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4,4′-Ethylenebipyridinium tetrachlorocuprate

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.006 Å
R factor = 0.043
wR factor = 0.127
Data-to-parameter ratio = 17.4

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

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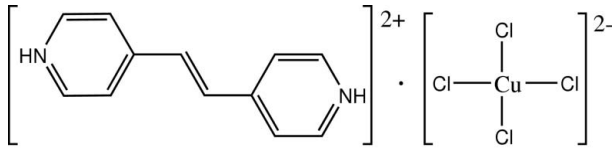
The crystal structure of the title compound, $(C_{12}H_{12}N_2)[CuCl_4]$, consists of Cu^{II} complex anions and diprotonated bis(4-pyridyl)ethylene. The cations and anions lie across individual inversion centers. The square-planar Cu^{II} complex anions link with cations *via* N—H···Cl hydrogen bonding.

Comment

As a part of our ongoing study on organic–inorganic hybrid crystal engineering involving transition metals with azoaromatic molecules, we report here the crystal structure of the title compound, (I).



(I)

The crystal structur of (I) (Fig. 1) consists of $[CuCl_4]^{2-}$ anions and diprotonated 1,2-bis(4-pyridyl)ethylene cations. The anion and cation lie across individual inversion centers. The Cu^{II} atom is coordinated by four Cl^- anions in a square-planar geometry (Table 1). The bis(4-pyridyl)ethylene cations link with the Cu^{II} complex anions *via* N—H···Cl hydrogen bonding (Table 2). The centroid-to-centroid distance of 3.498 (2) Å suggests the existence of π–π stacking between neighboring parallel pyridyl rings (Fig. 2).

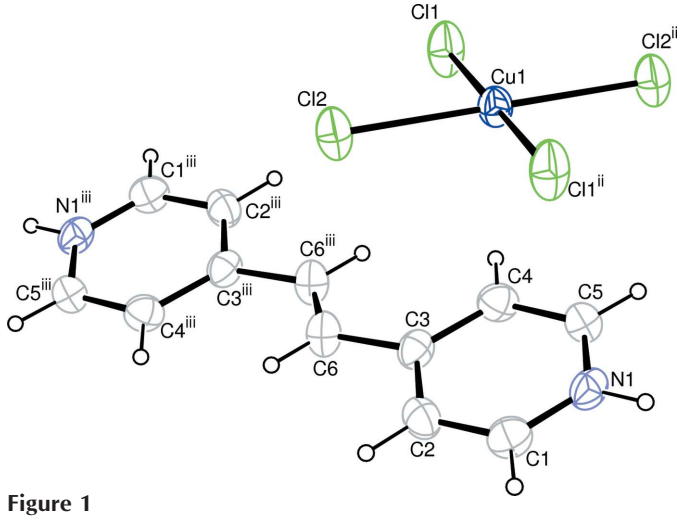


Figure 1
The molecular structure of (I), shown with 40% probability displacement ellipsoids (arbitrary spheres for H atoms). [Symmetry codes: (ii) $1-x, 1-y, 1-z$; (iii) $-x, 1-y, 2-z$.]

Experimental

Equimolar amounts of bis(4-pyridyl)ethylene and copper acetate were mixed in ethanol, followed by addition of several drops of concentrated HCl solution. Blue single crystals of (I) were obtained from the solution after 5 d.

Crystal data

$(C_{12}H_{12}N_2)[CuCl_4]$
M_r = 389.58
Triclinic, $P\overline{1}$
a = 7.0207 (14) Å
b = 7.0602 (11) Å
c = 8.1978 (19) Å
α = 68.66 (1)°
β = 73.748 (6)°
γ = 76.204 (11)°
V = 359.10 (12) Å^3
Z = 1
D_x = 1.801 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1725 reflections
θ = 3.1–27.1°
μ = 2.25 mm^{-1}
T = 273 (2) K
Block, blue
0.43 × 0.24 × 0.23 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.531, T_{max} = 0.603
3071 measured reflections
1547 independent reflections
1357 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 27.2°
$h = 0 \rightarrow 9$
$k = -8 \rightarrow 9$
$l = -9 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.127
S = 1.14
1547 reflections
89 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.069P)^2 + 0.374P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.086 (11)

Table 1
Selected geometric parameters (Å, °).

Cu1—Cl1	2.2489 (10)	Cu1—Cl2	2.2701 (10)
Cl1—Cu1—Cl2	89.90 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl1^{iv}	0.86	2.48	3.174 (3)	138
N1—H1···Cl2^{iv}	0.86	2.47	3.187 (3)	142

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

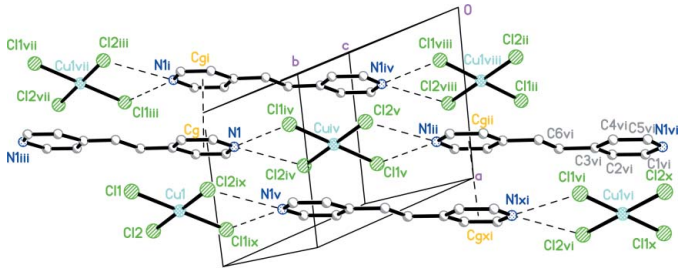


Figure 2
A packing diagram showing π–π stacking and hydrogen bonding (dashed lines). [symmetry codes: (i) $-x, -y, 2-z$; (ii) $x, -2+y, z$; (iii) $-x, 1-y, 2-z$; (iv) $x, -1+y, z$; (v) $1-x, -y, 1-z$; (vi) $1+x, -2+y, -1+z$; (vii) $-1+x, y, 1+z$; (viii) $x, -2+y, z$; (ix) $1-x, 1-y, 1-z$; (x) $2-x, -1-y, -z$; (xi) $1+x, -1+y, -1+z$.]

H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and refined in riding mode, with U_{iso}(H) = $1.2U_{eq}$(carrier).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 1999) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL*.

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