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(2,2′-Bipyridine)(4-bromo-2-formylphenolato)copper(II) perchlorate

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The title compound, [Cu($C_7H_4BrO_2$)($C_{10}H_8N_2$)]ClO_4, has been prepared by the reaction of 5-bromosalicylaldehyde and 2,2′-bipyridine with $Cu\{ClO_4)\cdot 6H_2O$. The two ligands coordinate the central Cu atom through two N [Cu—N = 1.981 (6) and 1.984 (7) Å] and two O [Cu—O = 1.888 (5) and 1.949 (6) Å] atoms. The coordination is completed by a perchlorate O atom, with a Cu—O distance of 2.533 (12) Å. The crystal packing is stabilized by weak Cu···O interactions and van der Waals forces.

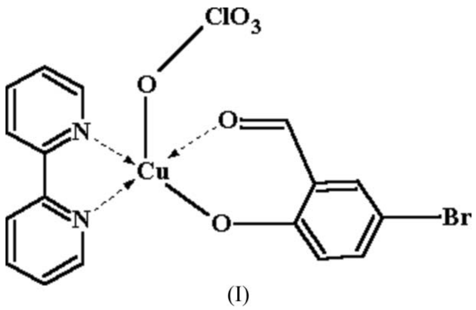
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.014 Å
Disorder in main residue
R factor = 0.059
wR factor = 0.181
Data-to-parameter ratio = 12.0

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

Comment

Schiff bases, particularly those derived from salicylaldehydes, and their metal complexes play a key role in our understanding of the chemistry of transition metal ions (Patel *et al.*, 2004). Copper(II) complexes containing *O*,*N*-donor atoms are very important owing to their significant catalytic activity in the preparative oxygenation of phenols and other substances, and their significant antibacterial and anticancer activity (Kurzak *et al.*, 1999). Complexes in which salicylaldehyde directly coordinates the metal ions are known (Janzen *et al.*, 2004), although reports of their crystal structures are rare. Intermolecular non-covalent interactions, such as weak Cu···O interactions (Sunirban & Samudranil, 2005), can play an important role in the self-assembly of the complex molecules, leading to interesting supramolecular structures. In this work, we have explored the self-assembly pattern of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The copper ion is coordinated by the two ligands in a distorted square geometry (Table 1) formed by two O atoms from 5-bromosalicylaldehyde and two N atoms from 2,2′-bipyridine. The coordination is completed by a perchlorate O atom, with a Cu1—O3 distance of 2.533 (12) Å. Copper(II) complexes may demonstrate a weak interaction between the metal ion and neighboring molecules (Sangeetha & Pal, 2000). The relatively short Cu1···O1^{i} [symmetry code: (i) $2 - x, -y, 2 - z$] distance of 2.822 (6) Å indicates the presence of such weak Cu···O interactions (Geraghty *et al.*, 1999) in (I), which stabilize the crystal packing (Fig. 2) along with van der Waals forces.

Experimental

The title compound was prepared by adding a methanol solution (5 ml) of copper(II) perchlorate (0.1 mmol) to a methanol solution (10 ml) of 5-bromosalicylaldehyde (0.1 mmol) neutralized by triethylamine. 2,2′-Bipyridine (0.1 mmol) was then added. The mixture was stirred for about 2 h and filtered. The filtrate was slowly evaporated at room temperture to yield green crystals of (I) suitable for X-ray analysis. Analysis calculated for $C_{17}H_{12}BrClCuN_2O_6$: C 39.32, H 2.33, N 5.40%; found: C 39.48, H 2.58, N 5.46%.

Crystal data

$[Cu(C_7H_4BrO_2)(C_{10}H_8N_2)]ClO_4$
$M_r = 519.19$
Triclinic, $P\overline{1}$
$a = 8.806$ (2) Å
$b = 10.512$ (3) Å
$c = 10.927$ (3) Å
$\alpha = 96.627$ (4)°
$\beta = 113.043$ (4)°
$\gamma = 92.835$ (4)°
$V = 919.5$ (4) Å^3
$Z = 2$
$D_x = 1.875$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.54$ mm^{-1}
$T = 294$ (2) K
Block, green
0.28 × 0.22 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.437$, $T_{\max} = 0.637$
4590 measured reflections
3193 independent reflections
2000 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.027$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.181$
$S = 1.01$
3193 reflections
266 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0877P)^2 + 2.119P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 1.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.64$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.890 (5)	Cu1—N2	1.986 (7)
Cu1—O2	1.947 (5)	Cu1—O3	2.533 (12)
Cu1—N3	1.981 (6)		
O1—Cu1—O2	92.2 (2)	C1—O1—Cu1	124.2 (5)
O1—Cu1—N3	172.6 (2)	C7—O2—Cu1	124.1 (5)
O2—Cu1—N3	92.8 (2)	C8—N2—Cu1	127.0 (6)
O1—Cu1—N2	93.3 (2)	C12—N2—Cu1	113.9 (6)
O2—Cu1—N2	174.3 (2)	C13—N3—Cu1	115.2 (5)
N3—Cu1—N2	81.6 (3)	C17—N3—Cu1	126.4 (5)

All H atoms were included in calculated positions and refined as riding on their parent atoms, with C—H = 0.93–0.98 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(parent atom). The highest residual peak is 1.01 Å from Br. The perchlorate group was refined as rotationally disordered over two orientations, with occupancies of 0.802 (9) and 0.198 (9).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); 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*.

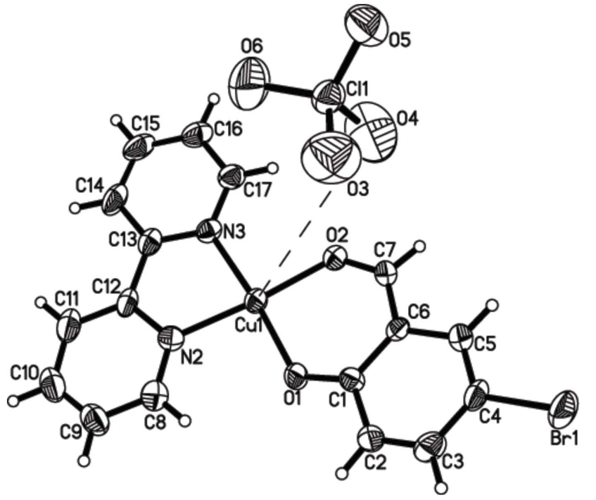


Figure 1
View of (I) with 30% probability displacement ellipsoids.

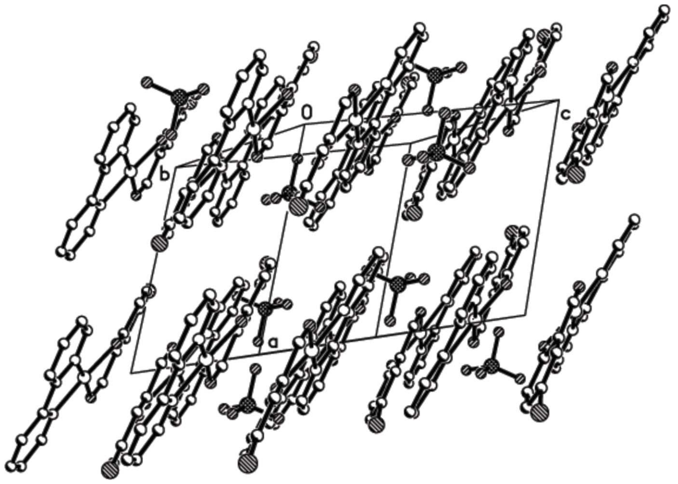


Figure 2
A perspective view of the crystal packing. H atoms have been omitted for clarity.

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