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Dichlorobis(3,5-dimethylpyrazole)copper(II)

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.009 Å
R factor = 0.067
wR factor = 0.211
Data-to-parameter ratio = 16.5

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

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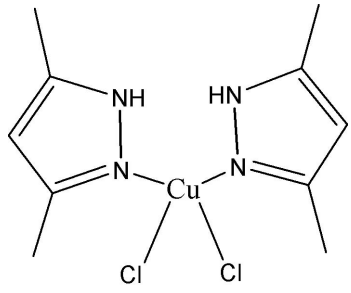
The title compound, $[CuCl_2(C_5H_8N_2)_2]$, has been synthesized as part of a project aimed at the synthesis and characterization of scorpionate ligands with cyano substituents. The structure shows the Cu ion coordinated by two 3,5-dimethylpyrazole ligands and two chloride ligands in a tetrahedral coordination geometry.

Comment

We are studying the synthesis of polypyrazolylborate compounds with cyano substituents on the pyrazole rings. The title compound, (I), was isolated as a by-product from the synthesis of metal compounds of 4-cyano-3,5-dimethylpyrazole to be used for studying magnetic interactions involving the cyanopyrazole moiety.



(I)

There have been a few crystal structures reported to date for four-coordinate Cu complexes containing two coordinated pyrazoles and two coordinated halides, *viz*. dichlorobis(1-phenyl-3,5-dimethylpyrazole)copper(II) (Francisco *et al.*, 1980; Costa-Filho *et al.*, 1999), dibromobis(3,5-diphenylpyrazole)copper(II) (Murray *et al.*, 1988), dibromobis(1-phenyl-3,5-dimethylpyrazole)copper(II) (Costa-Filho *et al.*, 1999), *trans*-dibromobis(5− t-butylpyrazole)copper(II) (Liu *et*

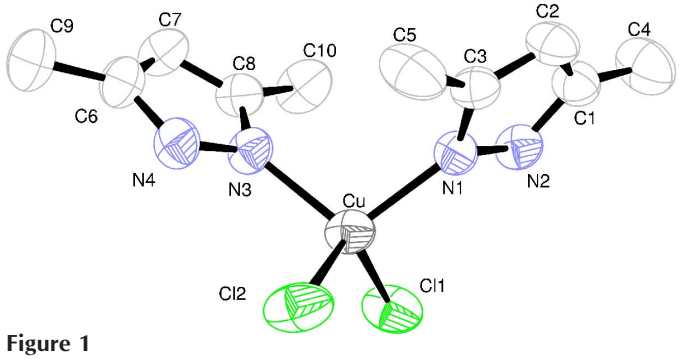


Figure 1
A view of the title compound, showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

al., 2001), bis(3-amino-4-acetyl-5-methylpyrazole)dichloro copper(II) (Hergold-Brundic *et al.*, 1991) and *trans*-bis(4-bromopyrazole)dichlorocopper(II) (Valle *et al.*, 1995). The bond lengths in the title compound are comparable with those in these structures, which show Cu—N bond lengths ranging from 1.94 to 2.02 Å and Cu—Cl bond lengths ranging from 2.23 to 2.34 Å.

Experimental

The title compound was isolated from a reaction to synthesize a copper complex of 4-cyano-3,5-dimethylpyrazole. Anhydrous $CuCl_2$ and 4-cyano-3,5-dimethylpyrazole were combined in THF in a 1:2 molar ratio. The isolated crystals represent a decomposition product of the ligand. Crystals were grown by slow evaporation of a dichloromethane solution.

Crystal data

$[CuCl_2(C_5H_8N_2)_2]$
M_r = 326.71
Monoclinic, $C2/c$
a = 15.023 (6) Å
b = 8.270 (7) Å
c = 24.038 (7) Å
β = 96.03 (3)°
V = 2970 (3) Å^3
Z = 8
D_x = 1.461 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
θ = 10–12°
μ = 1.82 mm^{-1}
T = 150 (2) K
Prism, blue
0.3 × 0.2 × 0.2 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Non–profiled $\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.449, T_{max} = 0.696
2697 measured reflections
2607 independent reflections
1907 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 25.0°
$h = 0 \rightarrow 17$
$k = 0 \rightarrow 9$
$l = -28 \rightarrow 28$
3 standard reflections
frequency: 60 min
intensity decay: −2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.067
$wR(F^2)$ = 0.211
S = 1.07
2607 reflections
158 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1478P)^2 + 1.1566P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.93 e Å^{-3}
$\Delta\rho_{min}$ = −1.14 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—N1	2.007 (5)	Cu—Cl2	2.2340 (18)
Cu—N3	2.010 (5)	Cu—Cl1	2.2404 (18)
N1—Cu—N3	105.5 (2)	N1—Cu—Cl1	101.26 (14)
N1—Cu—Cl2	115.49 (15)	N3—Cu—Cl1	115.39 (15)
N3—Cu—Cl2	101.20 (15)	Cl2—Cu—Cl1	117.95 (8)

H atoms were positioned geometrically and refined as riding on the atoms to which they are attached, with C—H distances in the range 0.93–0.96 Å and N—H distances of 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,*N*), or 1.5U_{eq}(C) for methyl atoms. The deepest hole is located 1.01 Å from the Cu atom.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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