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Bis[4-(dimethylamino)pyridinium] tetrabromidocuprate(II)

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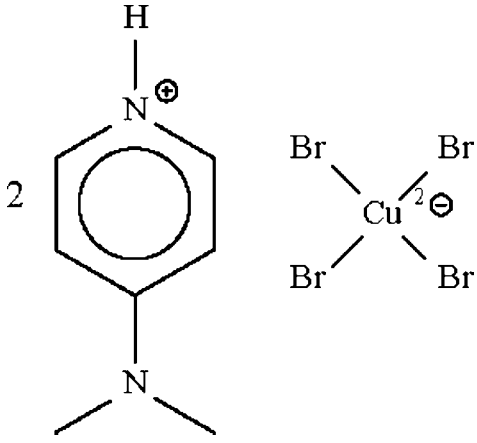
Key indicators: single-crystal X-ray study; T = 233 K; mean σ(C–C) = 0.009 Å; R factor = 0.043; wR factor = 0.123; data-to-parameter ratio = 21.6.

The metal atom in the anion of the title salt, $(C_7H_{11}N_2)_2[CuBr_4]$, shows a distorted tetrahedral coordination. The primary contacts between the ions are of the N—H···Br type.

Related literature

For other pyridinium tetrabromidocuprates, see: Coffey *et al.* (1996); Haddad & Al-Far (2008); Luque *et al.* (2001); Willet *et al.* (2000, 2003).



Experimental

Crystal data

$(C_7H_{11}N_2)_2[CuBr_4]$
M_r = 629.54
Triclinic, $P\overline{1}$
a = 8.1768 (2) Å
b = 9.2406 (3) Å
c = 14.3686 (4) Å
α = 93.689 (2)°
β = 94.814 (2)°
γ = 105.073 (2)°
V = 1040.42 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 8.73 mm^{-1}
T = 233 K
0.35 × 0.30 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.321, T_{max} = 0.746
(expected range = 0.180–0.418)
7224 measured reflections
4595 independent reflections
3168 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.123
S = 1.00
4595 reflections
213 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.84 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Br1	0.88	2.54	3.380 (7)	162
N3—H3···Br2	0.88	2.65	3.449 (6)	152

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2503).

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supporting information

Acta Cryst. (2009). E**65**, m972 [doi:10.1107/S1600536809028128]

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S1. Experimental

Copper sulfate pentahydrate (2.1 g, 8.3 mmol) dissolved in water (5 ml) was mixed with 4-dimethylaminopyridine hydrobromide perbromide (3 g, 8.3 mmol) dissolved in ethanol (10 ml). The mixture was heated for 30 min. The filtered green solution when allowed to evaporate yielded black crystals.

S2. Refinement

Hydrogen atoms were placed at calculated positions (C–H 0.94–0.97 Å; N–H 0.88 Å) and were treated as riding on their parent atoms, with U(H) set to 1.2–1.5U_{eq}(C, N).

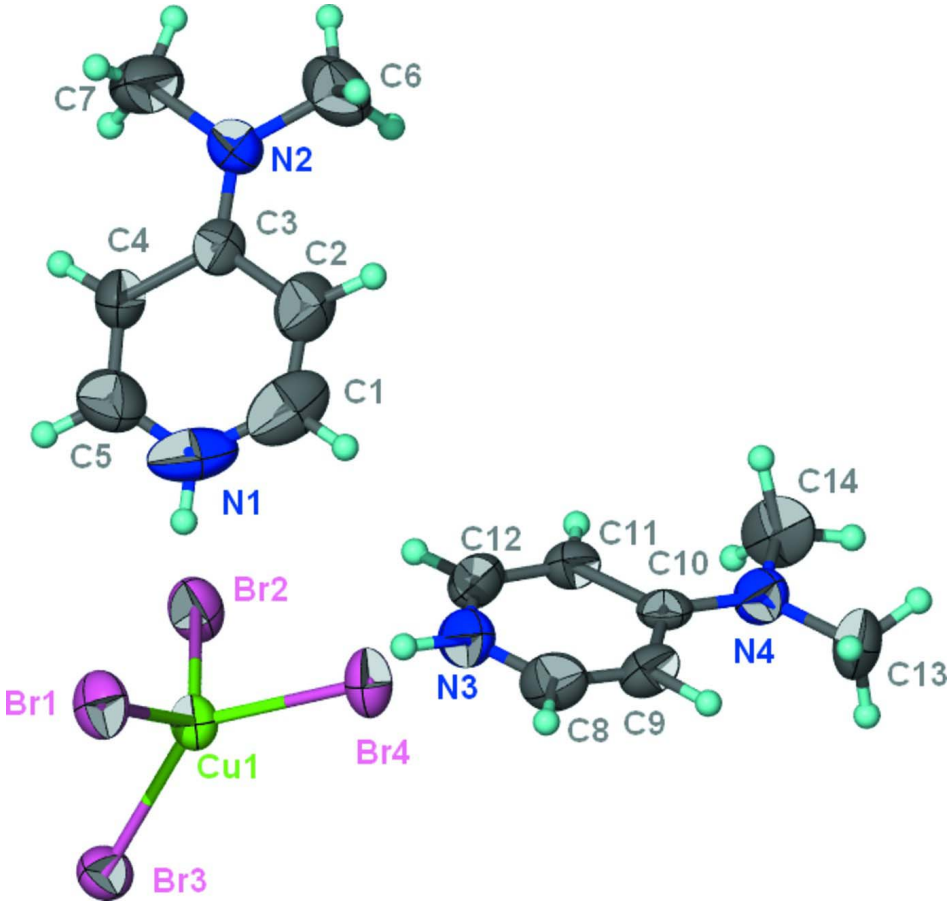

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of 2[$C_7H_{11}N_2$][$CuBr_4$] at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Bis[4-(dimethylamino)pyridinium] tetrabromidocuprate(II)

Crystal data

$(C_7H_{11}N_2)_2[CuBr_4]$
$M_r = 629.54$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.1768$ (2) Å
$b = 9.2406$ (3) Å
$c = 14.3686$ (4) Å
$\alpha = 93.689$ (2)°
$\beta = 94.814$ (2)°
$\gamma = 105.073$ (2)°
$V = 1040.42$ (5) Å^3
$Z = 2$
$F(000) = 606$
$D_x = 2.010$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2442 reflections
$\theta = 2.3$–27.5°
$\mu = 8.73$ mm^{-1}
$T = 233$ K
Block, black
0.35 × 0.30 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.321$, $T_{max} = 0.746$
7224 measured reflections
4595 independent reflections

3168 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.4°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 12$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.123$
$S = 1.00$
4595 reflections
213 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.84$ e Å^{-3}
$\Delta\rho_{min} = -0.82$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0078 (8)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.46757 (8)	0.23274 (7)	0.31534 (5)	0.04383 (19)
Br2	0.44673 (8)	0.69937 (7)	0.29470 (5)	0.0458 (2)
Br3	0.11950 (8)	0.35808 (7)	0.20247 (4)	0.03895 (18)
Br4	0.65667 (8)	0.48740 (7)	0.15029 (4)	0.04107 (19)
Cu1	0.41731 (9)	0.44301 (7)	0.23676 (5)	0.0323 (2)
N1	0.8043 (9)	0.5220 (8)	0.4011 (5)	0.067 (2)
H1	0.7335	0.4434	0.3685	0.081*
N2	1.1304 (7)	0.8919 (6)	0.5502 (4)	0.0466 (13)
N3	0.6251 (7)	0.8455 (6)	0.1004 (4)	0.0478 (13)
H3	0.5794	0.7776	0.1376	0.057*
N4	0.8436 (7)	1.1604 (6)	−0.0731 (3)	0.0415 (12)
C1	0.9472 (12)	0.5930 (9)	0.3673 (5)	0.063 (2)
H1A	0.9709	0.5576	0.3085	0.075*
C2	1.0582 (9)	0.7127 (9)	0.4141 (5)	0.0521 (18)
H2	1.1589	0.7596	0.3887	0.062*
C3	1.0231 (7)	0.7695 (7)	0.5032 (4)	0.0343 (13)
C4	0.8711 (8)	0.6903 (8)	0.5360 (5)	0.0465 (16)
H4	0.8409	0.7213	0.5942	0.056*
C5	0.7692 (9)	0.5702 (9)	0.4836 (5)	0.064 (2)
H5	0.6683	0.5179	0.5067	0.077*
C6	1.2928 (10)	0.9673 (9)	0.5180 (6)	0.067 (2)
H6A	1.2723	1.0101	0.4597	0.100*
H6B	1.3585	0.8951	0.5080	0.100*
H6C	1.3556	1.0469	0.5650	0.100*
C7	1.0967 (10)	0.9465 (9)	0.6426 (5)	0.062 (2)
H7A	0.9814	0.9571	0.6393	0.093*
H7B	1.1767	1.0433	0.6623	0.093*
H7C	1.1095	0.8752	0.6875	0.093*
C8	0.6803 (9)	0.8036 (7)	0.0201 (5)	0.0472 (17)

H8	0.6688	0.7008	0.0045	0.057*
C9	0.7497 (8)	0.9012 (7)	−0.0374 (4)	0.0409 (15)
H9	0.7858	0.8671	−0.0931	0.049*
C10	0.7710 (7)	1.0591 (6)	−0.0161 (4)	0.0328 (13)
C11	0.7118 (7)	1.1009 (7)	0.0682 (4)	0.0374 (14)
H11	0.7217	1.2026	0.0863	0.045*
C12	0.6401 (8)	0.9918 (8)	0.1234 (4)	0.0462 (17)
H12	0.5999	1.0200	0.1793	0.055*
C13	0.9027 (9)	1.1174 (9)	−0.1615 (5)	0.0558 (18)
H13A	0.9415	1.0274	−0.1553	0.084*
H13B	0.9960	1.1986	−0.1764	0.084*
H13C	0.8099	1.0977	−0.2112	0.084*
C14	0.8708 (10)	1.3216 (6)	−0.0511 (5)	0.059 (2)
H14A	0.9513	1.3551	0.0044	0.088*
H14B	0.7635	1.3424	−0.0398	0.088*
H14C	0.9158	1.3747	−0.1035	0.088*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0494 (4)	0.0387 (4)	0.0482 (4)	0.0151 (3)	0.0101 (3)	0.0186 (3)
Br2	0.0496 (4)	0.0355 (3)	0.0513 (4)	0.0073 (3)	0.0199 (3)	−0.0051 (3)
Br3	0.0337 (3)	0.0415 (3)	0.0407 (3)	0.0089 (3)	0.0043 (2)	0.0009 (3)
Br4	0.0450 (4)	0.0397 (3)	0.0446 (4)	0.0155 (3)	0.0205 (3)	0.0109 (3)
Cu1	0.0331 (4)	0.0319 (4)	0.0336 (4)	0.0095 (3)	0.0084 (3)	0.0061 (3)
N1	0.062 (5)	0.074 (5)	0.060 (4)	0.022 (4)	−0.024 (4)	−0.017 (4)
N2	0.034 (3)	0.058 (3)	0.042 (3)	0.002 (3)	0.004 (2)	0.003 (3)
N3	0.053 (4)	0.045 (3)	0.040 (3)	0.002 (3)	0.003 (3)	0.009 (3)
N4	0.050 (3)	0.035 (3)	0.036 (3)	0.005 (2)	0.005 (2)	0.005 (2)
C1	0.078 (6)	0.075 (5)	0.050 (4)	0.052 (5)	0.000 (4)	−0.010 (4)
C2	0.041 (4)	0.077 (5)	0.048 (4)	0.031 (4)	0.014 (3)	0.001 (4)
C3	0.028 (3)	0.046 (3)	0.034 (3)	0.019 (3)	0.005 (2)	0.006 (3)
C4	0.040 (4)	0.060 (4)	0.036 (3)	0.005 (3)	0.010 (3)	0.007 (3)
C5	0.043 (5)	0.083 (6)	0.059 (5)	0.004 (4)	−0.005 (4)	0.014 (5)
C6	0.054 (5)	0.063 (5)	0.074 (5)	−0.005 (4)	0.001 (4)	0.029 (4)
C7	0.058 (5)	0.068 (5)	0.052 (4)	0.009 (4)	−0.003 (4)	−0.011 (4)
C8	0.060 (5)	0.030 (3)	0.048 (4)	0.008 (3)	−0.003 (3)	0.003 (3)
C9	0.050 (4)	0.041 (3)	0.031 (3)	0.014 (3)	0.000 (3)	−0.003 (3)
C10	0.028 (3)	0.036 (3)	0.030 (3)	0.004 (2)	−0.007 (2)	0.001 (3)
C11	0.037 (3)	0.037 (3)	0.034 (3)	0.005 (3)	0.000 (3)	−0.003 (3)
C12	0.038 (4)	0.069 (5)	0.031 (3)	0.015 (3)	0.002 (3)	0.000 (3)
C13	0.060 (5)	0.070 (5)	0.037 (4)	0.009 (4)	0.016 (3)	0.016 (4)
C14	0.091 (6)	0.022 (3)	0.061 (5)	0.007 (3)	0.000 (4)	0.017 (3)

Geometric parameters (Å, º)

Br1—Cu1	2.4164 (9)	C4—H4	0.9400
Br2—Cu1	2.4039 (9)	C5—H5	0.9400

Br3—Cu1	2.3544 (9)	C6—H6A	0.9700
Br4—Cu1	2.3662 (9)	C6—H6B	0.9700
N1—C5	1.320 (10)	C6—H6C	0.9700
N1—C1	1.330 (11)	C7—H7A	0.9700
N1—H1	0.8800	C7—H7B	0.9700
N2—C3	1.339 (7)	C7—H7C	0.9700
N2—C6	1.458 (9)	C8—C9	1.314 (9)
N2—C7	1.463 (8)	C8—H8	0.9400
N3—C12	1.342 (8)	C9—C10	1.433 (8)
N3—C8	1.343 (9)	C9—H9	0.9400
N3—H3	0.8800	C10—C11	1.410 (8)
N4—C10	1.338 (7)	C11—C12	1.364 (9)
N4—C14	1.457 (7)	C11—H11	0.9400
N4—C13	1.464 (8)	C12—H12	0.9400
C1—C2	1.334 (10)	C13—H13A	0.9700
C1—H1A	0.9400	C13—H13B	0.9700
C2—C3	1.431 (8)	C13—H13C	0.9700
C2—H2	0.9400	C14—H14A	0.9700
C3—C4	1.404 (8)	C14—H14B	0.9700
C4—C5	1.341 (9)	C14—H14C	0.9700

Br1—Cu1—Br2	131.05 (4)	N2—C6—H6C	109.5
Br1—Cu1—Br3	99.47 (3)	H6A—C6—H6C	109.5
Br1—Cu1—Br4	97.82 (3)	H6B—C6—H6C	109.5
Br2—Cu1—Br3	100.27 (3)	N2—C7—H7A	109.5
Br2—Cu1—Br4	97.76 (3)	N2—C7—H7B	109.5
Br3—Cu1—Br4	136.48 (4)	H7A—C7—H7B	109.5
C5—N1—C1	119.7 (7)	N2—C7—H7C	109.5
C5—N1—H1	120.2	H7A—C7—H7C	109.5
C1—N1—H1	120.2	H7B—C7—H7C	109.5
C3—N2—C6	122.6 (6)	C9—C8—N3	122.3 (6)
C3—N2—C7	120.4 (6)	C9—C8—H8	118.9
C6—N2—C7	116.7 (6)	N3—C8—H8	118.9
C12—N3—C8	119.5 (6)	C8—C9—C10	120.8 (6)
C12—N3—H3	120.2	C8—C9—H9	119.6
C8—N3—H3	120.2	C10—C9—H9	119.6
C10—N4—C14	122.4 (5)	N4—C10—C11	122.2 (5)
C10—N4—C13	122.4 (5)	N4—C10—C9	121.7 (5)
C14—N4—C13	115.2 (6)	C11—C10—C9	116.1 (6)
C2—C1—N1	122.3 (7)	C12—C11—C10	119.2 (5)
C2—C1—H1A	118.9	C12—C11—H11	120.4
N1—C1—H1A	118.9	C10—C11—H11	120.4
C1—C2—C3	119.6 (7)	N3—C12—C11	122.1 (6)
C1—C2—H2	120.2	N3—C12—H12	118.9
C3—C2—H2	120.2	C11—C12—H12	118.9
N2—C3—C4	123.4 (5)	N4—C13—H13A	109.5
N2—C3—C2	120.7 (6)	N4—C13—H13B	109.5
C4—C3—C2	116.0 (6)	H13A—C13—H13B	109.5

C5—C4—C3	119.5 (6)	N4—C13—H13C	109.5
C5—C4—H4	120.2	H13A—C13—H13C	109.5
C3—C4—H4	120.2	H13B—C13—H13C	109.5
N1—C5—C4	122.9 (8)	N4—C14—H14A	109.5
N1—C5—H5	118.5	N4—C14—H14B	109.5
C4—C5—H5	118.5	H14A—C14—H14B	109.5
N2—C6—H6A	109.5	N4—C14—H14C	109.5
N2—C6—H6B	109.5	H14A—C14—H14C	109.5
H6A—C6—H6B	109.5	H14B—C14—H14C	109.5
C5—N1—C1—C2	−0.1 (12)	C12—N3—C8—C9	0.2 (10)
N1—C1—C2—C3	−0.9 (11)	N3—C8—C9—C10	0.5 (10)
C6—N2—C3—C4	176.1 (7)	C14—N4—C10—C11	1.6 (9)
C7—N2—C3—C4	2.7 (9)	C13—N4—C10—C11	−179.0 (5)
C6—N2—C3—C2	−4.6 (9)	C14—N4—C10—C9	−178.1 (6)
C7—N2—C3—C2	−178.0 (6)	C13—N4—C10—C9	1.3 (8)
C1—C2—C3—N2	−178.2 (6)	C8—C9—C10—N4	179.0 (6)
C1—C2—C3—C4	1.2 (9)	C8—C9—C10—C11	−0.7 (8)
N2—C3—C4—C5	178.9 (6)	N4—C10—C11—C12	−179.6 (5)
C2—C3—C4—C5	−0.5 (9)	C9—C10—C11—C12	0.2 (8)
C1—N1—C5—C4	0.8 (12)	C8—N3—C12—C11	−0.8 (9)
C3—C4—C5—N1	−0.4 (11)	C10—C11—C12—N3	0.6 (9)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Br1	0.88	2.54	3.380 (7)	162
N3—H3···Br2	0.88	2.65	3.449 (6)	152