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Bis(2-ethyl-1*H*-imidazol-3-ium) tetrachloridocuprate(II)

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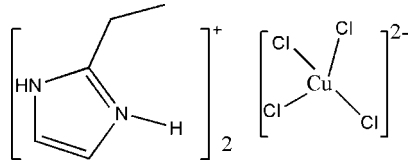
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.039; wR factor = 0.123; data-to-parameter ratio = 21.7.

In the crystal structure of the title salt, $(C_5H_9N_2)_2[CuCl_4]$, the organic cations and the tetrahedral $[CuCl_4]$ anions are linked into a three-dimensional network by N—H···Cl hydrogen bonds. The two 2-ethyl imidazolium cations in the asymmetric unit differ in the orientation of the ethyl group, with N—C—C—C torsion angles of −170.0 (4) and −87.6 (5)°.

Related literature

For general background to ferroelectric metal-organic frameworks, see: Fu *et al.* (2009); Ye *et al.* (2006); Zhang *et al.* (2008, 2010).



Experimental

Crystal data

$(C_5H_9N_2)_2[CuCl_4]$
M_r = 399.63
Triclinic, $P\overline{1}$
a = 7.992 (4) Å
b = 9.003 (4) Å
c = 12.216 (6) Å
α = 79.641 (14)°
β = 84.646 (14)°
γ = 72.154 (12)°
V = 822.4 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.97 mm^{-1}
T = 293 K
0.30 × 0.25 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.559, T_{max} = 0.674
9065 measured reflections
3775 independent reflections
3124 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.123
S = 1.17
3775 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl1^{i}	0.86	2.39	3.217 (3)	160
N2—H2A···Cl2	0.86	2.39	3.195 (3)	157
N3—H3A···Cl3	0.86	2.46	3.178 (3)	142
N4—H4C···Cl4^{ii}	0.86	2.32	3.149 (3)	164

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $-x+1, -y, -z+1$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

This work was supported by Southeast University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2067).

References

Fu, D.-W., Ge, J.-Z., Dai, J., Ye, H.-Y. & Qu, Z.-R. (2009). *Inorg. Chem. Commun.* **12**, 994–997.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Ye, Q., Song, Y.-M., Wang, G.-X., Chen, K. & Fu, D.-W. (2006). *J. Am. Chem. Soc.* **128**, 6554–6555.
Zhang, W., Xiong, R.-G. & Huang, S.-P. D. (2008). *J. Am. Chem. Soc.* **130**, 10468–10469.
Zhang, W., Ye, H.-Y., Cai, H.-L., Ge, J.-Z. & Xiong, R.-G. (2010). *J. Am. Chem. Soc.* **132**, 7300–7302.

supplementary materials

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Bis(2-ethyl-1*H*-imidazol-3-ium) tetrachloridocuprate(II)

R.-Q. Zhu

Comment

Dielectric constant measurements of compounds as a function of temperature is the basic method to find the materials which possess potential ferroelectric phase changes (Fu *et al.*, 2009; Ye *et al.*, 2006; Zhang *et al.*, 2008; Zhang *et al.*, 2010). The dielectric constant of the title compound has been measured, but showed no dielectric disuniformity in the range 93–365 K (m.p. 374–381 K).

X-ray crystallographic studies have been carried out for the complex $2[C_5N_2H_9]^{+}.CuCl_4^{2-}$ at 123 K. An view of the complex is shown in Fig. 1. The structure is consolidated by extensive intermolecular and intramolecular hydrogen bonds between Cl and N. This hydrogen bonding (Table 1, Fig. 2) produces a three-dimensional network. Within the $CuCl_4^{2-}$ tetrahedra the Cu-Cl distances are: Cu1—Cl1 = 2.2287 (13) Å, Cu1—Cl2 = 2.2625 Å,Cu1—Cl3 = 2.2688 (12) Å, Cu1—Cl4 = 2.2501 (13) Å.

The two 2-ethyl imidazolium cations in the asymmetric unit differ in the orientation of the ethyl group. In one cation all atoms except H atoms are situated in the same plane(dihedral angle N1—C3—C4—C5 = -170.0 (4)°), while in the other cation the dihedral angle N3—C8—C9—C10 is -87.6 (5) °.

Experimental

A mixture of $CuCl_2$ (4.26 g, 25 mmol), hydrochloric acid (50 mmol), and 2-ethyl imidazole (4.8 g, 50 mmol) in water was stirred for several days at room temperature, yellow block crystals were obtained.

Refinement

Hydrogen atom positions were calculated and allowed to ride on their respective C atoms and N atoms with C–H distances of 0.93–0.97Å and N–H = 0.86 Å, and with $U_{iso}(H)=1.2U_{eq}$(C or N).

Figures

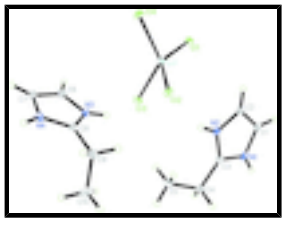

Fig. 1. The molecular structure of the title compound, with the displacement ellipsoids drawn at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines.

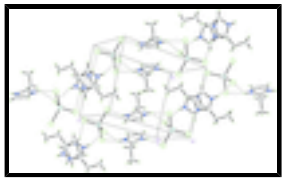

Fig. 2. Packing diagram of the title compound, showing the structure along the *b* axis. Hydrogen bonds are shown as dashed lines.

Bis(2-ethyl-1*H*-imidazol-3-ium) tetrachloridocuprate(II)

Crystal data

$(C_5H_9N_2)_2[CuCl_4]$	$Z = 2$
$M_r = 399.63$	$F(000) = 406$
Triclinic, $P\overline{1}$	$D_x = 1.614$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.992$ (4) Å	Cell parameters from 2088 reflections
$b = 9.003$ (4) Å	$\theta = 2.4$–$27.5°$
$c = 12.216$ (6) Å	$\mu = 1.97$ mm^{-1}
$\alpha = 79.641$ (14)°	$T = 293$ K
$\beta = 84.646$ (14)°	Block, yellow
$\gamma = 72.154$ (12)°	0.30 × 0.25 × 0.20 mm
$V = 822.4$ (7) Å^3	

Data collection

Rigaku SCXmini diffractometer	3775 independent reflections
Radiation source: fine-focus sealed tube	3124 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.035$
CCD_Profile_fitting scans	$\theta_{max} = 27.5°$, $\theta_{min} = 1.7°$
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)	$h = -10 \rightarrow 10$
$T_{min} = 0.559$, $T_{max} = 0.674$	$k = -11 \rightarrow 11$
9065 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H-atom parameters constrained
$wR(F^2) = 0.123$	$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.17$	$(\Delta/\sigma)_{max} = 0.001$
3775 reflections	$\Delta\rho_{max} = 0.59$ e Å^{-3}
174 parameters	$\Delta\rho_{min} = -0.66$ e Å^{-3}
0 restraints	Extinction correction: *SHELXL97* (Sheldrick, 2008)

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.0014 (1)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.91120 (5)	0.05748 (5)	0.21071 (3)	0.01639 (14)
C1	0.8790 (5)	0.4965 (4)	−0.1245 (3)	0.0203 (7)
H1	0.9490	0.4905	−0.1897	0.024*
C2	0.8332 (5)	0.3759 (4)	−0.0584 (3)	0.0192 (7)
H2	0.8657	0.2709	−0.0691	0.023*
C3	0.7099 (4)	0.5947 (4)	0.0167 (3)	0.0183 (7)
C4	0.6042 (5)	0.7072 (4)	0.0911 (3)	0.0250 (8)
H4A	0.5023	0.7782	0.0523	0.030*
H4B	0.6747	0.7704	0.1076	0.030*
C5	0.5432 (5)	0.6239 (5)	0.1994 (3)	0.0285 (9)
H5A	0.4760	0.5588	0.1835	0.043*
H5B	0.4713	0.7010	0.2426	0.043*
H5C	0.6436	0.5591	0.2406	0.043*
C6	0.7322 (5)	0.0989 (4)	0.5488 (3)	0.0223 (8)
H6	0.8545	0.0669	0.5483	0.027*
C7	0.6228 (5)	0.0601 (4)	0.6319 (3)	0.0208 (7)
H7	0.6544	−0.0045	0.6998	0.025*
C8	0.4588 (5)	0.2168 (4)	0.4944 (3)	0.0177 (7)
C9	0.3058 (5)	0.3210 (4)	0.4307 (3)	0.0257 (8)
H9A	0.2071	0.2783	0.4487	0.031*
H9B	0.3347	0.3231	0.3517	0.031*
C10	0.2529 (6)	0.4888 (5)	0.4567 (4)	0.0397 (11)
H10A	0.2191	0.4877	0.5343	0.060*
H10B	0.1557	0.5535	0.4126	0.060*
H10C	0.3507	0.5311	0.4397	0.060*
Cl1	1.16150 (11)	0.01933 (9)	0.10773 (7)	0.01903 (19)
Cl2	0.61789 (11)	0.16204 (10)	0.18983 (7)	0.0194 (2)
Cl3	0.94259 (11)	0.24838 (10)	0.29860 (7)	0.0204 (2)
Cl4	0.91629 (11)	−0.19331 (10)	0.27848 (8)	0.0233 (2)
N1	0.8018 (4)	0.6294 (3)	−0.0763 (2)	0.0193 (6)
H1A	0.8113	0.7219	−0.1024	0.023*

N2	0.7279 (4)	0.4409 (3)	0.0285 (2)	0.0187 (6)
H2A	0.6811	0.3891	0.0823	0.022*
N3	0.6284 (4)	0.1948 (3)	0.4648 (2)	0.0201 (6)
H3A	0.6673	0.2350	0.4020	0.024*
N4	0.4552 (4)	0.1350 (3)	0.5963 (2)	0.0186 (6)
H4C	0.3608	0.1298	0.6347	0.022*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0145 (2)	0.0147 (2)	0.0195 (2)	−0.00468 (17)	0.00088 (16)	−0.00158 (16)
C1	0.0197 (18)	0.0200 (17)	0.0211 (18)	−0.0069 (14)	−0.0028 (14)	−0.0008 (14)
C2	0.0228 (18)	0.0141 (16)	0.0215 (18)	−0.0061 (14)	0.0004 (14)	−0.0046 (13)
C3	0.0176 (17)	0.0170 (16)	0.0219 (18)	−0.0063 (14)	−0.0059 (14)	−0.0029 (13)
C4	0.029 (2)	0.0196 (18)	0.027 (2)	−0.0036 (16)	−0.0039 (16)	−0.0077 (15)
C5	0.029 (2)	0.029 (2)	0.025 (2)	0.0003 (17)	−0.0018 (16)	−0.0111 (16)
C6	0.0176 (17)	0.0208 (18)	0.026 (2)	−0.0031 (14)	0.0002 (15)	−0.0040 (15)
C7	0.0209 (18)	0.0199 (17)	0.0191 (18)	−0.0021 (14)	−0.0051 (14)	−0.0012 (14)
C8	0.0213 (18)	0.0142 (16)	0.0181 (17)	−0.0053 (14)	0.0002 (14)	−0.0046 (13)
C9	0.0232 (19)	0.0235 (19)	0.028 (2)	0.0009 (16)	−0.0101 (16)	−0.0062 (16)
C10	0.042 (3)	0.023 (2)	0.048 (3)	0.0048 (19)	−0.020 (2)	−0.0072 (19)
Cl1	0.0178 (4)	0.0166 (4)	0.0227 (4)	−0.0061 (3)	0.0043 (3)	−0.0042 (3)
Cl2	0.0147 (4)	0.0207 (4)	0.0209 (4)	−0.0052 (3)	−0.0015 (3)	0.0019 (3)
Cl3	0.0213 (4)	0.0221 (4)	0.0206 (4)	−0.0103 (3)	0.0030 (3)	−0.0061 (3)
Cl4	0.0208 (4)	0.0152 (4)	0.0293 (5)	−0.0035 (3)	0.0054 (4)	0.0017 (3)
N1	0.0217 (15)	0.0157 (14)	0.0206 (15)	−0.0080 (12)	−0.0038 (12)	0.0027 (12)
N2	0.0195 (15)	0.0158 (14)	0.0195 (15)	−0.0052 (12)	−0.0007 (12)	0.0006 (11)
N3	0.0221 (16)	0.0188 (14)	0.0177 (15)	−0.0058 (12)	0.0012 (12)	0.0000 (12)
N4	0.0161 (14)	0.0221 (15)	0.0181 (15)	−0.0067 (12)	0.0034 (12)	−0.0048 (12)

Geometric parameters (Å, °)

Cu1—Cl1	2.2287 (13)	C6—C7	1.346 (5)
Cu1—Cl4	2.2501 (13)	C6—N3	1.374 (4)
Cu1—Cl2	2.2625 (14)	C6—H6	0.9300
Cu1—Cl3	2.2688 (12)	C7—N4	1.374 (4)
C1—C2	1.355 (5)	C7—H7	0.9300
C1—N1	1.375 (5)	C8—N4	1.330 (4)
C1—H1	0.9300	C8—N3	1.333 (4)
C2—N2	1.391 (4)	C8—C9	1.481 (5)
C2—H2	0.9300	C9—C10	1.523 (5)
C3—N2	1.330 (4)	C9—H9A	0.9700
C3—N1	1.335 (5)	C9—H9B	0.9700
C3—C4	1.493 (5)	C10—H10A	0.9600
C4—C5	1.516 (6)	C10—H10B	0.9600
C4—H4A	0.9700	C10—H10C	0.9600
C4—H4B	0.9700	N1—H1A	0.8600
C5—H5A	0.9600	N2—H2A	0.8600
C5—H5B	0.9600	N3—H3A	0.8600

C5—H5C	0.9600	N4—H4C	0.8600
Cl1—Cu1—Cl4	101.08 (4)	C6—C7—N4	106.2 (3)
Cl1—Cu1—Cl2	139.56 (4)	C6—C7—H7	126.9
Cl4—Cu1—Cl2	98.32 (4)	N4—C7—H7	126.9
Cl1—Cu1—Cl3	97.91 (4)	N4—C8—N3	105.9 (3)
Cl4—Cu1—Cl3	130.13 (5)	N4—C8—C9	126.9 (3)
Cl2—Cu1—Cl3	96.09 (4)	N3—C8—C9	127.0 (3)
C2—C1—N1	106.7 (3)	C8—C9—C10	111.8 (3)
C2—C1—H1	126.7	C8—C9—H9A	109.3
N1—C1—H1	126.7	C10—C9—H9A	109.3
C1—C2—N2	106.1 (3)	C8—C9—H9B	109.3
C1—C2—H2	127.0	C10—C9—H9B	109.3
N2—C2—H2	127.0	H9A—C9—H9B	107.9
N2—C3—N1	106.5 (3)	C9—C10—H10A	109.5
N2—C3—C4	126.7 (3)	C9—C10—H10B	109.5
N1—C3—C4	126.8 (3)	H10A—C10—H10B	109.5
C3—C4—C5	112.6 (3)	C9—C10—H10C	109.5
C3—C4—H4A	109.1	H10A—C10—H10C	109.5
C5—C4—H4A	109.1	H10B—C10—H10C	109.5
C3—C4—H4B	109.1	C3—N1—C1	110.5 (3)
C5—C4—H4B	109.1	C3—N1—H1A	124.7
H4A—C4—H4B	107.8	C1—N1—H1A	124.7
C4—C5—H5A	109.5	C3—N2—C2	110.3 (3)
C4—C5—H5B	109.5	C3—N2—H2A	124.9
H5A—C5—H5B	109.5	C2—N2—H2A	124.9
C4—C5—H5C	109.5	C8—N3—C6	110.3 (3)
H5A—C5—H5C	109.5	C8—N3—H3A	124.8
H5B—C5—H5C	109.5	C6—N3—H3A	124.8
C7—C6—N3	106.8 (3)	C8—N4—C7	110.8 (3)
C7—C6—H6	126.6	C8—N4—H4C	124.6
N3—C6—H6	126.6	C7—N4—H4C	124.6

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···Cl1^{i}	0.86	2.39	3.217 (3)	160
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Symmetry codes: (i) −*x*+2, −*y*+1, −*z*; (ii) −*x*+1, −*y*, −*z*+1.

Fig. 1

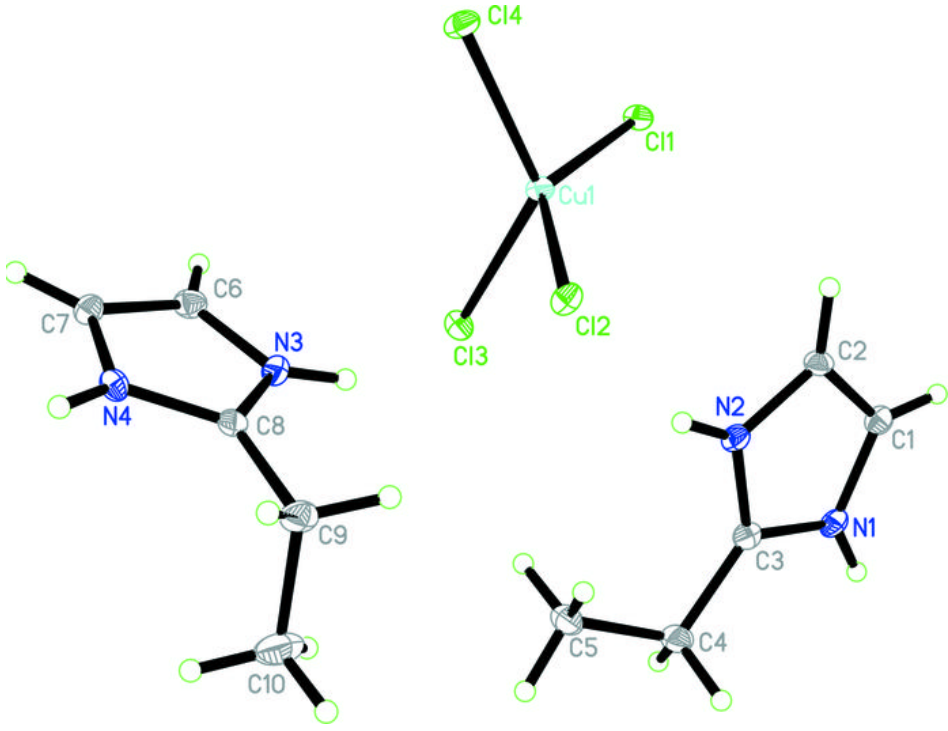

Fig. 2