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Diaquabis(4-fluorobenzoato-κO)bis(nicotinamide-κN^1)cobalt(II)

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.093
Data-to-parameter ratio = 13.2

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

The title Co^{II} complex, [Co($C_7H_4FO_2$)$_2$($C_6H_6N_2O$)$_2$(H_2O)$_2$], is monomeric and centrosymmetric. It contains two 4-fluorobenzoate and two nicotinamide ligands and two water molecules, all ligands being monodentate. The four O atoms in the equatorial plane around the Co atom form a slightly distorted square-planar arrangement, while the distorted octahedral coordination is completed by the two N atoms in the axial positions. In the crystal structure, O—H···O and N—H···O hydrogen bonds link the molecules, to form a two-dimensional network parallel to the ($10\overline{1}$) plane.

Comment

Transition metal complexes with biochemical molecules show interesting physical and/or chemical properties, through which they may find applications in biological systems (Antolini *et al.*, 1982). 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. Victims of pellagra show unusually high serum and urinary copper levels (Krishnamachari, 1974).

The structures of Co complexes having different benzoic and/or nicotinic acid derivatives as ligands have been the subject of much interest in our laboratory; examples are [Co($C_7H_5O_3$)$_2$(DENA)$_2$(H_2O)$_2$], (II) (where DENA is diethylnicotinamide, $C_{10}H_{14}N_2O$; Hökelek & Necefoğlu, 1997), [Co($C_7H_4NO_4$)$_2$(NA)$_2$(H_2O)$_2$], (III) ($C_6H_6N_2O$; Hökelek & Necefoğlu, 1998), [Co(C_7H_6NO)$_2$(NA)$_2$(H_2O)$_2$], (IV) (Hökelek & Necefoğlu, 1999*a*), [Co($C_7H_5O_2$)$_2$(NA)$_2$(H_2O)$_2$], (V) (Hökelek & Necefoğlu, 1999*b*), and [Co($C_7H_5O_3$)$_2$(NA)$_2$(H_2O)$_2$], (VI) (Hökelek & Necefoğlu, 1999*c*).

The structure–function–coordination relationships of the arylcarboxylate ion in Co^{II} complexes of benzoic acid deri-

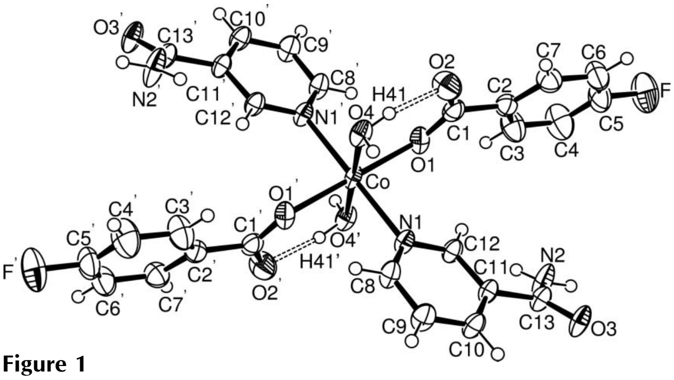
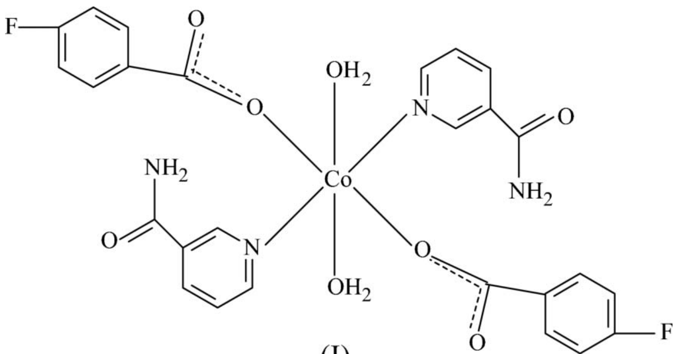


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as double dashed lines. Primed atoms are generated by the symmetry operator (−x, −y, −z).

vatives change, depending on the nature and position of the substituted groups on the benzene ring, the nature of the additional ligand molecule or solvent, and the medium of synthesis (Nadzhafov *et al.*, 1981; Shnulin *et al.*, 1981; Antsyshkina *et al.*, 1980; Amiraslanov *et al.*, 1979; Adiwidjaja *et al.*, 1978).

The structure determination of the title compound, (I), a cobalt complex with two fluorobenzoate (FB) and two NA ligands, and two water molecules, was undertaken in order to determine the properties of the FB and NA ligands and also to compare the results obtained with those reported previously.



(I)

Compound (I) is a monomeric complex, with the Co atom on a centre of symmetry. It contains two FB, two NA ligands and two water molecules (Fig. 1). All ligands are monodentate. The four O atoms (O1, O4, and the symmetry-related atoms O1′ and O4′) in the equatorial plane around the Co atom form a slightly distorted square-planar arrangement, while the slightly distorted octahedral coordination is completed by the two N atoms of the NA ligands (N2, N2′) in the axial positions (Table 1, Fig. 1), as observed in compounds (II)–(VI).

The near equality of the C1—O1 [1.268 (3) Å] and C1—O2 [1.253 (3) Å] bonds in the carboxylate group indicates a delocalized bonding arrangement, rather than localized single and double bonds, as in bis(4-hydroxybenzoato-κO)bis(nicotinamide-κN)zinc(II) (Necefoğlu *et al.*, 2002), tetraaquabis[4-(dimethylamino)benzoato-κO]manganese(II) dihydrate (Hökelek & Necefoğlu, 2007*a*) and diaquabis[4-(dimethylamino)benzoato-κO](nicotinamide-κN^1)cobalt(II) dihydrate (Hökelek & Necefoğlu, 2007*b*). This may be due to the intramolecular O—H···O hydrogen bonding of the carboxylate O atoms (Table 2). The Co atom is displaced out of the least-squares plane of the carboxylate group (O1/C1/O2) by 0.530 (2) Å. The dihedral angle between the carboxylate group and the benzene ring C2–C7 is 8.67 (11)°, while that between rings C2–C7 and N2/C8–C12 is 77.13 (6)°.

The molecules of (I) are linked into a two-dimensional network parallel to the $(10\overline{1})$ plane by O—H···O and N—H···O intermolecular hydrogen bonds (Table 2).

Experimental

Compound (I) was prepared by the reaction of $CoSO_4$ (1.55 g, 10 mmol) and nicotinamide (2.44 g, 20 mmol) in H_2O (100 ml) with sodium *p*-fluorobenzoate (3.24 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

$[Co(C_7H_4FO_2)_2(C_6H_6N_2O)_2(H_2O)_2]$
$M_r = 617.43$
Monoclinic, $P2_1/n$
$a = 12.003$ (2) Å
$b = 8.928$ (4) Å
$c = 12.4219$ (18) Å
$\beta = 90.434$ (13)°

$V = 1331.2$ (7) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.72$ mm^{-1}
$T = 294$ (2) K
0.25 × 0.20 × 0.15 mm

Data collection

Enraf–Nonius TurboCAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.782$, $T_{max} = 0.898$
2815 measured reflections

2685 independent reflections
2184 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.093$
$S = 1.03$
2685 reflections
203 parameters

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—O1	2.0683 (14)	Co—N1	2.1704 (17)
Co—O4	2.1307 (15)		
O1—Co—O4	91.04 (6)	O4—Co—N1^i	89.09 (6)
O1—Co—O4^i	88.96 (6)	O1—Co—N1	89.27 (6)
O1—Co—N1^i	90.73 (6)	O4—Co—N1	90.91 (6)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H21···O3^{ii}	0.83 (3)	2.27 (4)	2.886 (3)	132 (3)
N2—H22···O4^{iii}	0.83 (3)	2.30 (2)	2.969 (3)	138 (2)
O4—H41···O2	0.87 (4)	1.72 (4)	2.580 (2)	168 (4)
O4—H42···O3^{iv}	0.86 (3)	1.93 (3)	2.778 (2)	165 (3)

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

H atoms of the water molecule and NH_2 group were located in a difference map and refined isotropically [O—H = 0.86 (3) and 0.87 (4) Å and U_{iso}(H) = 0.060 (8) and 0.082 (11) Å^2; N—H = 0.83 (3) and 0.83 (3) Å and U_{iso}(H) = 0.049 (7) and 0.077 (10) Å^2]. The remaining H atoms were positioned geometrically and constrained to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(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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References

Adiwidjaja, G., Rossmanith, E. & Küppers, H. (1978). *Acta Cryst.* B**34**, 3079–3083.

Amiraslanov, I. R., Mamedov, Kh. S., Movsumov, E. M., Musaev, F. N. & Nadzhafov, G. N. (1979). *Zh. Strukt. Khim.* **20**, 1075–1080. (In Russian.)

Antolini, L., Battaglia, L. P., Corradi, A. B., Marcotrigiano, G., Menabue, L., Pellacani, G. C. & Saladini, M. (1982). *Inorg. Chem.* **21**, 1391–1395.

Antsyshkina, A. S., Chiragov, F. M. & Poray-Koshits, M. A. (1980). *Koord. Khim.* **15**, 1098–1103. (In Russian.)

Enraf–Nonius (1994). *CAD-4 EXPRESS*. Enraf–Nonius, Delft, The Netherlands.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.

Harms, K. & Wocadlo, S. (1995). *XCAD4*. University of Marburg, Germany.

Hökelek, T. & Necefoğlu, H. (1997). *Acta Cryst.* C**53**, 187–189.

Hökelek, T. & Necefoğlu, H. (1998). *Acta Cryst.* C**54**, 1242–1244.

Hökelek, T. & Necefoğlu, H. (1999*a*). *Anal. Sci.* **15**, 1043–1044.

Hökelek, T. & Necefoğlu, H. (1999*b*). *Acta Cryst.* C**55**, 545–547.

Hökelek, T. & Necefoğlu, H. (1999*c*). *Acta Cryst.* C**55**, 1438–1440.

Hökelek, T. & Necefoğlu, H. (2007*a*). *Acta Cryst.* E**63**, m821–m823.

Hökelek, T. & Necefoğlu, H. (2007*b*). *Acta Cryst.* E**63**, m1078–m1080.

Krishnamachari, K. A. V. R. (1974). *Am. J. Clin. Nutr.* **27**, 108–111.

Nadzhafov, G. N., Shnulin, A. N. & Mamedov, Kh. S. (1981). *Zh. Strukt. Khim.* **22**, 124–128. (In Russian.)

Necefoğlu, H., Hökelek, T., Ersanlı, C. C. & Erdönmez, A. (2002). *Acta Cryst.* E**58**, m758–m761.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Shnulin, A. N., Nadzhafov, G. N., Amiraslanov, I. R., Usubaliev, B. T. & Mamedov, Kh. S. (1981). *Koord. Khim.* **7**, 1409–1416. (In Russian.)

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