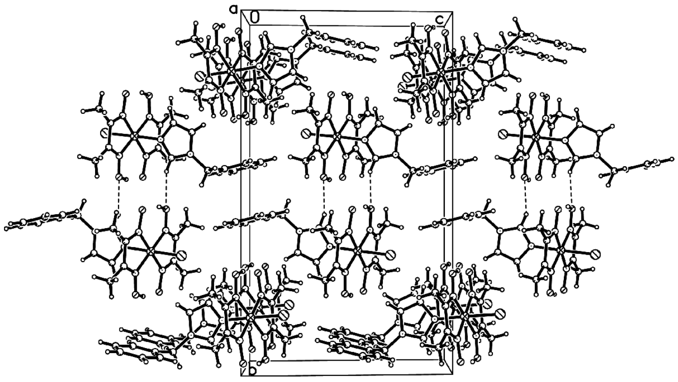


Figure 2
A view of the packing along the *a* axis. Dashed lines indicate hydrogen bonds.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors acknowledge the State Key Laboratory of Inorganic Synthesis and Preparative Chemistry for support of this work. We also thank Professor Long-Guan Zhu for his help.

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Acta Cryst. (2005). E**61**, m936–m938 Shen *et al.* • $[Co(C_4H_7N_2O_2)_2Cl(C_{10}H_{10}N_2)]$ **m937**

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