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Diaquabis(4-chlorobenzoato-κO)bis(nicotinamide-κN)cobalt(II)

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Key indicators

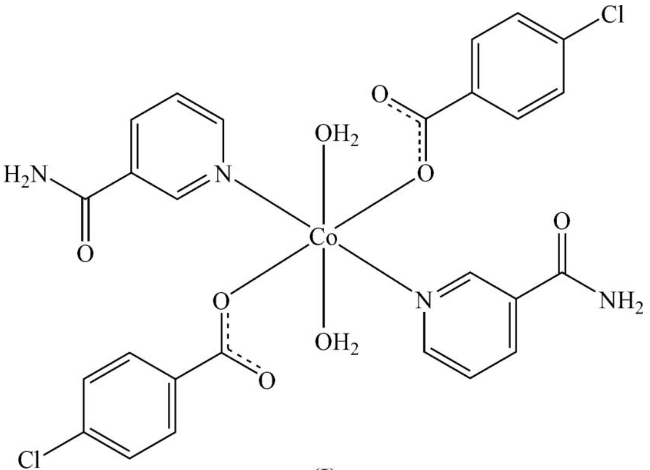
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
R factor = 0.046
wR factor = 0.131
Data-to-parameter ratio = 14.1

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

In the title compound, $[Co(C_7H_4ClO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$, the Co^{II} atom lies on a centre of inversion and is coordinated in a distorted octahedral geometry by two 4-chlorobenzoate anions, two nicotinamide molecules and two water molecules, all of which act as monodentate ligands. Intermolecular O—H···O and N—H···O hydrogen bonds link the molecules into two-dimensional sheets.

Comment

Nicotinamide (NA) is one form of niacin and a deficiency of this vitamin leads to loss of copper from the body, known as pellagra disease. The nicotinic acid derivative *N*,*N*-diethylnicotinamide (DENA) is an important respiratory stimulant. Transition-metal complexes with biochemical molecules show interesting physical and/or chemical properties, which may find applications in biological systems (Antolini *et al.*, 1982). To the best of our knowledge, only a few structures of Co^{II} complexes with nicotinic and/or benzoic acid derivatives as ligands have been reported to date (Amiraslanov *et al.*, 1979; Nadzhafov *et al.*, 1981; Mikelashvili, 1982; Hökelek & Necefoğlu, 1997; 1998; 1999*a*,*b*,*c*, 2007*a*).



(I)

In the title compound, (I), the Co^{II} atom lies on a centre of inversion and is coordinated by two 4-chlorobenzoic acid anions, two NA molecules and two water molecules (Fig. 1 and Table 1), all of which act as monodentate ligands. The slightly distorted octahedral coordination geometry is comparable to that in similar compounds (Hökelek & Necefoğlu, 1997; 1998; 1999*a*,*b*,*c*, 2007*a*). The near equality of the C1—O1 [1.251 (4) Å] and C1—O2 [1.257 (4) Å] bonds of the carboxylate group indicates a delocalized bonding arrangement,

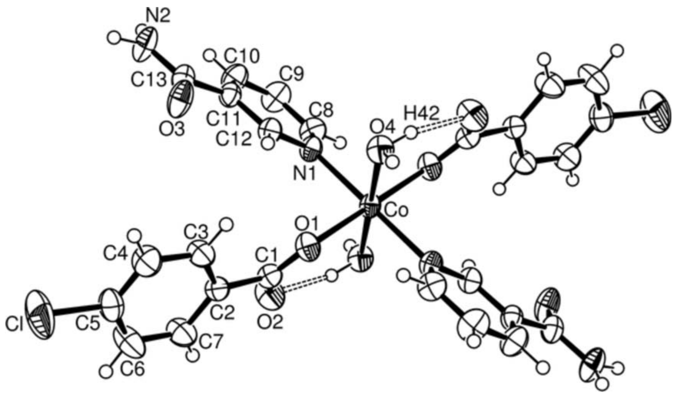


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level for non-H atoms. Unlabelled atoms are related to labelled atoms by the symmetry code ($-x$, $-y$, $-z$). Dashed lines denote O—H···O hydrogen bonds.

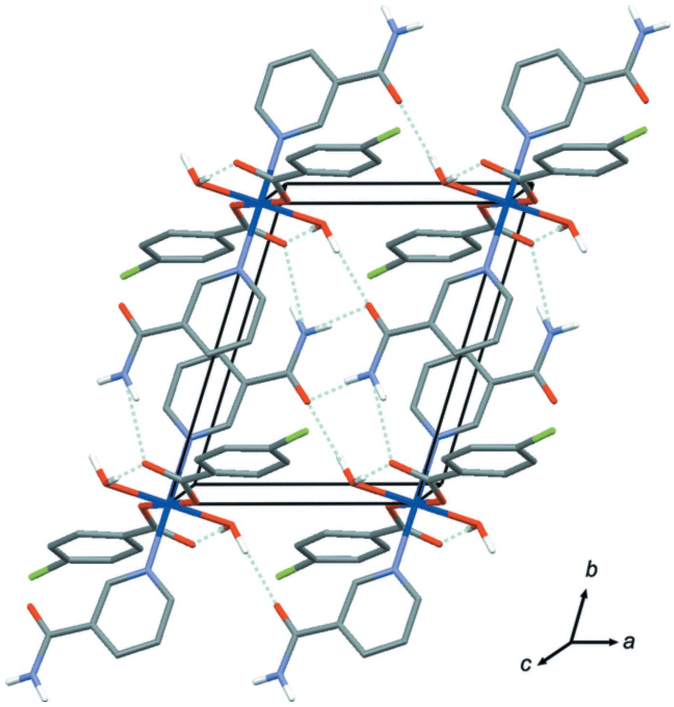


Figure 2
Partial packing diagram of (I), showing hydrogen bonds (dashed lines) linking the complexes into 2-dimensional sheets in the *ab* planes. H atoms not involved in hydrogen bonding are omitted.

rather than localized single and double bonds as has been observed in, for example, bis(4-hydroxybenzoato-κO)bis(nicotinamide-κN)zinc(II) (Necefoğlu *et al.*, 2002), diaquabis[4-(dimethylamino)benzoato-κO]bis(nicotinamide-κN)cobalt(II) dihydrate (Hökelek & Necefoğlu, 2007*a*) and tetraaquabis[4-(dimethylamino)benzoato-κO]manganese(II) dihydrate (Hökelek & Necefoğlu, 2007*b*). This may be influenced by the intra- and intermolecular O—H···O and N—H···O hydrogen bonds involving the carboxylate O atoms (Fig. 2 and Table 2).

In the crystal structure, the amide groups of the NA molecules form centrosymmetric hydrogen-bonded dimers (Fig. 2). O—H···O and N—H···O hydrogen bonds further link the molecules into two-dimensional sheets lying parallel to the *ab* plane (Fig. 2).

Experimental

The title compound, (I), was prepared by reaction of $CoSO_4$ (1.55 g, 10 mmol) and NA (2.44 g, 20 mmol) in H_2O (100 ml) with sodium 4-chlorobenzoate (3.11 g, 20 mmol) in H_2O (100 ml). The mixture was filtered and set aside to crystallize at ambient temperature for several days, giving pink single crystals.

Crystal data

$[Co(C_7H_4ClO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$
$M_r = 650.32$
Triclinic, $P\overline{1}$
$a = 7.5945$ (2) Å
$b = 9.9333$ (2) Å
$c = 10.0701$ (3) Å
$\alpha = 78.90$ (1)°
$\beta = 86.84$ (1)°
$\gamma = 71.55$ (2)°
$V = 707.13$ (9) Å^3
$Z = 1$
Mo $K\alpha$ radiation
$\mu = 0.85$ mm^{-1}
$T = 294$ (2) K
0.30 × 0.25 × 0.20 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.788$, $T_{max} = 0.842$
3086 measured reflections
2862 independent reflections
2259 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
3 standard reflections frequency: 120 min intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.131$
$S = 1.03$
2862 reflections
203 parameters
8 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -0.71$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—O1	2.074 (2)	Co—N1	2.146 (3)
Co—O4	2.134 (2)		
O1—Co—O4^{i}	92.53 (9)	O1^{i}—Co—N1	89.65 (9)
O1—Co—O4	87.47 (9)	O4^{i}—Co—N1	92.93 (9)
O1—Co—N1	90.35 (9)	O4—Co—N1	87.07 (9)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H42···O2	0.90 (4)	1.74 (5)	2.632 (4)	167 (5)
O4—H41···O3^{ii}	0.95 (3)	1.95 (3)	2.887 (4)	169 (3)
N2—H21···O2^{iii}	0.91 (3)	2.03 (3)	2.885 (4)	155 (3)
N2—H22···O3^{iv}	0.89 (4)	2.07 (4)	2.923 (5)	161 (3)

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

H atoms of the water molecule and NH_2 group were located in difference Fourier maps and refined isotropically with the O—H and N—H distances restrained to 0.92 (2) Å, and with the H···H

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distances restrained to 1.52 (4) Å. The remaining H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atoms, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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