Diaquabis(1*H*-imidazole-κN^3)bis(4-nitro-benzoato-κO)cobalt(II)

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Key indicators

Single-crystal X-ray study

T = 295 K

Mean σ(C–C) = 0.003 Å

R factor = 0.025

wR factor = 0.066

Data-to-parameter ratio = 11.6

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

The title complex, $[Co(C_7H_4NO_4)_2(C_3H_4N_2)_2(H_2O)_2]$, assumes an octahedral coordination geometry with the Co atom located on an inversion center. The overlapped arrangement of parallel imidazole ligands of neighboring complex molecules, with an interplanar distance of 3.555 (14) Å, suggests the existence of π–π stacking between imidazole rings.

Comment

Aromatic polycyclic compounds, such as phenanthroline, benzimidazole and quinoline, usually exhibit π–π stacking in metal complexes. As part of an investigation of the π–π stacking in metal complexes, a series of metal complexes incorporating imidazole has been prepared in our laboratory, and the crystal structure of the title Co^{II} complex, (I), is presented here; it shows π–π stacking between imidazole rings.

(I)
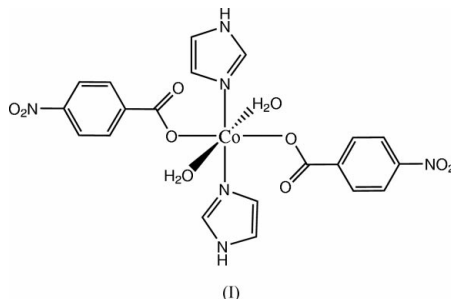
The molecular structure of (I) is shown in Fig. 1. The Co^{II} atom is located on an inversion center and has an octahedral coordination geometry (Table 1), formed by nitrobenzoate
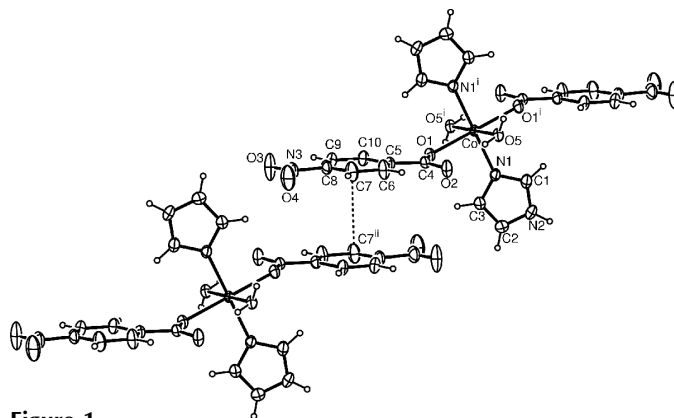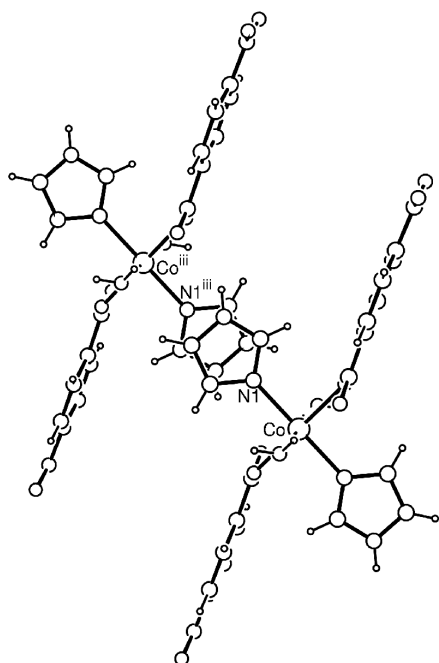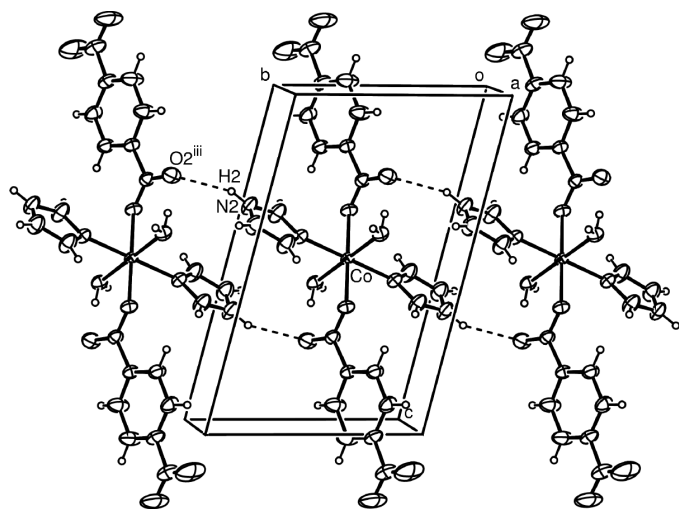

Figure 1

The molecular structure of (I), shown with 40% probability displacement ellipsoids. The dashed line indicates the shortest intermolecular C···C contact of 3.405 (3) Å. [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $2 - x, 1 - y, 2 - z$.]

Figure 2
$\pi-\pi$ stacking between imidazole rings. [Symmetry code: (iii) $1 - x, 2 - y, 1 - z$.]

Figure 3
Molecular packing diagram of (I). Dashed lines indicate intermolecular N—H···O hydrogen bonds. [Symmetry code: (iii) $1 - x, 2 - y, 1 - z$.]

anions, imidazole and water molecules. The nitrobenzoate assumes a nearly planar configuration and the nitro and carboxy groups are coplanar with the benzene plane, the maximum atomic deviation being 0.0800 (13) Å (for atom O2). The nitrobenzoate mean plane is tilted by 23.36 (5)° with respect to the equatorial coordination plane formed by the four O atoms. This is similar to the situation found in the Ni^{II} analog (Xu & Xu, 2004). The C7···C7^{ii} distance of 3.405 (3) Å [symmetry code: (ii) $2 - x, 1 - y, 1 - z$] shows that there is a short contact between neighboring parallel benzene rings, which may be the reason for the tilt of the nitrobenzoate plane.

An overlapped arrangement of parallel imidazole ligands in neighboring complex molecules is observed in the crystal structure (Fig. 2). The interplanar distance of 3.555 (14) Å suggests the existence of $\pi-\pi$ stacking between imidazole rings. The molecular packing is illustrated in Fig. 3. The complex molecules are linked to each other *via* intermolecular hydrogen bonds, either between imidazole and carboxyl groups or between coordinated water and the carboxyl group. Weak C—H···O hydrogen bonding occurs between imidazole and the carboxyl group (Table 2).

Experimental

CoCl$_2$·6H$_2$O (0.24 g, 1 mmol) was dissolved in an aqueous solution (10 ml) containing nitrobenzoic acid (0.33 g, 2 mmol) and NaOH (0.08 g, 2 mmol). The solution was refluxed for 20 min, then an ethanol solution (10 ml) of imidazole (0.14 g, 2 mmol) was added with continuous stirring. The resulting solution was refluxed for a further 3 h. After cooling to room temperature, the solution was filtered. Red single crystals were obtained from the filtrate after one week.

Crystal data

[Co(C$_7$H$_4$NO$_4$)$_2$(C$_3$H$_4$N$_2$)$_2$(H$_2$O)$_2$]	$Z = 1$
$M_r = 563.36$	$D_x = 1.666$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 5.6482$ (10) Å	Cell parameters from 2629
$b = 8.0559$ (12) Å	reflections
$c = 12.7628$ (11) Å	$\theta = 2.8-25.0°$
$\alpha = 75.619$ (2)°	$\mu = 0.84$ mm^{-1}
$\beta = 87.920$ (2)°	$T = 295$ (2) K
$\gamma = 86.9180$ (10)°	Prism, red
$V = 561.56$ (14) Å^3	$0.20 \times 0.14 \times 0.13$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer	1963 independent reflections
ω scans	1851 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.013$
	$\theta_{max} = 25.0°$
$T_{min} = 0.85, T_{max} = 0.90$	$h = -6 \rightarrow 6$
4259 measured reflections	$k = -9 \rightarrow 9$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.025$	$+ 0.148P]$
$wR(F^2) = 0.066$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
1963 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
169 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Co—O1	2.1827 (11)	Co—N1	2.0944 (14)
Co—O5	2.1208 (11)		
O1—Co—O5	93.11 (4)	N1—Co—O5	89.40 (5)
N1—Co—O1	92.75 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^i	0.86	2.32	3.076 (2)	146
O5—H5A···O2	0.80	1.88	2.6430 (17)	158
O5—H5B···O1^{iv}	0.84	2.03	2.8439 (16)	161
C3—H3···O5^v	0.93	2.40	3.305 (2)	165

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

Water H atoms were located in a difference Fourier map and refined fixed in those positions with isotropic displacement parameters of 0.05 Å^2. 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 $U_{iso}(H) = 1.2U_{eq}$ of the carrier atom.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/ MSC, 2002); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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