

Tris(1*H*-benzimidazole- κN^3)(oxydiacetato- $\kappa^3 O, O', O''$)cobalt(II)**Lei Cao[‡] and Duan-Jun Xu***Department of Chemistry, Zhejiang University,
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Key indicatorsSingle-crystal X-ray study
 $T = 295$ K
Mean $\sigma(C-C) = 0.005$ Å
 R factor = 0.041
 wR factor = 0.114
Data-to-parameter ratio = 13.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title complex, $[Co(C_4H_4O_5)(C_7H_6N_2)_3]$, one tridentate oxydiacetate dianion and three benzimidazole molecules coordinate to the Co^{II} cation, resulting in a distorted octahedral geometry. The oxydiacetate ligand chelates to the Co^{II} cation with a facial configuration and the $Co-O$ (ether) bond distance is longer than the average $Co-O$ (carboxyl) bond distance by 0.185 (3) Å. A network of $N-H\cdots O$ hydrogen bonds helps to establish the crystal packing.

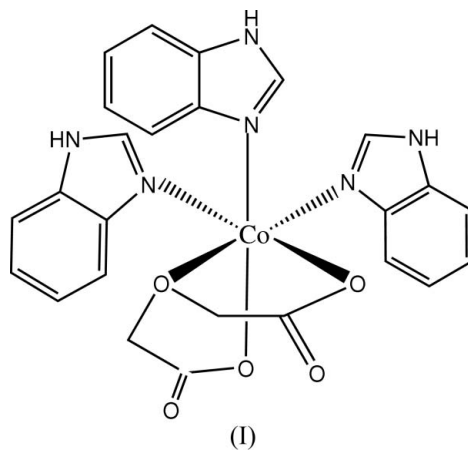
Received 20 September 2005

Accepted 21 September 2005

Online 28 September 2005

Comment

Several reported crystal structures of metal complexes incorporating the benzimidazole ($C_7H_6N_2$; BZIM) ligand have shown the existence of $\pi-\pi$ stacking between neighbouring aromatic rings in these structures (Chen *et al.*, 2003; Liu & Xu, 2004; Bukowska-Strzyżewska & Tosik, 1983). As part of our ongoing investigations of the nature of $\pi-\pi$ stacking (Li *et al.*, 2005), the title BZIM/ODA (ODA is the oxydiacetate dianion, $C_4H_4O_5^{2-}$) complex of Co^{II} , (I), has been prepared in our laboratory, and its structure is presented here.



The molecular structure of (I) is illustrated in Fig. 1. The combination of three BZIM ligands and a tridentate chelating ODA ligand results in a distorted octahedral coordination for the Co^{II} cation (Table 1). The facial configuration of the ODA anion in (I) differs from the meridional configuration found in most Co complexes with a chelating ODA ligand (CSD, Version 5.26; Allen, 2002), but agrees with that found in diaqua(nitrobenzimidazole)(ODA)cobalt(II) (Zhang *et al.*, 2005). It is notable that the $Co-O$ (ether) bond is significantly longer than the $Co-O$ (carboxyl) bonds in (I).

As shown in the packing diagram (Fig. 2), the uncoordinated ODA carboxyl atoms, O2 and O5, form links with the BZIM ligands of neighbouring complexes by accepting $N-$

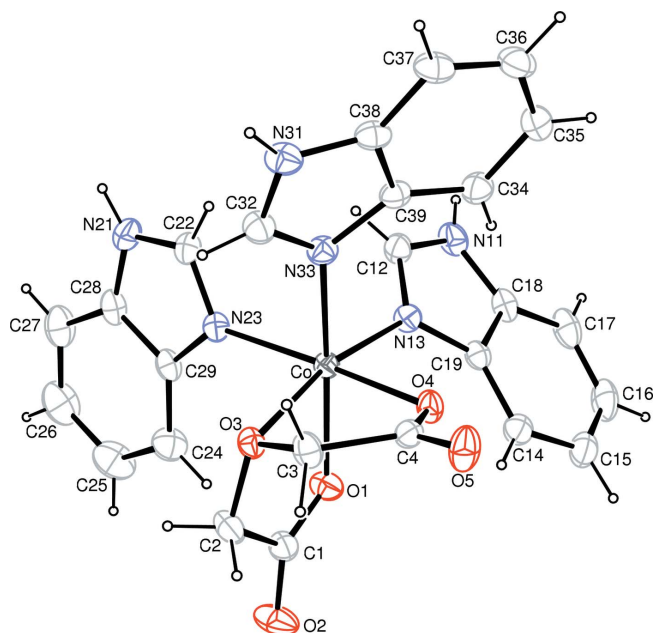


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

H \cdots O hydrogen bonds (Table 2), which results in a long centroid-to-centroid separation ($> 5 \text{ \AA}$) for the latter species. Thus, no π - π stacking occurs between parallel BZIM ligands in the crystal structure of (I).

Experimental

An aqueous solution (15 ml) of $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ (1 mmol), H_2ODA (1 mmol) and Na_2CO_3 (1 mmol) was mixed with an ethanol solution (5 ml) of BZIM (2 mmol). The solution was refluxed for 5 h and then filtered. Red single crystals of (I) were obtained after 2 d.

Crystal data

$[\text{Co}(\text{C}_4\text{H}_4\text{O}_3)(\text{C}_7\text{H}_6\text{N}_2)_3]$	$D_x = 1.486 \text{ Mg m}^{-3}$
$M_r = 545.42$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 11165 reflections
$a = 12.2152(4) \text{ \AA}$	$\theta = 2.3\text{--}26.5^\circ$
$b = 10.3120(2) \text{ \AA}$	$\mu = 0.75 \text{ mm}^{-1}$
$c = 19.3617(4) \text{ \AA}$	$T = 295(2) \text{ K}$
$\beta = 91.257(1)^\circ$	Rod, red
$V = 2438.27(11) \text{ \AA}^3$	$0.26 \times 0.09 \times 0.06 \text{ mm}$
$Z = 4$	

Data collection

Rigaku R-Axis RAPID diffractometer	4587 independent reflections
ω scans	3430 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$R_{\text{int}} = 0.048$
$T_{\text{min}} = 0.918$, $T_{\text{max}} = 0.955$	$\theta_{\text{max}} = 25.6^\circ$
19382 measured reflections	$h = -14 \rightarrow 14$
	$k = -12 \rightarrow 12$
	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.041$	$w = 1/[\sigma^2(F_o^2) + (0.066P)^2]$
$wR(F^2) = 0.114$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{\text{max}} = 0.001$
4587 reflections	$\Delta\rho_{\text{max}} = 0.62 \text{ e \AA}^{-3}$
334 parameters	$\Delta\rho_{\text{min}} = -0.56 \text{ e \AA}^{-3}$

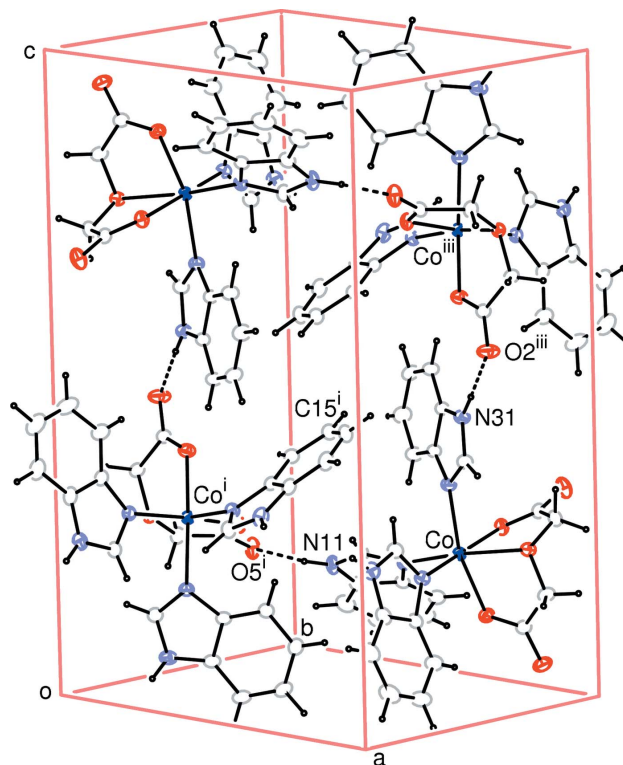


Figure 2
A packing diagram for (I). Dashed lines indicate intermolecular hydrogen bonds. [Symmetry codes: (i) $1 - x, -\frac{1}{2} + y, \frac{1}{2} - z$; (iii) $x, \frac{3}{2} - y, \frac{1}{2} + z$.]

Table 1

Selected geometric parameters (\AA , $^\circ$).

Co—O1	2.039 (2)	Co—N13	2.085 (2)
Co—O3	2.269 (2)	Co—N23	2.178 (2)
Co—O4	2.1294 (19)	Co—N33	2.134 (2)
O1—Co—O3	77.60 (8)	O3—Co—N33	88.88 (8)
O1—Co—O4	87.68 (8)	O4—Co—N13	94.91 (8)
O1—Co—N13	94.47 (9)	O4—Co—N23	172.95 (8)
O1—Co—N23	93.63 (9)	O4—Co—N33	83.58 (8)
O1—Co—N33	165.29 (9)	N13—Co—N23	91.89 (9)
O3—Co—O4	76.89 (7)	N13—Co—N33	98.03 (9)
O3—Co—N13	168.69 (8)	N33—Co—N23	93.65 (9)
O3—Co—N23	96.61 (8)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
N11—H11 \cdots O4 ⁱ	0.86	2.23	3.039 (3)	157
N11—H11 \cdots O5 ⁱ	0.86	2.39	3.018 (3)	131
N21—H21 \cdots O5 ⁱⁱ	0.86	1.96	2.762 (3)	154
N31—H31 \cdots O2 ⁱⁱⁱ	0.86	1.90	2.756 (3)	178

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

H atoms were placed in calculated positions, with C—H = 0.97 \AA (methylene), C—H = 0.93 \AA (aromatic) and N—H = 0.86 \AA . They were included in the final cycles of refinement in riding mode, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This project was supported by the National Natural Science Foundation of China (grant No. 20443003).

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