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Diaqua(5-nitro-1*H*-benzimidazole-κN^3)(oxydiacetato-$\kappa O,O',O''$)cobalt(II) monohydrate

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Key indicators

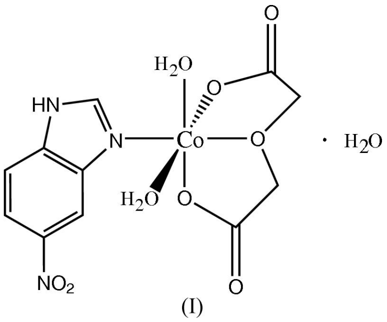
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.110
Data-to-parameter ratio = 15.3

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

In the title compound, $[Co(C_4H_4O_5)(C_7H_5N_3O_2)(H_2O)_2]\cdot H_2O$, the Co^{II} atom is coordinated by one tridentate oxydiacetate dianion, one monodentate nitrobenzimidazole molecule and two water molecules in a distorted octahedral geometry. The face-to-face distance of 3.345 (14) Å between parallel nitrobenzimidazole ligands of neighboring complexes indicates the existence of π–π stacking.

Comment

The π–π stacking interaction between aromatic rings is correlated with the electron-transfer process in some biological systems (Deisenhofer & Michel, 1989). In such systems, the face-to-face distance between parallel aromatic rings is significantly shorter than the van der Waals thickness for the aromatic ring. In order to investigate further the nature of π–π stacking, a series of metal complexes incorporating aromatic compounds such as phenanthroline (Li *et al.*, 2002), quinoline (Pan & Xu, 2004) and benzimidazole (Li *et al.*, 2005) have been prepared in our laboratory. In this article, we present the crystal structure of a new Co^{II} complex, (I), incorporating nitrobenzimidazole (NBZIM), in order to study the influence of a substituent group of the aromatic compound on the resulting π–π stacking.



(I)

The molecular structure of (I) is shown in Fig. 1. The Co^{II} atom is coordinated by one oxydiacetate (ODA) dianion, one NBZIM molecule and two water molecules in a distorted octahedral geometry (Table 1). The tridentate ODA anion chelates to the Co^{II} atom in a facial configuration. Both five-membered chelating rings of ODA have a similar envelope conformation, with the ether O atom (O3) lying in the flap position and deviating from the mean planes formed by the other four atoms by 0.358 (4) and 0.279 (4) Å for the O1 and O4 rings, respectively. The bond angles at atom O3 indicate the normal sp^3-hybridization for the ether O atom, while the Co—O3 bond distance is significantly longer than the Co—O(carboxyl) bonds (Table 1).

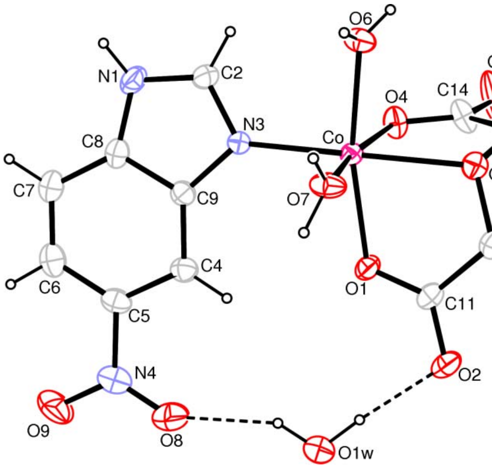


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). Dashed lines indicate hydrogen bonds.

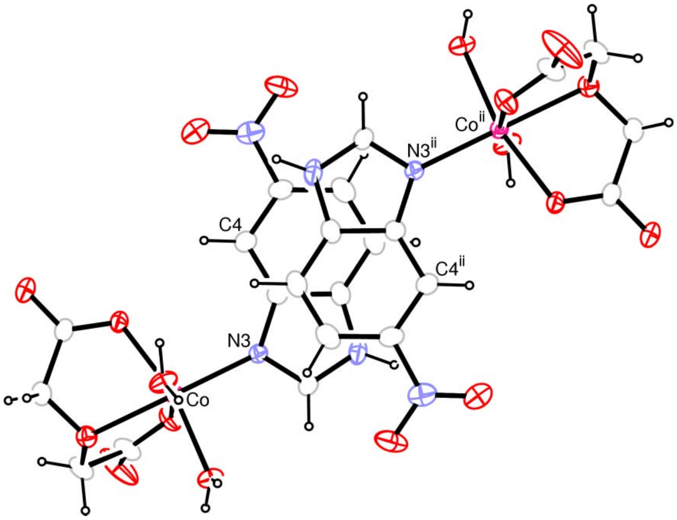


Figure 2
π–π stacking of NBZIM rings between neighboring molecules. [Symmetry code: (ii) $1 - x, 2 - y, 1 - z$.]

The nitro group is coplanar with the benzimidazole (BZIM) ring, the maximum atomic deviation being 0.034 (2) Å for atom O8. The NBZIM ligand coordinates in a monodentate fashion to the Co^{II} atom. The Co—N3 bond distance of 2.089 (2) Å in (I) is shorter than the 2.114 (3) Å found in a corresponding Co^{II} complex with the BZIM ligand, $[Co(BZIM)(malonato)(H_2O)]_n$, (Xue *et al.*, 2003).

A partially overlapped arrangement between neighboring parallel NBZIM ligands is observed in (I) (Fig. 2). The face-to-face distance of 3.345 (14) Å is smaller than the 3.42 (2) Å found in the corresponding Co^{II} complex with the BZIM ligand (Xue *et al.*, 2003) and suggests the existence of strong π–π stacking interactions in (I).

An extensive hydrogen-bonding network occurs in (I) (Fig. 3). Atom H2 is involved in a bifurcated C—H···O bond (Table 2).

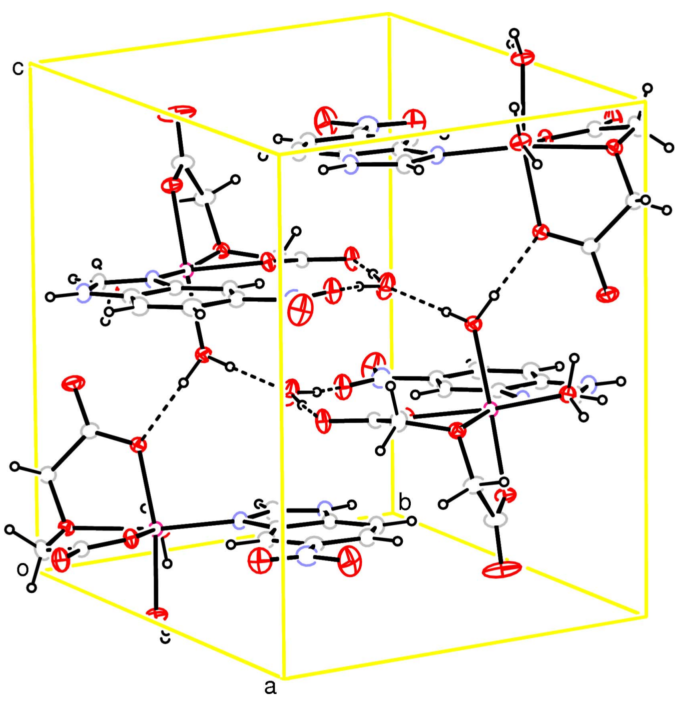


Figure 3
The packing of (I), showing the intermolecular hydrogen bonding (dashed lines).

Experimental

An aqueous solution (15 ml) of $CoCl_2·6H_2O$ (1 mmol), H_2ODA (1 mmol) and Na_2CO_3 (1 mmol) was mixed with an aqueous solution (5 ml) of NBZIM (2 mmol). The solution was refluxed for 4 h and then filtered. Red single crystals of (I) were obtained from the filtrate after 6 d.

Crystal data

$[Co(C_4H_4O_5)(C_7H_5N_3O_2)(H_2O)_2]·H_2O$
$M_r = 408.19$
Monoclinic, $P2_1/c$
$a = 11.5641\ (5)$ Å
$b = 10.2592\ (5)$ Å
$c = 12.7556\ (6)$ Å
$\beta = 90.3721\ (12)^\circ$
$V = 1513.27\ (12)$ Å^3
$Z = 4$
$D_x = 1.792$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10 912 reflections
$\theta = 2.4$–25.0°
$\mu = 1.20$ mm^{-1}
$T = 295\ (2)$ K
Plate, red
0.31 × 0.20 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.740$, $T_{max} = 0.902$
14 228 measured reflections
3468 independent reflections
2938 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.5^\circ$
$h = -15 \rightarrow 15$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.110$
$S = 1.10$
3468 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 1.5881P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

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Table 1
Selected interatomic distances (Å).

Co—O1	2.0541 (19)	Co—O6	2.0876 (19)
Co—O3	2.1824 (19)	Co—O7	2.120 (2)
Co—O4	2.103 (2)	Co—N3	2.089 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	1.88	2.715 (3)	164
O1*W*—H1*A*···O2	0.90	1.86	2.746 (3)	171
O1*W*—H1*B*···O8	0.90	2.07	2.891 (4)	151
O6—H6*A*···O5^{ii}	0.89	1.76	2.621 (3)	162
O6—H6*B*···O9^{iii}	0.82	2.18	2.998 (3)	173
O7—H7*A*···O1*W*^{iv}	0.90	1.82	2.709 (3)	171
O7—H7*B*···O4^{ii}	0.86	1.99	2.853 (3)	174
C2—H2···O6	0.93	2.54	3.069 (4)	116
C2—H2···O5^{v}	0.93	2.31	3.199 (5)	160
C7—H7···O1*W*^{i}	0.93	2.58	3.498 (4)	168

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

C- and N-bound H atoms were placed in calculated positions, with C—H = 0.97 (methylene) and 0.93 Å (aromatic) and N—H = 0.86 Å, and included in the final cycles of refinement as riding atoms with the constraint $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier) applied. Water H atoms were located in a difference Fourier map and refined as riding in their as-found positions relative to their carrier O atoms, with fixed isotropic displacement parameters of 0.05 Å^2.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); 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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