metal-organic papers

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Bis(2-aminopyridine)dibenzoatocobalt(II)

The title compound, $[Co(C_7H_5O_2)_2(C_5H_6N_2)_2]$, contains Co^{II} cations bonded to two bidentate benzoate ligands and two 2-aminopyridine ligands, resulting in highly distorted *cis*-CoN_2O_4 octahedra. The crystal structure is stabilized by N—H···O hydrogen bonds.

Comment

Cobalt complexes are of great interest in coordination chemistry in relation to catalysis and enzymatic reactions, magnetism, and molecular architectures (Billson *et al.*, 2000; Fritsky *et al.*, 2003; Kotera *et al.*, 2003). Cobalt complexes with benzoic acid and various *N*-heterocyclic compounds or amines have been reported (Brechin *et al.*, 1996; Saussine *et al.*, 1985; Singh *et al.*, 2005; Yamami *et al.*, 1997). As an extension of this work, the crystal structure of the title compound, (I) (Fig. 1), is reported here.

(I)
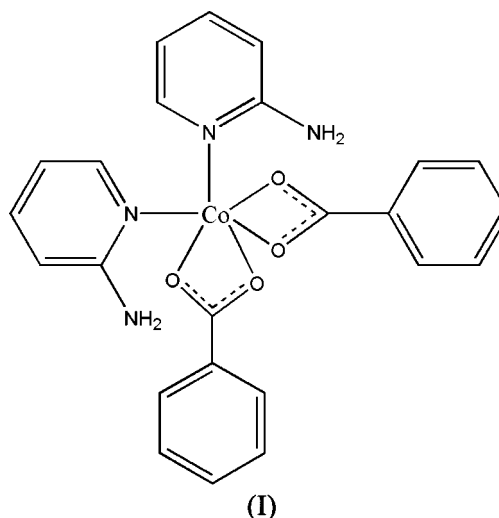
The Co^{II} ion in (I) is six-coordinated by four O atoms from two bidentate benzoate ligands and by two N atoms from two 2-aminopyridine molecules, resulting in a highly distorted *cis*-CoN_2O_4 octahedron (Table 1). The C—O bond lengths indicate that the negative charges of the benzoate –CO_2^- groups are completely delocalized. The acute Co—O—C bond angles cover the narrow range from 86.95 (9) to 91.49 (8)°.

In the crystal structure, the stabilization of (I) is supported by N—H···O hydrogen bonds (Table 2).

Experimental

A mixture of $CoCO_3$ (0.3 mmol, 35.7 mg) and benzoic acid (0.1 mmol, 12.2 mg) in a H_2O–EtOH solution (2:1 *v/v*, 20 ml) was heated with stirring for 1 h in an open beaker, then 2-aminopyridine (0.1 mmol, 9.4 mg) was added. The solution was heated for 30 min and the

remaining solid phase was filtered off. After allowing the solution to stand in air for 5 d, red block-shaped crystals of (I) were formed on slow evaporation of the solvent. Analysis found: C 58.88, H 4.56, N 11.47%; calculated for $C_{24}H_{22}CoN_4O_4$: C 58.90, H 4.53, N 11.45%.

Crystal data

$[Co(C_7H_5O_2)_2(C_5H_6N_2)_2]$	$Z = 8$
$M_r = 489.39$	$D_x = 1.373$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 25.097 (5)$ Å	$\mu = 0.76$ mm^{-1}
$b = 10.991 (2)$ Å	$T = 293 (2)$ K
$c = 17.499 (3)$ Å	Block, red
$\beta = 101.28 (3)°$	$0.28 \times 0.23 \times 0.16$ mm
$V = 4733.7 (15)$ Å^3	

Data collection

Bruker APEX area-detector diffractometer	19355 measured reflections
φ and ω scans	5137 independent reflections
Absorption correction: multi-scan	4599 reflections with $I > 2\sigma(I)$
(*SADABS*; Bruker, 2001)	$R_{int} = 0.018$
$T_{min} = 0.815$, $T_{max} = 0.888$	$\theta_{max} = 27.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0529P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.031$	$+ 1.2499P]$
$wR(F^2) = 0.086$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.018$
5137 reflections	$\Delta\rho_{max} = 0.37$ e Å^{-3}
298 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Co1—N3	2.0579 (14)	Co1—O3	2.1746 (12)
Co1—N1	2.0644 (14)	C1—O1	1.2680 (18)
Co1—O4	2.0726 (11)	C1—O2	1.2638 (16)
Co1—O2	2.1150 (13)	C8—O3	1.2625 (16)
Co1—O1	2.1268 (11)	C8—O4	1.2643 (17)
O2—Co1—O1	61.99 (4)	C1—O2—Co1	89.64 (9)
O4—Co1—O3	61.79 (4)	C8—O3—Co1	86.95 (9)
C1—O1—Co1	89.00 (8)	C8—O4—Co1	91.49 (8)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N4—H4$C\cdots$O1	0.90	2.08	2.9536 (19)	164
N4—H4$B\cdots$O3^i	0.90	2.17	2.9791 (17)	150
N2—H2$B\cdots$O4	0.90	1.98	2.849 (2)	161
N2—H2$A\cdots$O2^{ii}	0.90	2.12	2.9178 (18)	147

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

All H atoms were placed in idealized positions (C—H = 0.93–0.97 Å and N—H = 0.90 Å) and refined as riding, with U_{iso}(H) = $1.2U_{eq}$(C) and $1.5U_{eq}$(N).
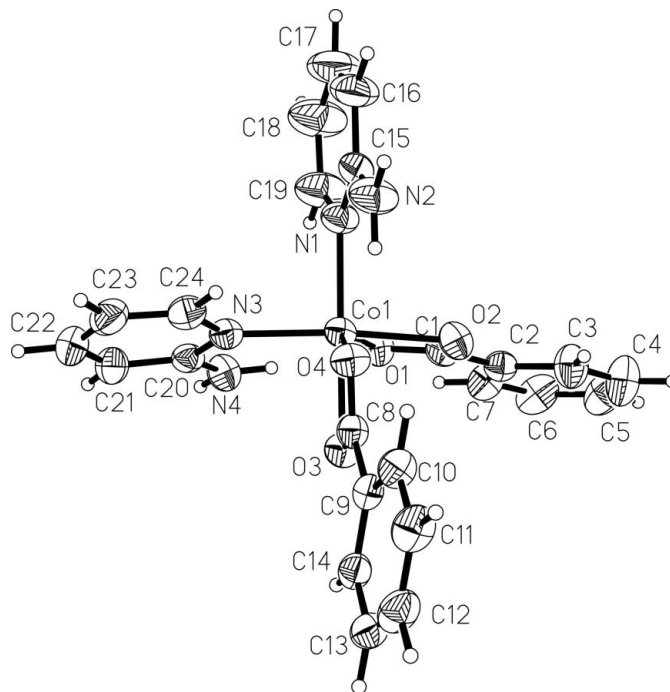

Figure 1
The structure of (I), showing 35% probability displacement ellipsoids (arbitrary spheres for the H atoms).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXL97*.

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