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Dichlorotetrakis(4-methylimidazole)copper(II)

Christian Näther,* Mario Wriedt and Inke Jeß

Institut für Anorganische Chemie, Christian-Albrechts-Universität Kiel, Olshausenstr. 40, D-24098 Kiel, Germany

Correspondence e-mail:
cnaether@ac.uni-kiel.de

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.101
Data-to-parameter ratio = 24.4

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

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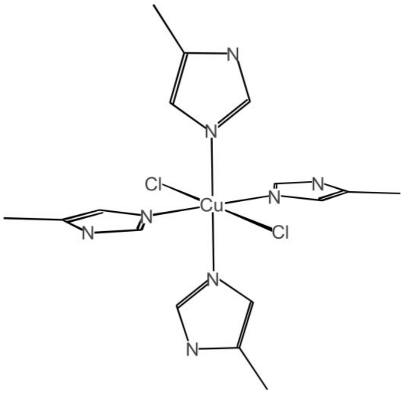
In the structure of the title compound, $[CuCl_2(C_4H_6N_2)_4]$, the copper(II) cation is surrounded by four 4-methylimidazole ligands within a slightly distorted square plane. The coordination sphere is completed by two contacts to Cl atoms which are elongated due to the Jahn–Teller distortion. The coordination polyhedron around the copper(II) cations can be described as a strongly distorted octahedron. The copper(II) cations are located on centres of inversion, whereas the two crystallographically independent 4-methylimidazole ligands and the chloride anion occupy general positions. There are short N—H···Cl distances to the Cl atoms indicating hydrogen bonding.

Comment

In the crystal structure of the title compound, (I), the copper(II) cations are coordinated by four N atoms of 4-methylimidazole ligands, forming a slightly distorted square plane. The Cu—N distances of 2.0148 (14) and 2.0124 (13) Å are comparable to those in other compounds retrieved from the Cambridge Structural Database (Conquest Version 1.3, 2001; Allen & Kennard, 1993). The coordination sphere of the copper(II) cation is completed by two symmetry-equivalent Cl atoms located above and below the square plane. The Cu—Cl distance of 3.0373 (6) Å is strongly elongated due to Jahn–Teller distortion and the coordination polyhedron around the copper(II) cation can be described as a strongly distorted octahedron.



(I)

The asymmetric unit contains two crystallographically independent 4-methylimidazole ligands and one chloride anion located in general positions and one copper(II) cation which is located on a centre of inversion. There are short H···Cl distances between the H atoms bound to nitrogen and the chloride anions of 2.309 Å. The N···Cl distances of 3.165 and 3.131 Å and the N—H···Cl angles of 173.7 and 159.9°

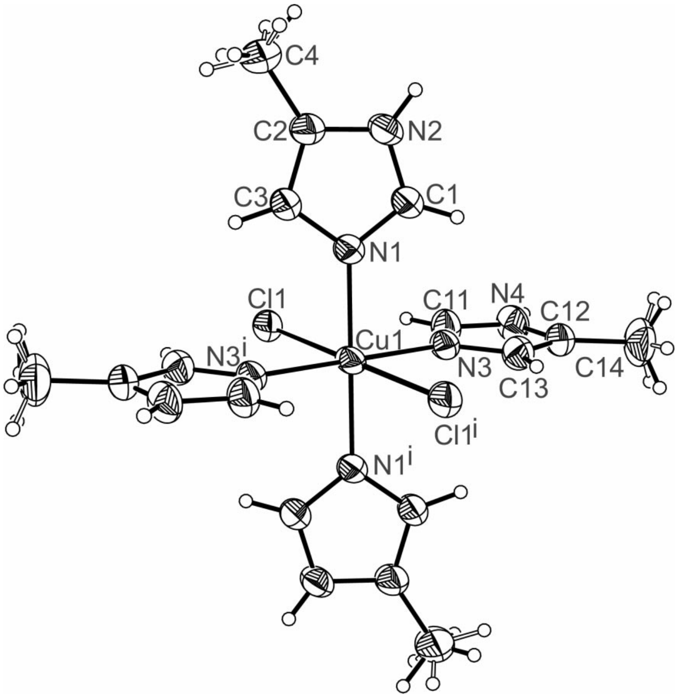


Figure 1
The crystal structure of the title compound with the atom labelling and displacement ellipsoids drawn at the 50% probability level. The disordering of the H atoms is shown as solid and open bonds. [Symmetry code: (i) $-x+1$, $-y+1$, $-z+1$.]

indicate hydrogen bonding. There are two comparable copper(II) complexes described in the literature. In tetrakis(4-methylimidazolyl)bis(perchlorato-*O*)copper(II) (Su *et al.*, 1992), the copper(II) cations are sixfold coordinated by four 4-methylimidazole ligands and two perchlorate anions, and in tetrakis(4-methylimidazol-1-yl)bis(cyanamidonitrate)copper(II), two cyanamidonitrate anions act as the counter-anions (Kohout *et al.*, 1999).

Experimental

The title compound was prepared by the reaction of 167.6 mg (4 mmol) 4-methylimidazole and 85.24 mg (0.5 mmol) copper(II) chloride dihydrate in 5 ml acetonitrile. The reaction mixture was stirred for 2 d, and the precipitate filtered off and washed with dimethyl ether. The precipitate is phase pure which was 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

$[CuCl_2(C_4H_6N_2)_4]$
$M_r = 462.87$
Monoclinic, $P2_1/c$
$a = 8.0925\ (8)$ Å
$b = 11.8347\ (7)$ Å
$c = 11.3012\ (11)$ Å
$\beta = 93.063\ (12)^\circ$
$V = 1080.80\ (16)$ Å^3
$Z = 2$

$D_x = 1.422$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 130 reflections
$\theta = 15$–19.5°
$\mu = 1.28$ mm^{-1}
$T = 293\ (2)$ K
Block, blue
$0.12 \times 0.09 \times 0.05$ mm

Data collection

Stoe AED-II four-circle diffractometer
ω–θ scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)
$T_{min} = 0.782$, $T_{max} = 0.846$
5869 measured reflections
3152 independent reflections
2550 reflections with $I > 2\sigma(I)$

$R_{int} = 0.027$
$\theta_{max} = 30.0^\circ$
$h = 0 \rightarrow 11$
$k = -16 \rightarrow 10$
$l = -15 \rightarrow 15$
4 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.101$
$S = 1.03$
3152 reflections
129 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.2887P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.86$ e Å^{-3}
$\Delta\rho_{min} = -0.54$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0055 (14)

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	2.0124 (13)	Cu1—N1	2.0148 (14)
N3—Cu1—N3^i	180.0	N3—Cu1—N1	90.24 (6)
N3—Cu1—N1^i	89.76 (6)	N1^i—Cu1—N1	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 site-occupation factors which were refined to 0.30 (4) and 0.70 (4) for the H atoms attached to C4, and to 0.63 (4) and 0.37 (4) for the H atoms attached to C14. All H atoms were refined with fixed isotropic displacement parameters; $U_{iso}(H) = 1.5U_{eq}C(methyl) = 1.2U_{eq}C(aromatic)$.

Data collection: *DIF*4 (Stoe & Cie, 1992); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1992); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CIFTAB* in *SHELXL*97.

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