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Key indicators

<table>
<thead>
<tr>
<th>Single-crystal X-ray study</th>
<th>T = 295 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean σ(C–C) = 0.006 Å</td>
<td>R factor = 0.055</td>
</tr>
<tr>
<td>wR factor = 0.180</td>
<td>Data-to-parameter ratio = 13.9</td>
</tr>
</tbody>
</table>

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

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The Cu atom in the title compound, \([\text{Cu}(\text{C}_{16}\text{H}_{10}\text{BrN}_{4}\text{O}_{3})_{2}(\text{C}_{3}\text{H}_{7}\text{NO})_{2}]\), lies on a special position of \(\bar{T}\) site symmetry in a grossly elongated \(\text{CuN}_{2}\text{O}_{4}\) octahedral geometry [\(\text{Cu} \cdots \text{O}_{\text{DMF}} = 3.014 (4) \text{Å}\)]. The Cu atom is also \(\text{N,O}\)-chelated by the hydrazonate ligand. An \(\text{N} \cdots \text{H} \cdots \text{O}\) hydrogen bond helps to consolidate the crystal packing.

Comment

A previous report (Ali et al., 2005a) described the crystal structure of the Schiff base that is synthesized by condensing 5-bromoindole-3-carbaldehyde with 2-nitrobenzoylhydrazone. In the title compound, (I) (Fig. 1), two of these deprotonated Schiff bases chelate to copper (site symmetry \(\bar{T}\)) in a square-planar geometry (Table 1). However, the O atom of the DMF molecule lies at a distance of 3.014 (4) Å from the Cu atom; thus, the copper coordination geometry can also be regarded as grossly distorted octahedral. The molecules of (I) are linked by an \(\text{N} \cdots \text{H} \cdots \text{O}_{\text{DMF}}\) hydrogen bond (Table 2) into a chain.

The nickel derivative of 5-bromoindole-3-carbaldehyde benzoylhydrazone was recrystallized from pyridine to afford the bis-pyridine adduct; the geometry of the metal atom coordination is an essentially regular octahedron, and the pyridine N atoms are \(\text{cis}\) to each other (Ali et al., 2005b).

Experimental

5-Bromoindole-3-carboxaldehyde was condensed with 2-nitrobenzoylhydrazide to form the Schiff base 5-bromo-1\(H\)-indole-3-carbaldehyde 2-nitrobenzoylhydrazone (Ali et al., 2005b). This
reactant (0.40 g, 1.0 mmol) and copper(II) acetate dihydrate (0.11 g, 0.5 mmol) were heated in ethanol (50 ml) for several hours. The solid that separated from solution was purified by recrystallization from DMF. Green crystals of (I) were isolated after two weeks.

**Crystal data**

\[
[\text{Cu(C}_{16}\text{H}_{10}\text{BrN}_{4}\text{O}_{3})_{2}(\text{C}_{3}\text{H}_{7}\text{NO})_{2}] \]

\[M_1 = 982.11\]

Triclinic, \(P\overline{1}\)

\[a = 8.643 (5) \text{ Å}\]

\[b = 9.102 (5) \text{ Å}\]

\[c = 14.302 (9) \text{ Å}\]

\[\alpha = 99.84 (2)^\circ\]

\[\beta = 99.27 (1)^\circ\]

\[\gamma = 106.43 (1)^\circ\]

\[V = 1037 (1) \text{ Å}^3\]

**Data collection**

Rigaku Mercury CCD
diffactometer

3797 independent reflections

Mo Ka radiation

Cell parameters from 3209 reflections

\[\theta_{max} = 25.5^\circ\]

\[h = -10 \rightarrow 10\]

\[k = -10 \rightarrow 11\]

\[l = -17 \rightarrow 15\]

17658 measured reflections

**Refinement**

Refinement on \(F^2\)

\[R(F^2 > 2\sigma(F^2)) = 0.055\]

\[wR(F^2) = 0.180\]

\[S = 1.10\]

\[3797\] reflections

\[274\] parameters

\[H\) atoms treated by a mixture of independent and constrained refinement

\[w = 1/[\sigma^2(F^2) + (0.1064P)^2 + 0.1574P]\]

\[w = 1/[\sigma^2(F^2) + (0.1064P)^2 + 0.1574P]\]

\[P = (F^2 + 2F^2)/3\]

\[\Delta\rho_{max} = 0.001\]

\[\Delta\rho_{min} = 0.87 \text{ e Å}^{-3}\]

\[\Delta\rho_{min} = -0.64 \text{ e Å}^{-3}\]

\[U_{eq(C)} = \frac{1}{3}(U_{11} + U_{22} + U_{33})\]

\[U_{eq(H)} = 1.2\]

**Table 1**

Selected geometric parameters (Å, °).

<table>
<thead>
<tr>
<th>Bond</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu1—O1</td>
<td>1.930 (3)</td>
</tr>
<tr>
<td>Cu1—O4</td>
<td>3.014 (4)</td>
</tr>
<tr>
<td>Cu1—N3</td>
<td>1.937 (3)</td>
</tr>
<tr>
<td>O1—Cu1—O4</td>
<td>85.0 (1)</td>
</tr>
<tr>
<td>O1—Cu1—N3</td>
<td>81.8 (1)</td>
</tr>
<tr>
<td>O1—Cu1—N3°C</td>
<td>92.8 (1)</td>
</tr>
</tbody>
</table>

Symmetry code: (i) \(-x + 1, -y + 1, -z + 1\).

**Table 2**

Hydrogen-bond geometry (Å, °).

<table>
<thead>
<tr>
<th>D—H—A</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>N4—H4e—O4°C</td>
<td>0.85 (1)</td>
</tr>
<tr>
<td>N4—H4e—O4°C</td>
<td>1.95 (2)</td>
</tr>
<tr>
<td>N4—H4e—O4°C</td>
<td>2.777 (4)</td>
</tr>
<tr>
<td>N4—H4e—O4°C</td>
<td>163 (5)</td>
</tr>
</tbody>
</table>

Symmetry code: (8) \(x, y + 1, z\).

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**References**


