Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bromotetrakis(1*H*-imidazole-κN^3)copper(II) bromide

Moayad Hossaini Sadr,[a] Davood Zare,[a] William Lewis,[b] Jan Wikaira,[b] Ward T. Robinson[b] and Seik Weng Ng[c]*

[a]Department of Chemistry, Tarbiat Moallem University of Azarbaijan, Tabriz, Iran, [b]Department of Chemistry, University of Canterbury, Christchurch, New Zealand, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Received 28 July 2004
Accepted 9 August 2004
Online 28 August 2004

The monoclinic unit cell of the title compound, $[CuBr(C_3H_4N_2)_4]Br$, emulates an orthorhombic cell as its β angle is close to 90°; the crystal structure is twinned with approximately equal contributions of the two components. The Cu atom is five-coordinate in a square-pyramidal geometry. The cation interacts with the bromide anion through hydrogen bonds, which give rise to a layer structure.

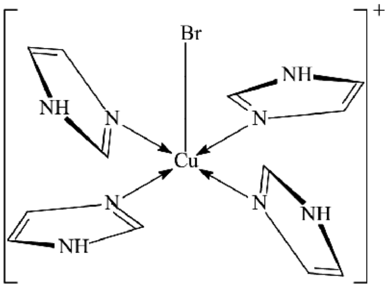
Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.009 Å
R factor = 0.053
wR factor = 0.168
Data-to-parameter ratio = 16.0

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

Comment

Following our interest in the copper complexes of polypyrazolylborate ligands (Beheshti *et al.*, 2002; Hossaini Sadr *et al.*, 2004), we have synthesized new complexes of poly(pyrazolyl)silane ligands, which are the neutral analogs of the poly(pyrazolyl)borates (Pullen *et al.*, 1999; Richburg *et al.*, 2000; Hossaini Sadr *et al.*, 2004). An attempt to synthesize the dimethylsilyl adduct of copper dibromide yielded the title blue salt, (I).



(I)

The direct reaction of copper(II) bromide and imidazole in ethanol afforded a centrosymmetric complex of an identical elemental composition (Parker & Breneman, 1995). If the extremely long Cu···Br interaction reported for this structure [3.3767 (4) Å] is considered as a bond, the geometry of copper is distorted octahedral. The geometry of the Cu atom is clearly square-pyramidal in the title complex: the Cu atom is linked to only one Br atom [Cu1—Br1 = 2.755 (1) Å], the other Br atom being more than 4 Å away. It is also linked to four imidazole ligands in a square-pyramidal environment, as shown in Fig. 1. The Cu1—Br1 bond is significantly longer than the covalent bond [2.408 (1) Å] found in the four-coordinate bis(2-chloroimidazole) adduct (Valle *et al.*, 1993). A square-planar geometry is found for copper in the anhydrous as well as in the dihydrated tetrakis(4-methylimidazole) adducts (Näther *et al.*, 2002*a*,*b*). Both Br atoms engage in hydrogen-bonding interactions, resulting in a layered structure.

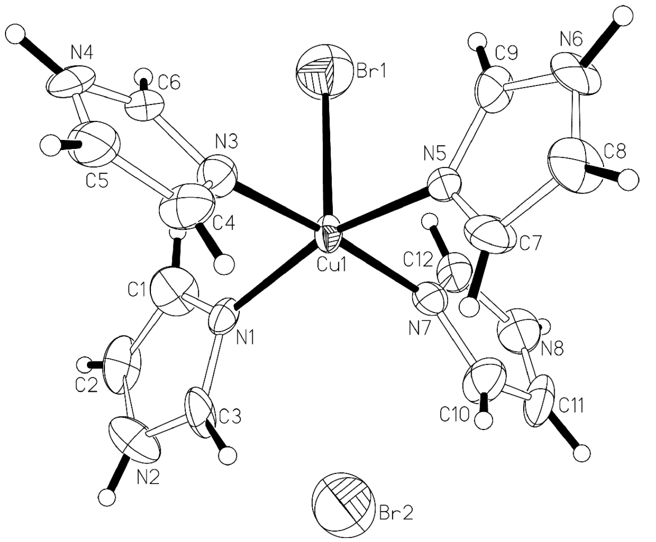


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 90% probability level. H atoms are drawn as spheres of arbitrary radii.

A copper(II) bromide adduct with four imidazole ligands has been synthesized by reacting cupric oxide with imidazole in the presence of bromide ions (Bhattacharjee & Choudhury, 1998), but it is not clear whether the compound is that already structurally verified (Parker & Breneman, 1995) or the title salt.

Experimental

The title compound was obtained adventitiously as block-shaped crystals along with an uncharacterized white compound when copper dibromide was treated with an equimolar quantity of diimidazolyldimethylsilane. The specimen used for the measurements was cut from a large block.

Crystal data

$[CuBr(C_3H_4N_2)_4]Br$
$M_r = 495.69$
Monoclinic, $P2_1/n$
$a = 8.9625\ (3)$ Å
$b = 13.2140\ (5)$ Å
$c = 13.9889\ (5)$ Å
$\beta = 90.052\ (1)°$
$V = 1656.7\ (1)$ Å^3
$Z = 4$
$D_x = 1.987$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7789 reflections
$\theta = 2.7$–$26.4°$
$\mu = 6.15$ mm^{-1}
$T = 113\ (2)$ K
Plate, blue
0.48 × 0.38 × 0.07 mm

Data collection

Siemens *P*4/CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.337$, $T_{max} = 0.653$
14 285 measured reflections
3343 independent reflections
3081 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 26.4°$
$h = -11 \rightarrow 11$
$k = -16 \rightarrow 14$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.168$
$S = 1.07$
3343 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1271P)^2 + 5.3184P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.30$ e Å^{-3}
$\Delta\rho_{min} = -2.23$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—Br1	2.755 (1)	Cu1—N5	2.018 (5)
Cu1—N1	2.016 (5)	Cu1—N7	1.995 (6)
Cu1—N3	2.000 (6)		
N1—Cu1—N3	89.4 (3)	N3—Cu1—N7	174.0 (2)
N1—Cu1—N5	162.0 (2)	N3—Cu1—Br1	93.5 (2)
N1—Cu1—N7	89.5 (3)	N5—Cu1—N7	89.6 (3)
N1—Cu1—Br1	100.4 (1)	N5—Cu1—Br1	97.7 (1)
N3—Cu1—N5	89.6 (3)	N7—Cu1—Br1	92.5 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*n*···Br1^{i}	0.88	2.52	3.346 (6)	156
N4—H4*n*···Br2^{ii}	0.88	2.48	3.355 (6)	170
N6—H6*n*···Br2^{iii}	0.88	2.55	3.227 (5)	134
N8—H8*n*···Br2^{iv}	0.88	2.46	3.341 (6)	174

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

The β angle of the unit cell is close to 90°. The cell emulated an orthorhombic cell, and this necessitated the use of the twin law matrix $(100,0\bar{1}0,00\bar{1})$. The second twin component refined to 0.474 (3). Measurements on a smaller crystal gave identical results. For each imidazole ring, the five bond distances were restrained to be within ±0.01 Å. The twinning problem led to elongated ellipsoids for some of the C and N atoms. The displacement parameters of pairs of connected atoms were restrained by a DELU 0.005 command in *SHELXL*97 (Sheldrick, 1997) to avoid the displacement ellipsoids becoming too elongated. In the final difference Fourier map, the largest peak was 0.2 Å from Cu1 and the deepest hole about 0.3 Å from Br2. H atoms were positioned geometrically [C—H = 0.95 Å, N—H = 0.88 Å and $U_{iso}(H) = 1.2U_{eq}$(C or N)] and were included in the refinement in the riding-model approximation.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

The authors thank the Research Office of Tarbiat Moallem University, the University of Canterbury and the University of Malaya for supporting this work.

References

Beheshti, A., Clegg, W. & Hossaini Sadr, M. (2002). *Inorg. Chim. Acta*, **335**, 21–26.

Bhattacharjee, C. R. & Choudhury, P. K. (1998). Transition *Met. Chem.* **23**, 561–564.

Bruker (2001). *SADABS, SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.

Hossaini Sadr, M. (2004). Unpublished results.

Hossaini Sadr, M., Clegg, W. & Bijhanzade, H. R. (2004). *Polyhedron*, **23**, 637–641.

Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Acta Cryst. (2004). E**60**, m1324–m1326 Moayad Hossaini Sadr *et al.* • $[CuBr(C_3H_4N_2)_4]Br$ **m1325**

Näther, C., Wriedt, M. & Jeß, I. (2002*a*). *Acta Cryst.* E**58**, m63–m64.

Näther, C., Wriedt, M. & Jeß, I. (2002*b*). *Acta Cryst.* E**58**, m107–m109.

Parker, O. J. & Breneman, G. L. (1995). *Acta Cryst.* C**51**, 1097–1077.

Pullen, E. E., Rheingold, A. L. & Rabinovich, D. (1999). *Inorg. Chem. Commun.* **2**, 194–197.

Richburg, L. M., Farouq, J. A., Incarvito, C. D., Rheingold, A. L. & Rabinovich, D. (2000). *Polyhedron*, **19**, 1815–1820.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Valle, G., González, A. S. & Ettorre, R. (1993). *Acta Cryst.* C**49**, 1298–1300.

m1326 Moayad Hossaini Sadr *et al.* • $[CuBr(C_3H_4N_2)_4]Br$ *Acta Cryst.* (2004). E**60**, m1324–m1326