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Diaquabis[*N*-benzoyl-*N*′-(isonicotinoyl)-hydrazine]dichlorocobalt(II) dihydrate

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Key indicators

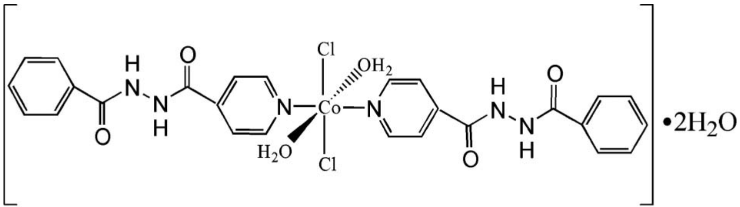
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.077
wR factor = 0.157
Data-to-parameter ratio = 13.7

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

In the title complex, $[CoCl_2(C_{13}H_{11}N_3O_2)_2(H_2O)_2]\cdot 2H_2O$, each Co^{II} atom occupies an inversion center and is coordinated by two water molecules, two Cl^- anions and two *N*-benzoyl-*N*′-(isonicotinoyl)hydrazine ligands in a distorted octahedral geometry. The asymmetric unit contains two half-complexes. The three-dimensional supramolecular architecture is stabilized by intermolecular hydrogen bonding.

Comment

The chemical properties of hydrazide and its analogs have been intensively investigated in several research areas because of their chelating capability and pharmacological application (Sreeja *et al.*, 2004). As part of a continuing study (Bian *et al.*, 2005), we have synthesized the title Co^{II} complex, (I), and present its structure here.



(I)

The molecular structure of (I) is shown in Fig. 1. The asymmetric unit contains half each of two independent centrosymmetric Co^{II} complex molecules with the Co^{II} ions located on inversion centers. Each Co^{II} ion is coordinated by two water molecules, two Cl^- anions and two *N*-benzoyl-*N*′-(isonicotinoyl)hydrazine ligands with an elongated octahedral coordination geometry (Table 1). The coordination geometry of (I) is similar to that found in diaquadichlorobis[*N*-(hydroxymethyl)nicotinamide]cobalt(II) (Shamuratov *et al.*, 1991).

The three-dimensional supramolecular architecture is stabilized by an extensive hydrogen-bonding network involving uncoordinated water, coordinated water and hydrazine molecules and Cl^- anions (Table 2).

Experimental

N-Benzoyl-*N*6′-(isonicotinoyl)hydrazine (*L*) was prepared according to Bian *et al.* (2005). A mixture of $CoCl_2\cdot 6H_2O$ (0.3 mmol) in water (1 ml) and *L* (0.6 mmol) in methanol (10 ml) was refluxed for 1 h. The resulting dark-red solution was filtered. The filtrate was then left to stand at room temperature for two weeks to obain single crystals of (I).

Crystal data

$[CoCl_2(C_{13}H_{11}N_3O_2)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 684.39$
Monoclinic, $P2_1/n$
$a = 22.06$ (4) Å
$b = 6.251$ (11) Å
$c = 22.73$ (4) Å
$\beta = 97.89$ (3)°
$V = 3105$ (10) Å^3
$Z = 4$
$D_x = 1.464$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.78$ mm^{-1}
$T = 293$ (2) K
Block, dark red
0.24 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.835$, $T_{max} = 0.885$
12298 measured reflections
5366 independent reflections
3328 reflections with $I > 2\sigma(I)$
$R_{int} = 0.070$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.077$
$wR(F^2) = 0.157$
$S = 1.11$
5366 reflections
391 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 6.4187P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co1—O3	2.074 (4)	Co2—O6	2.109 (5)
Co1—N1	2.193 (5)	Co2—N4	2.185 (5)
Co1—Cl1	2.501 (3)	Co2—Cl2	2.469 (3)
O3—Co1—N1^{i}	88.81 (19)	O6—Co2—N4^{ii}	91.55 (19)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O8	0.86	2.15	2.811 (9)	134
N3—H3···O1^{iii}	0.86	1.99	2.834 (8)	165
N5—H5*C*···O7	0.86	2.08	2.813 (9)	143
N6—H6···O5^{iv}	0.86	1.99	2.831 (8)	165
O3—H3*A*···O4^{v}	0.85	1.89	2.710 (7)	163
O3—H3*B*···Cl1^{vi}	0.85	2.31	3.085 (7)	151
O6—H6*A*···O2^{vii}	0.85	1.91	2.726 (7)	160
O6—H6*B*···Cl2^{vi}	0.85	2.42	3.212 (7)	155
O7—H7*A*···Cl1^{v}	0.86	2.48	3.233 (8)	147
O7—H7*B*···O4^{vi}	0.85	2.21	2.821 (8)	129
O8—H8*A*···Cl2^{viii}	0.85	2.46	3.291 (8)	167
O8—H8*B*···O1^{ix}	0.86	2.46	3.090 (9)	130
O8—H8*B*···O2^{ix}	0.86	2.28	3.033 (9)	146

Symmetry codes: (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (vi) $x, y+1, z$; (vii) $x-1, y, z$; (viii) $x+1, y, z$; (ix) $x, y-1, z$.

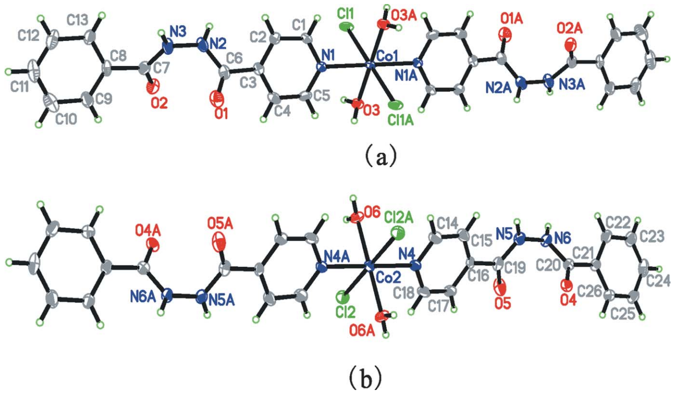


Figure 1
The two independent molecules (*a* and *b*) in (I), shown with 30% probability displacement ellipsoids [symmetry codes: (*a*) $2-x, 1-y, -z$; (b) $-x, 1-y, 1-z$].

H atoms of water molecules were located in a difference Fourier map and constrained to O—H = 0.85–0.86 Å, with U_{iso}(H) = 1.2U_{eq}(O). Other H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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, 1997); software used to prepare material for publication: *SHELXTL*.

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m1222 Yu *et al.* • $[CoCl_2(C_{13}H_{11}N_3O_2)_2(H_2O)_2]$ *Acta Cryst.* (2006). E**62**, m1221–m1222