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Diaquabis(4-chlorobenzoato-*κO*)bis(1*H*-imidazole-*κN*^{3})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 = 0.030
wR factor = 0.081
Data-to-parameter ratio = 17.6

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

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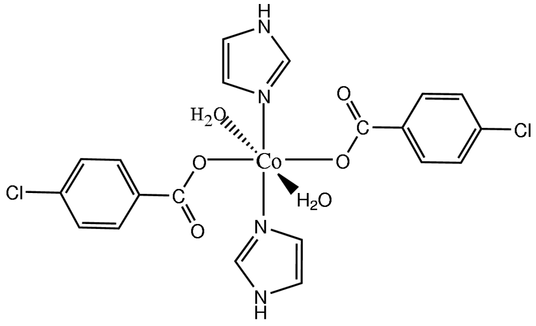
In the title complex, $[Co(C_7H_4ClO_2)_2(C_3H_4N_2)_2(H_2O)_2]$, the Co^{II} atom is located on an inversion center and assumes an octahedral coordination geometry. The chlorobenzoate plane is inclined to the equatorial plane with a dihedral angle of 20.34 (7)°. Weak C—H···Cl hydrogen bonding occurs between the chlorobenzoate ligands of neighboring molecules.

Comment

π–π Stacking between aromatic rings is related to the electron-transfer process in some biological systems (Deisenhofer & Michel, 1989). Aromatic polycyclic compounds, such as phenanthroline, benzimidazole and quinoline, have commonly shown π–π stacking in metal complexes (Wu *et al.*, 2003; Pan & Xu, 2004). Imidazole and benzoate have been used in the title cobalt(II) complex, (I), but the crystal structure shows that no π–π stacking occurs between aromatic rings.



(I)

The molecular structure of (I) is shown in Fig. 1. The Co^{II} atom is located on an inversion center and is surrounded by two imidazole molecules, two water molecules and two chlorobenzoate anions in an octahedral coordination geometry (Table 1). The benzoate anion is planar, the maximum atomic deviation being 0.0093 (12) Å for atom O2. The benzoate plane is tilted with respect to the equatorial plane formed by four O atoms by 20.34 (7)°, which is similar to the angle of 23.36 (5)° found in a nitrobenzoate–cobalt(II) complex (Xu & Xu, 2004).

The molecular packing is illustrated in Fig. 2. Conventional intramolecular and intermolecular O—H···O and N—H···O hydrogen bonds occur between molecules, as expected. Weak C—H···O hydrogen bonding also occurs between imidazole and coordinated water molecules of neighboring molecules (Table 2). Moreover, the C9—H9···Cl angle, which is close to linear, suggests weak hydrogen bond between chlorobenzoate ligands of neighboring molecules, although the C—H···Cl contact is rather long (Desiraju & Steiner, 1999). No π–π stacking occurs between aromatic rings in (I).

Experimental

An acetonitrile–water solution (10 ml) containing $CoSO_4 \cdot 7H_2O$ (0.28 g, 1 mmol), 4-chlorobenzoic acid (1.56 g, 10 mmol) and NaOH (0.40 g, 10 mmol) was refluxed for 30 min. Imidazole (0.13 g, 2 mmol) was then added to the above solution. The resulting solution was refluxed for 4 h and filtered. Red single crystals of (I) were obtained from the filtrate after 10 d.

Crystal data

$[Co(C_7H_4ClO_2)_2(C_3H_4N_2)_2(H_2O)_2]$
$M_r = 542.22$
Monoclinic, $P2_1/c$
$a = 13.2773$ (11) Å
$b = 5.4948$ (6) Å
$c = 16.0402$ (14) Å
$\beta = 95.7432$ (18)°
$V = 1164.36$ (19) Å^3
$Z = 2$
$D_x = 1.547$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7806 reflections
$\theta = 2.5$–$26.0°$
$\mu = 1.01$ mm^{-1}
$T = 295$ (2) K
Prism, red
0.36 × 0.32 × 0.27 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.698$, $T_{\max} = 0.766$
10379 measured reflections
2653 independent reflections
2360 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 27.4°$
$h = -17 \rightarrow 17$
$k = -7 \rightarrow 6$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.081$
$S = 1.04$
2653 reflections
151 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0431P)^2 + 0.5201P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.26$ e Å^{-3}
$\Delta\rho_{\min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Co—O3	2.1014 (12)	Co—O1	2.1472 (11)
Co—N1	2.1309 (13)		
O1—Co—N1	91.77 (5)	O3—Co—O1	87.16 (4)
O3—Co—N1	92.42 (5)		

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D\cdots A$	D—H$\cdots$$A$
O3—H3$A$$\cdots$O2$^{\rm i}$	0.88	1.83	2.6586 (18)	155
O3—H3$B$$\cdots$O1$^{\rm ii}$	0.88	1.91	2.7740 (16)	167
N2—H2N$\cdots$O2$^{\rm iii}$	0.86	2.00	2.802 (2)	154
C1—H1$\cdots$O3$^{\rm ii}$	0.93	2.40	3.247 (3)	152
C9—H9$\cdots$Cl$^{\rm iv}$	0.93	3.08	4.001 (2)	173

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

H atoms on aromatic rings were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and were included in the final cycles of refinement in a riding model, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$ of the carrier atom. Water H atoms were located in a difference Fourier map and refined as riding in their as-found positions relative to the O atom, with fixed isotropic displacement parameters of 0.05 Å^2.

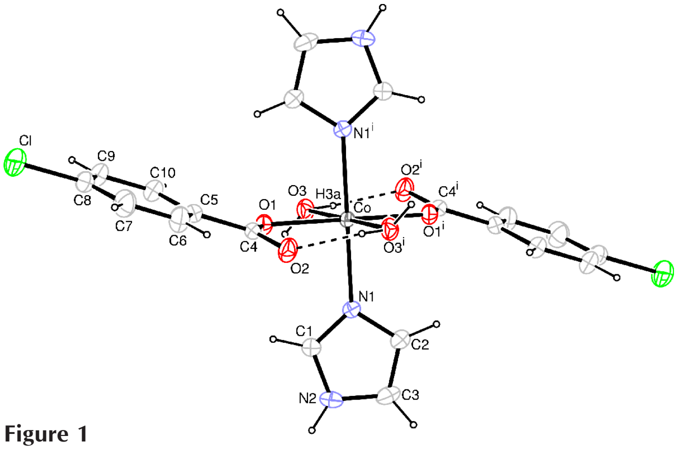


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids. Dashed lines indicate the intramolecular hydrogen bonding. [Symmetry code: (i) $1-x, -y, 1-z$.]

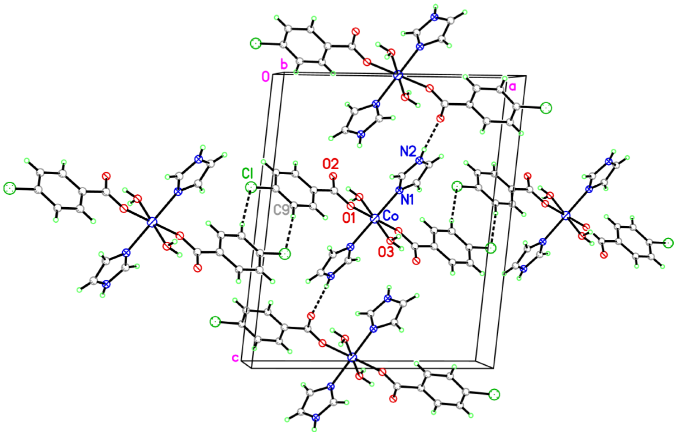


Figure 2
The crystal packing, showing intermolecular hydrogen bonding (dashed lines).

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) and *XP* (Siemens, 1994); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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