

**{2-[2-(1*H*-1,3-Benzimidazol-2-yl)ethylimino-
methyl]-2,4-dibromophenolato}(1,10-
phenanthroline)copper(II) tetrafluoroborate****Xiao-Hang Qiu,* Jun Zhao and
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Key indicators

Single-crystal X-ray study

 $T = 294$ KMean $\sigma(\text{C}-\text{C}) = 0.008$ Å

Disorder in solvent or counterion

 R factor = 0.047 wR factor = 0.119

Data-to-parameter ratio = 14.1

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

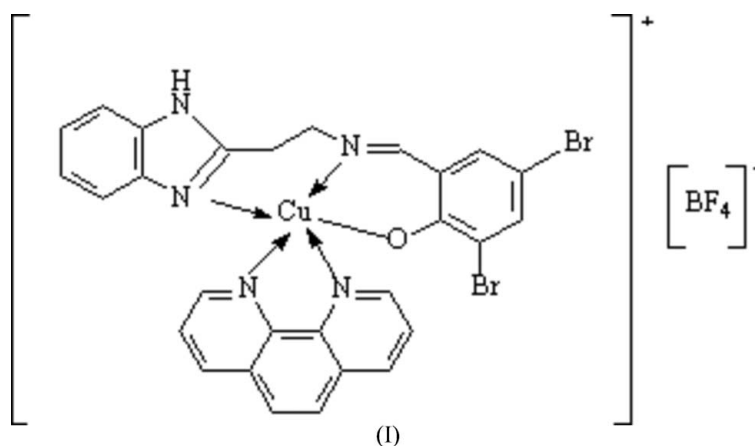
In the title compound, $[\text{Cu}(\text{C}_{18}\text{H}_{12}\text{Br}_2\text{N}_3\text{O})(\text{C}_{10}\text{H}_8\text{N}_2)]\text{BF}_4$, the Cu atom is pentacoordinated by three atoms, *viz.* N, N and O of the tridentate 2-[2-(1*H*-1,3-benzimidazol-2-yl)ethyliminomethyl]-2,4-dibromophenolate ligand and two N atoms of the 1,10-phenanthroline ligand. The Cu coordination geometry is highly distorted trigonal bipyramidal, with Cu—O and Cu—N bond lengths of 1.916 (3) and 1.954 (4)–2.212 (4) Å, respectively. The axial positions are occupied by two N atoms which form an N—Cu—N angle of 170.29 (16)°.

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Comment

Mixed-ligand complexes with metal ions bound to two different and biologically important ligands have interest as models for metalloenzymes (Hoshino *et al.*, 1979). Mixed-ligand complexes of metal ions have been extensively studied following the recognition of their important role in biological processes (Patel *et al.*, 2004). There has been substantial interest in the rational design of novel transition metal complexes which bind and cleave duplex DNA with high sequence or structure selectivity (Gonzalez-Alvarez *et al.*, 2002). In this paper, we present the title compound, (I), a new mixed-ligand copper(II) complex, which may be of interest with respect to both of the above-mentioned areas.



The crystal structure of (I) is composed of $[\text{CuL}(\text{phen})]^+$ cations and BF_4^- anions ($L = 2\text{-}\{2\text{-}(3,5\text{-dibromosalicyl-
idene)amino}\text{ethyl}\}\text{-}1H\text{-}1,3\text{-benzimidazole}$ and $\text{phen} = 1,10\text{-phenanthroline}$). The structure of the cation is shown in Fig. 1. The Cu atom is pentacoordinated by five atoms, *viz.* N, N and O of the tridentate ligand L and two N atoms of phen. The structure index parameter is 0.74 ($\tau = 0$ for a square pyramid and $\tau = 1$ for a trigonal bipyramid; Addison *et al.*, 1984), suggesting that the coordination geometry is highly distorted

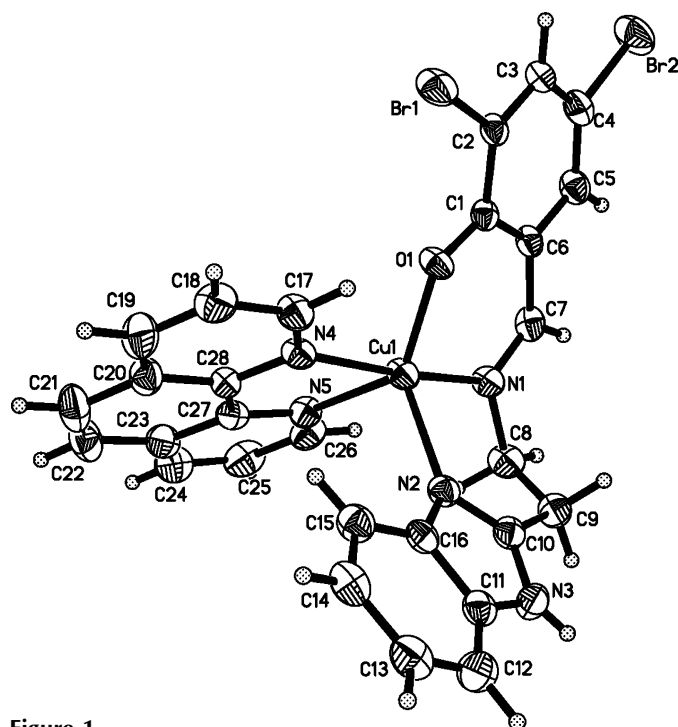


Figure 1
A view of the cation of the title compound, shown with 30% probability displacement ellipsoids.

trigonal bipyramidal. Atoms N2, N5 and O1 lie in the equatorial plane, while atoms N1 and N4 occupy axial positions, with an N1—Cu1—N4 angle of 170.29 (16)° (Table 1). The Cu atom lies 0.10 (1) Å out of the mean plane of the equatorial donors. The Cu—N distances lie in the range 1.954 (4)–2.158 (4) Å (Table 1), in agreement with those observed previously in copper(II) complexes (Zhang *et al.*, 2005). The Cu—O(phenolate) bond distance of 1.916 (3) Å is also consistent with those reported in the literature (Xie *et al.*, 2002).

Experimental

The title compound was prepared by adding a methanol solution (5 ml) of copper(II) tetrafluoroborate (0.1 mmol) and a methanol solution (5 ml) of 1,10-phenanthroline (0.1 mmol) to a methanol solution (10 ml) of 2-{2-[(3,5-dibromosalicylidene)amino]ethyl}-1*H*-1,3-benzimidazole (Das & Dash, 1995) (0.1 mmol), and neutralizing the reaction mixture with triethylamine (0.1 mmol). The mixture was stirred for about 2 h and filtered. The filtrate was evaporated slowly at room temperature to yield green block-shaped crystals of (I). Analysis calculated for C₂₈H₂₀BBr₂CuF₄N₅O: C 44.68, H 2.68, N 9.31%; found: C 44.42, H 2.71, N 9.39%.

Crystal data

[Cu(C ₁₈ H ₁₂ Br ₂ N ₃ O)(C ₁₀ H ₈ N ₂)]BF ₄	$D_x = 1.789 \text{ Mg m}^{-3}$
$M_r = 752.66$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 4857 reflections
$a = 25.568 (3) \text{ \AA}$	$\theta = 2.4\text{--}26.5^\circ$
$b = 15.730 (2) \text{ \AA}$	$\mu = 3.70 \text{ mm}^{-1}$
$c = 16.664 (2) \text{ \AA}$	$T = 294 (2) \text{ K}$
$\beta = 123.520 (2)^\circ$	Block, green
$V = 5587.5 (12) \text{ \AA}^3$	$0.24 \times 0.22 \times 0.20 \text{ mm}$
$Z = 8$	

Data collection

Bruker SMART CCD area-detector diffractometer	5882 independent reflections
φ and ω scans	3801 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.037$
$T_{\text{min}} = 0.427$, $T_{\text{max}} = 0.477$	$\theta_{\text{max}} = 26.7^\circ$
15693 measured reflections	$h = -32 \rightarrow 31$
	$k = -15 \rightarrow 19$
	$l = -18 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0425P)^2 + 19.5623P]$
$R[F^2 > 2\sigma(F^2)] = 0.047$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.119$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.88 \text{ e \AA}^{-3}$
5882 reflections	$\Delta\rho_{\text{min}} = -0.62 \text{ e \AA}^{-3}$
417 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.916 (3)	Cu1—N2	2.158 (4)
Cu1—N1	1.954 (4)	Cu1—N5	2.212 (4)
Cu1—N4	2.014 (4)		
O1—Cu1—N1	91.99 (14)	C1—O1—Cu1	128.2 (3)
O1—Cu1—N4	86.03 (13)	C7—N1—Cu1	125.7 (3)
N1—Cu1—N4	170.29 (16)	C8—N1—Cu1	116.9 (3)
O1—Cu1—N2	126.07 (14)	C10—N2—Cu1	122.1 (3)
N1—Cu1—N2	90.77 (15)	C16—N2—Cu1	132.5 (3)
N4—Cu1—N2	98.08 (15)	C17—N4—Cu1	125.3 (3)
O1—Cu1—N5	129.58 (14)	C28—N4—Cu1	116.3 (3)
N1—Cu1—N5	95.57 (15)	C26—N5—Cu1	132.7 (4)
N4—Cu1—N5	78.52 (14)	C27—N5—Cu1	110.0 (3)
N2—Cu1—N5	103.64 (14)		

H atoms were included in calculated positions and refined as riding, with C—H = 0.93–0.98 Å, N—H = 0.86 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$. The BF₄[−] anion was treated as disordered over two orientations with refined occupancies of 0.751 (9) and 0.249 (9). The B—F bond lengths were restrained to 1.36 (4) Å.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

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