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## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
Disorder in main residue  
 $R$  factor = 0.038  
 $wR$  factor = 0.106  
Data-to-parameter ratio = 13.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis(1*H*-benzimidazole- $\kappa N^3$ )bis(4-hydroxybenzoato- $\kappa^2 O, O'$ )copper(II)

In the title complex,  $[\text{Cu}(\text{C}_7\text{H}_5\text{O}_3)_2(\text{C}_7\text{H}_6\text{N}_2)_2]$ , (I), the  $\text{Cu}^{\text{II}}$  atom, located on an inversion center, is surrounded by two 4-hydroxybenzoate anions and two benzimidazole molecules in an elongated octahedral geometry, the longer Cu—O distance being 2.618 (2) Å in the axial direction. The partially overlapped arrangement and the short face-to-face distance of 3.405 (6) Å suggest  $\pi$ – $\pi$  stacking between benzimidazole ligands of neighboring molecules.

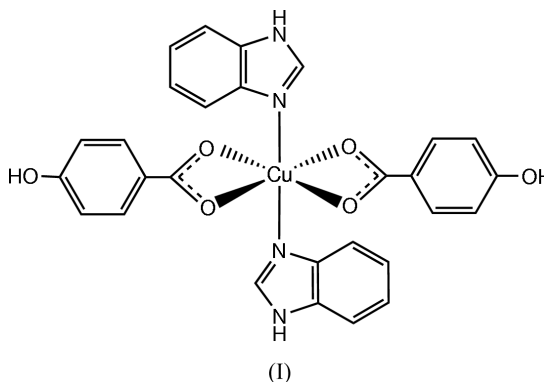
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## Comment

$\pi$ – $\pi$  stacking is an important intermolecular non-covalent interaction and is correlated with electron transfer in some biological systems (Deisenhofer & Michel, 1989). As part of an ongoing investigation into  $\pi$ – $\pi$  stacking in metal complexes (Pan & Xu, 2004; Liu *et al.*, 2004), we have prepared the title  $\text{Cu}^{\text{II}}$  complex, (I), and present its crystal structure here.



The molecular structure of (I) is illustrated in Fig. 1. The  $\text{Cu}^{\text{II}}$  atom is located on an inversion center and assumes an elongated octahedral coordination geometry. Two N atoms of benzimidazole (bzim) ligands and two O atoms (O1) of 4-hydroxybenzoate anions form the equatorial plane, with normal bond distances (Table 1). The other carboxyl O atoms (O2) coordinate axially, with a longer Cu—O2 distance, 2.618 (2) Å; the bond distances in the axial direction are usually longer than those in the equatorial plane by about 0.2–0.6 Å. The difference of 0.656 (3) Å in Cu—O distances found in (I) is greater than those found in most  $\text{Cu}^{\text{II}}$  complexes, but the Cu—O1—C1 bond angle, 106.11 (15)°, which is much smaller than the 120° expected for an O atom with normal  $sp^2$  hybridization, suggests the existence of a genuine bonding interaction between atoms Cu and O2 (Li *et al.*, 2005). Thus the coordination geometry in (I) is best described as elongated octahedral rather than as square planar.

A partially overlapped arrangement is observed between parallel N13-bzim and N13<sup>iv</sup>-bzim rings [symmetry code: (iv)



**Table 1**

Selected geometric parameters (Å, °).

Cu—O1	1.9619 (17)	Cu—N13	1.989 (2)
Cu—O2	2.618 (2)		
O1—Cu—O2	55.43 (7)	O2—Cu—N13	86.63 (7)
O1—Cu—N13	89.09 (8)	C1—O1—Cu	106.11 (15)

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O3 <i>A</i> —H3···O2 <sup>i</sup>	0.90	1.77	2.639 (4)	160
O3 <i>B</i> —H3···O2 <sup>i</sup>	0.87	1.77	2.589 (5)	154
N11—H11···O3 <i>A</i> <sup>ii</sup>	0.86	2.03	2.767 (5)	144
N11—H11···O3 <i>B</i> <sup>ii</sup>	0.86	2.09	2.910 (5)	160

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

Two 4-hydroxyphenyl rings with different spatial orientations and the same coordinates for atoms C6 and C7 were found in a difference Fourier map. These were refined isotropically and the occupancies converged to 0.488 (4) and 0.512 (4), respectively. They were each fixed at 0.5 in the final cycles of refinement. The common H atom of the disordered hydroxy groups was located in a difference Fourier map and included in the structure factor calculations with fixed positional parameters and isotropic displacement parameter  $U_{\text{iso}}(\text{H}) = 0.05 \text{ \AA}^2$ . H atoms on the 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 riding mode, with  $U_{\text{iso}}(\text{H})$  values of  $1.2U_{\text{eq}}$  of the carrier atoms.

Data collection: *PROCESS-AUTO* (Rigaku Corporation, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK & Rigaku Corporation, 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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