

**(2,2'-Bipyridine)bromodiimidazolecopper(II)
bromide****Feng-Yi Xia,^a Xin-Hua Li^{b*} and
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325027, People's Republic of ChinaCorrespondence e-mail: lixinhua01@126.com**Key indicators**Single-crystal X-ray study
T = 298 K
Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$
R factor = 0.034
wR factor = 0.108
Data-to-parameter ratio = 14.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title compound, $[\text{CuBr}(\text{C}_3\text{H}_4\text{N}_2)_2(\text{C}_{10}\text{H}_8\text{N}_2)]\text{Br}$, consists of bromodiimidazole(2,2'-bipyridine)copper(II) cations and bromide anions that are linked by hydrogen bonds into a network structure. Two imidazoles, a 2,2'-bipyridine and a bromide anion are coordinated by the Cu atom, whose geometry is distorted towards octahedral because of the second bromide anion.

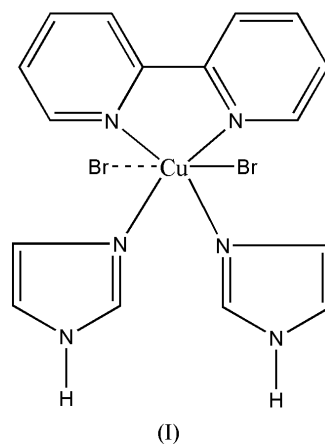
Received 17 November 2004

Accepted 22 November 2004

Online 27 November 2004

Comment

Much interest is focused on the synthesis of coordination polymers (Carlucci *et al.*, 1994; Munakata *et al.*, 1999; Hirsch *et al.*, 1997; Hoskins & Robson, 1990); occasionally, the products are not the expected compounds. In the present study, the title compound contains two imidazole molecules that come from the decomposition of the starting 1,1'-carbonyldiimidazole ligand. The Cu atom of the $[\text{Cu}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{C}_3\text{H}_4\text{N}_2)_2\text{Br}]^+$ cation is five-coordinated by the two imidazole molecules, a 2,2'-bipyridine and a bromide anion; the geometry is distorted towards octahedral, as the second bromide anion is 3.324 (4) Å away. The cations and anions interact through $\text{N}-\text{H}\cdots\text{Br}$ hydrogen bonds involving the imidazole, generating a three-dimensional network structure (Table 2).

**Experimental**

Copper bromide (0.5 g, 2 mmol) was dissolved in water (10 ml) and the solution was mixed with a dimethylformamide solution (10 ml) of 2,2'-bipyridine (0.3 g, 2 mmol), terephthalic acid (0.4 g, 2 mmol) and 1,1'-carbonyldiimidazole (0.3 g, 2 mmol) at room temperature. The reaction mixture was filtered; blue prism-shaped crystals separated from the solution after about three months.

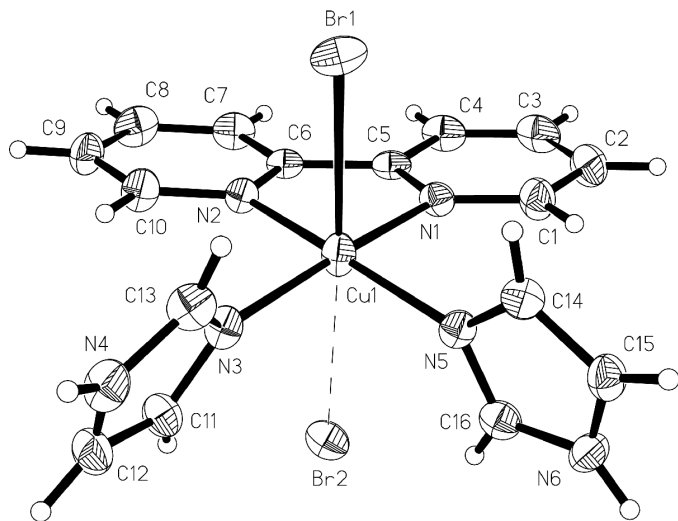


Figure 1
ORTEP (Johnson, 1976) plot of the title compound, with the atom numbering, showing 50% probability displacement ellipsoids.

Crystal data

[CuBr(C₃H₄N₂)₂(C₁₀H₈N₂)]Br
M_r = 515.71
 Monoclinic, *P*₂₁/*c*
a = 13.121 (5) Å
b = 8.731 (3) Å
c = 16.205 (6) Å
 β = 97.560 (6)°
V = 1840.2 (11) Å³
Z = 4

D_x = 1.861 Mg m⁻³
 Mo Kα radiation
 Cell parameters from 3180 reflections
 θ = 1.6–25.1°
 μ = 5.54 mm⁻¹
T = 298 (2) K
 Prism, blue
 0.25 × 0.19 × 0.15 mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
*T*_{min} = 0.50, *T*_{max} = 0.82
 8504 measured reflections

3180 independent reflections
 2536 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.028
 θ_{max} = 25.1°
h = -15 → 10
k = -10 → 10
l = -18 → 19

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.034
wR(*F*²) = 0.108
S = 1.05
 3180 reflections
 226 parameters

H-atom parameters constrained
w = 1/[σ²(*F*_o²) + (0.0650*P*)²]
 where *P* = (*F*_o² + 2*F*_c²)/3
 (Δ/*σ*)_{max} = 0.001
 Δρ_{max} = 0.54 e Å⁻³
 Δρ_{min} = -0.38 e Å⁻³

Table 1
Selected geometric parameters (Å, °).

Br1—Cu1	2.8189 (10)	Cu1—N2	2.013 (3)
Cu1—N5	1.991 (3)	Cu1—N1	2.031 (3)
Cu1—N3	2.002 (3)		
N5—Cu1—N3	90.96 (13)	N2—Cu1—N1	80.01 (13)
N5—Cu1—N2	169.17 (13)	N5—Cu1—Br1	96.25 (10)
N3—Cu1—N2	95.70 (13)	N3—Cu1—Br1	93.75 (10)
N5—Cu1—N1	92.28 (13)	N2—Cu1—Br1	91.83 (10)
N3—Cu1—N1	171.65 (13)	N1—Cu1—Br1	93.54 (9)

Table 2
Hydrogen-bonding 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>
N4—H4N···Br2 ⁱ	0.86	2.53	3.320 (4)	152
N6—H6N···Br1 ⁱⁱ	0.86	2.45	3.254 (4)	156

Symmetry codes: (i) 2 - *x*, ½ + *y*, ½ - *z*; (ii) *x*, *y* - 1, *z*.

H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.86 (N—H) and 0.93 Å (C—H), with *U*_{iso} = 1.2*U*_{eq} (parent atom).

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXTL (Bruker, 2000); software used to prepare material for publication: SHELXL97.

We acknowledge financial support by Wenzhou Normal College and the Education Office of Zhejiang province (No. 20040336 and 2003Z17) and the ‘551’ Distinguished Person Foundation of Wenzhou.

References

Bruker (2000). SMART, SAINT, SADABS and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
 Carlucci, L., Ciani, G. & Proserpio, D. M. (1994). Chem. Commun. pp. 2755–2757.
 Hirsch, K. A., Wilson, S. C. & Moore, J. S. (1997). Chem. Eur. J. 3, 765–771.
 Hoskins, B. F. & Robson, R. (1990). J. Am. Chem. Soc. 112, 1546–1551.
 Johnson, C. K. (1976). ORTEP. Report ORNL-5138. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.
 Munakata, M., Wu, L. P. & Kuroda-Sowa, T. (1999). Adv. Inorg. Chem. 46, 173–178.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.