

Dibromotetrakis(4-methylimidazole)copper(II)

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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
Disorder in main residue
 R factor = 0.038
 wR factor = 0.104
Data-to-parameter ratio = 25.8

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

In the structure of the title compound, $[\text{CuBr}_2(\text{C}_4\text{H}_6\text{N}_2)_4]$, the copper(II) cations are coordinated by four 4-methylimidazole ligands and two bromide anions within a distorted octahedron. The Cu—Br distances are elongated due to Jahn–Teller distortion. The two crystallographically independent 4-methylimidazole ligands and the single independent Br are located in general positions, whereas the copper(II) cation is located on a centre of inversion. There are short N—H \cdots Br contacts to the bromide ligands, indicating hydrogen bonding.

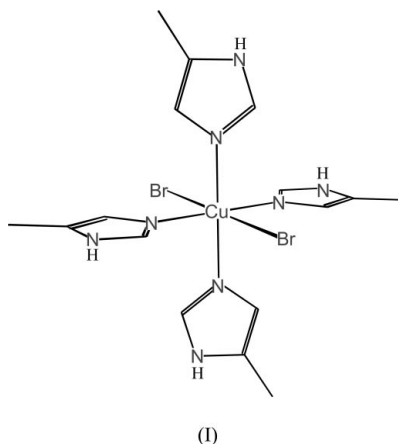
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Comment

The title compound, (I), is isotypic with dichlorotetrakis(4-methylimidazole)copper(II) (Näther *et al.*, 2002). In its crystal structure, the copper(II) cations are coordinated by four N atoms of the 4-methylimidazole ligands within a slightly distorted square-planar arrangement. The Cu—N distances of 2.014 (3) and 2.017 (2) Å are comparable to those in dichlorotetrakis(4-methylimidazole)copper(II) (Näther *et al.*, 2002) and to those in known 4-methylimidazole–copper(II) complexes such as tetrakis(4-methylimidazolyl)bis-(perchlorato-*O*)copper(II) (Su *et al.*, 1992) and tetrakis(4-methylimidazol-1-yl)bis(cyanamidonitrate)copper(II) (Kohout *et al.*, 1999). The coordination sphere of the copper(II) cation is completed by two long contacts to two symmetry-equivalent bromide anions [3.2371 (5) Å]; these contacts are strongly elongated due to Jahn–Teller distortion. The coordination polyhedron around the copper(II) cation can be described as a strongly distorted octahedron.



The asymmetric unit of the title compound contains one copper(II) cation which is located on a centre of inversion, one Br anion and two crystallographically independent 4-methylimidazole ligands, which are located in general positions.

There are short Br \cdots H distances between the bromide anions and the N—H atoms of both ligands, of 2.45 and 2.46 Å. The Br \cdots N distances of 3.309 (3) and 3.284 (3) Å, and the Br \cdots H—N angles of 177 and 161°, indicate hydrogen bonding.

Experimental

The title compound was prepared by the reaction of 167.6 mg (2 mmol) 4-methylimidazole and 111.7 mg (0.5 mmol) copper(II) bromide in 5 ml acetonitrile. The reaction mixture was stirred over 2 d, and the solid product was filtered off and washed with dimethyl ether. The precipitate is phase pure, as proved by X-ray powder diffraction. It consists of a blue crystalline powder and a few blue single crystals which are suitable for X-ray structure determination.

Crystal data

[CuBr ₂ (C ₄ H ₆ N ₂) ₄]	$D_x = 1.626 \text{ Mg m}^{-3}$
$M_r = 551.79$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 78 reflections
$a = 8.2657 (9) \text{ \AA}$	$\theta = 10.0\text{--}17.5^\circ$
$b = 12.053 (1) \text{ \AA}$	$\mu = 4.53 \text{ mm}^{-1}$
$c = 11.338 (1) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 94.06 (1)^\circ$	Block, blue
$V = 1126.73 (18) \text{ \AA}^3$	$0.10 \times 0.10 \times 0.08 \text{ mm}$
$Z = 2$	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{\text{int}} = 0.039$
ω scans	$\theta_{\text{max}} = 30.1^\circ$
Absorption correction: numerical (<i>X-SHAPE</i> ; Stoe & Cie, 1998)	$h = 0 \rightarrow 11$
$T_{\text{min}} = 0.687$, $T_{\text{max}} = 0.881$	$k = -16 \rightarrow 6$
5129 measured reflections	$l = -15 \rightarrow 15$
3300 independent reflections	3 standard reflections
2136 reflections with $I > 2\sigma(I)$	frequency: 240 min
	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 0.9319P]$
$R[F^2 > 2\sigma(F^2)] = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.104$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.00$	$\Delta\rho_{\text{max}} = 1.23 \text{ e \AA}^{-3}$
3300 reflections	$\Delta\rho_{\text{min}} = -0.95 \text{ e \AA}^{-3}$
128 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Selected geometric parameters (Å, °).

Cu1—N1	2.014 (3)	Cu1—N3	2.017 (2)
N1 ⁱ —Cu1—N1	180.0	N1—Cu1—N3	90.30 (10)
N1 ⁱ —Cu1—N3	89.70 (10)	N3—Cu1—N3 ⁱ	180.0

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

The aromatic H atoms were positioned with idealized geometry and refined using a riding model. The methyl H atoms were disordered and were refined as idealized disordered methyl groups with two positions rotated from each other by 60° and occupation factors

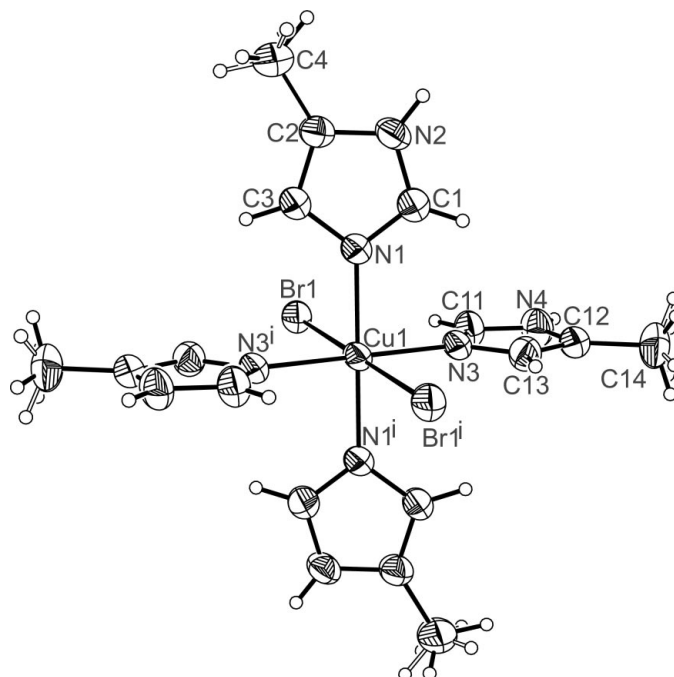


Figure 1

The crystal structure of the title compound with labelling, and with displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) $-x+1, -y+1, -z+1$.]

which refined to 0.30 (6) and 0.70 (6) for the H atoms attached to C4 and to 0.57 (6) and 0.43 (6) for the H atoms attached to C14. All H atoms were refined with fixed isotropic displacement parameters; $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}[\text{C(methyl)}]$ or $1.2U_{\text{eq}}[\text{C(methylene)}]$.

Data collection: *SDP* (Enraf–Nonius, 1985); cell refinement: *SDP*; data reduction: *XCAD4* in *SDP*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CIFTAB* in *SHELXL97*.

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References

- Bruker (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Enraf–Nonius (1985). *Structure Determination Package*. Enraf–Nonius, Delft, The Netherlands.
- Kohout, J., Hvastijová, M., Kožíšek, J., Díaz, J. G., Valko, M., Jäger, L. & Svoboda, I. (1999). *Inorg. Chim. Acta*, **287**, 186–192.
- Näther, C., Wriedt, M. & Jeß, I. (2002). *Acta Cryst.* **E58**, m39–m40.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Stoe & Cie (1998). *X-SHAPE*. Version 1.03. Stoe & Cie, Darmstadt, Germany.
- Su, C.-C., Chen, J.-H., Hwang, K.-Y., Liu, S.-J., Wang, S.-W., Wang, S.-L. & Liu, S.-N. (1992). *Inorg. Chim. Acta*, **196**, 231–236.