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# Bromobis(2,3-lutidine)copper(I)

**Peter G. Jones* and Eva-Maria Zerbe**

Institut für Anorganische und Analytische
Chemie, Technische Universität Braunschweig,
Postfach 3329, 38023 Braunschweig, Germany

Correspondence e-mail: p.jones@tu-bs.de

**Key indicators**

Single-crystal X-ray study
*T* = 133 K
Mean $\sigma$(C–C) = 0.003 Å
*R* factor = 0.025
*wR* factor = 0.062
Data-to-parameter ratio = 26.1

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

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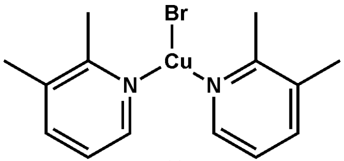
The title compound, [$CuBr(C_7H_9N)_2$], consists of monomeric molecules in which the Cu atom displays trigonal planar coordination, with Cu—N = 1.9970 (15) and 1.9946 (14) Å, and Cu—Br = 2.3422 (3) Å. The packing involves layer formation parallel to ($10\bar{2}$) by C—H$\cdots$Br interactions.

## Comment

We are interested in the synthesis and structure of complexes of the coinage metals with nitrogen ligands. Recently, we published the structure of [di(methanesulfonyl)amido]bis(2-picoline)copper(I) (Jones *et al.*, 2004), but the preparation of such materials proved difficult. One such experiment led to the title compound, (I), in poor yield, starting from copper(I) dimesylamide (presumably contaminated by bromide) and 2,3-lutidine.



(I)

The molecule of (I) is shown in Fig. 1. The copper centre exhibits planar three-coordination by two lutidine N atoms and the Br atom (the r.m.s. deviation of the four atoms from the mean plane through them is 0.0003 Å). The dimensions of the lutidine ligands may be regarded as normal; the ring angles at the N atom are slightly less than the ideal 120° (Table 1). The lutidine ligands make angles of 76.91 (4) and 65.78 (4)° with the $CuN_2Br$ plane.

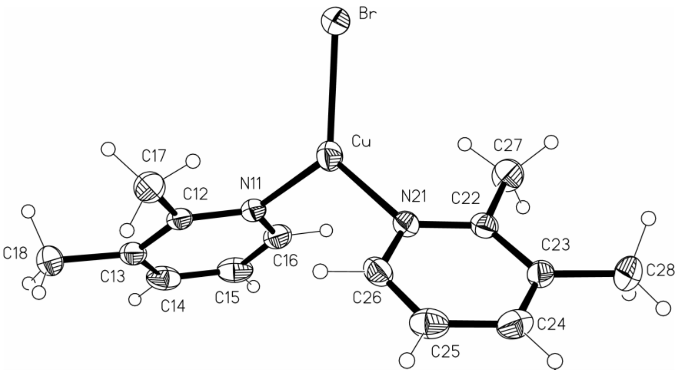


**Figure 1**
The molecule of the title compound in the crystal structure. Displacement ellipsoids are drawn at the 50% probability level and H-atom radii are arbitrary.

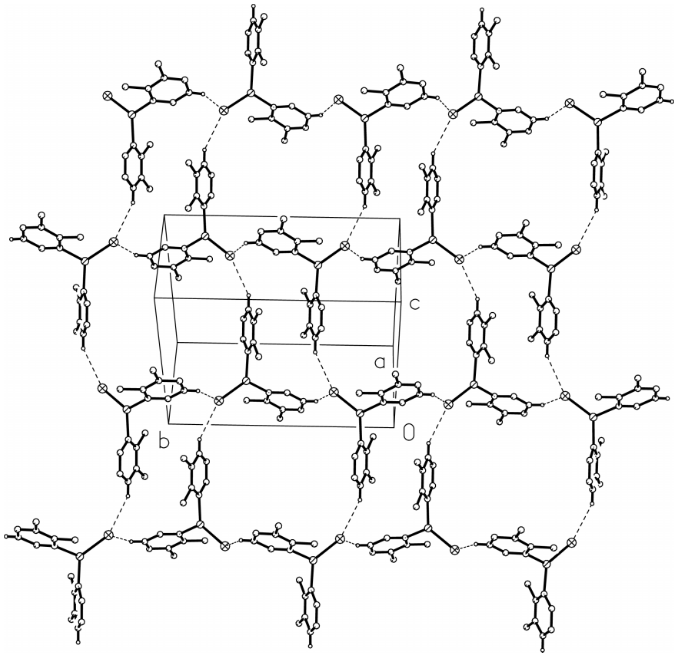


**Figure 2**
The layer formation in the title compound. Hydrogen bonds are indicated by dashed lines. H atoms not involved in hydrogen bonds have been omitted. The view direction is perpendicular to ($10\bar{2}$).

Näther & Beck (2004) have recently presented the structure of the related molecule chlorobis(piperidine)copper(I), which is also trigonal planar at copper, but with a wide N—Cu—N angle of 135.37 (7)°.

The packing of the title compound involves short C—H···Br contacts that may be classified as weak hydrogen bonds (Table 2). The two shortest contacts combine to form layers of molecules parallel to ($10\bar{2}$) (Fig. 2).

## Experimental

See *Comment* section. The reaction mixture in dichloromethane was layered with diethyl ether, after which small crystals grew slowly.

### *Crystal data*

$[CuBr(C_7H_9N)_2]$
$M_r = 357.75$
Monoclinic, $P2_1/c$
$a = 7.5168$ (6) Å
$b = 15.1240$ (10) Å
$c = 13.1804$ (10) Å
$\beta = 94.610$ (4)°
$V = 1493.55$ (19) Å$^3$
$Z = 4$

$D_x = 1.591$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 5859 reflections
$\theta = 2$–30.5°
$\mu = 4.12$ mm$^{-1}$
$T = 133$ (2) K
Prism, colourless
0.33 × 0.18 × 0.14 mm

### *Data collection*

Bruker SMART 1000 CCD diffractometer
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.609$, $T_{max} = 0.703$
30 827 measured reflections

4367 independent reflections
3613 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 30.0°$
$h = -10 \rightarrow 10$
$k = -21 \rightarrow 20$
$l = -18 \rightarrow 18$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.062$
$S = 1.06$
4367 reflections
167 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0266P)^2 + 0.8705P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cu—N21 | 1.9946 (14) | Cu—Br | 2.3422 (3) |
| Cu—N11 | 1.9970 (15) | | |
| N21—Cu—N11 | 115.65 (6) | C12—N11—Cu | 124.29 (12) |
| N21—Cu—Br | 121.95 (4) | C26—N21—C22 | 118.59 (15) |
| N11—Cu—Br | 122.41 (4) | C26—N21—Cu | 117.11 (12) |
| C16—N11—C12 | 118.54 (15) | C22—N21—Cu | 124.22 (12) |
| C16—N11—Cu | 117.16 (12) | | |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C14—H14···Br$^{i}$ | 0.95 | 2.90 | 3.7791 (19) | 155 |
| C24—H24···Br$^{ii}$ | 0.95 | 3.15 | 4.0264 (19) | 154 |
| C15—H15···Br$^{iii}$ | 0.95 | 3.13 | 3.879 (2) | 137 |
| C25—H25···Br$^{iv}$ | 0.95 | 2.94 | 3.7045 (19) | 139 |

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

Methyl H atoms were identified in difference syntheses, idealized and refined as rigid groups allowed to rotate but not tip. Other H atoms were included using a riding model. C—H bond lengths were fixed at 0.98 (methyl) or 0.95 Å (aromatic), and methyl H—C—H angles were fixed at 109.5°. $U_{iso}$(H) values were fixed at $1.2U_{eq}$ of the parent atom.

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: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

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## References

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