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

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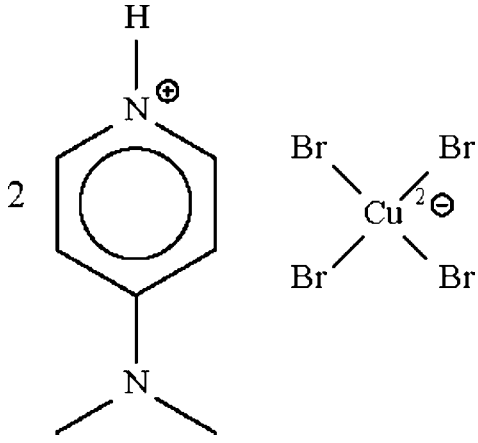
Key indicators: single-crystal X-ray study; T = 233 K; mean σ(C–C) = 0.009 Å; R factor = 0.043; wR factor = 0.123; data-to-parameter ratio = 21.6.

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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supplementary materials

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

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

K. M. Lo and S. W. Ng

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.

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).

Figures

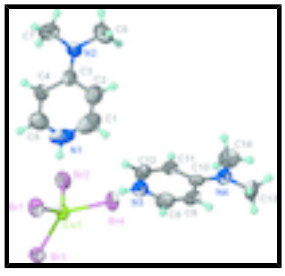


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of 2[$C_7H_{11}N_2$][$CuBr_4$] at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

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

Crystal data

$(C_7H_{11}N_2)_2[Cu_1Br_4]$	$Z = 2$
$M_r = 629.54$	$F_{000} = 606$
Triclinic, $P\overline{1}$	$D_x = 2.010$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.1768$ (2) Å	Cell parameters from 2442 reflections
$b = 9.2406$ (3) Å	$\theta = 2.3$–27.5º
$c = 14.3686$ (4) Å	$\mu = 8.73$ mm^{-1}
$\alpha = 93.689$ (2)º	$T = 233$ K
$\beta = 94.814$ (2)º	Block, black
$\gamma = 105.073$ (2)º	0.35 × 0.30 × 0.10 mm
$V = 1040.42$ (5) Å^3	

Data collection

Bruker SMART APEX diffractometer	4595 independent reflections
Radiation source: fine-focus sealed tube	3168 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.042$
$T = 233$ K	$\theta_{max} = 27.5^{o}$
ω scans	$\theta_{min} = 1.4^{o}$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{min} = 0.321$, $T_{max} = 0.746$	$k = -10 \rightarrow 12$
7224 measured reflections	$l = -18 \rightarrow 18$

Refinement

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

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 (Å^2)

	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, °)

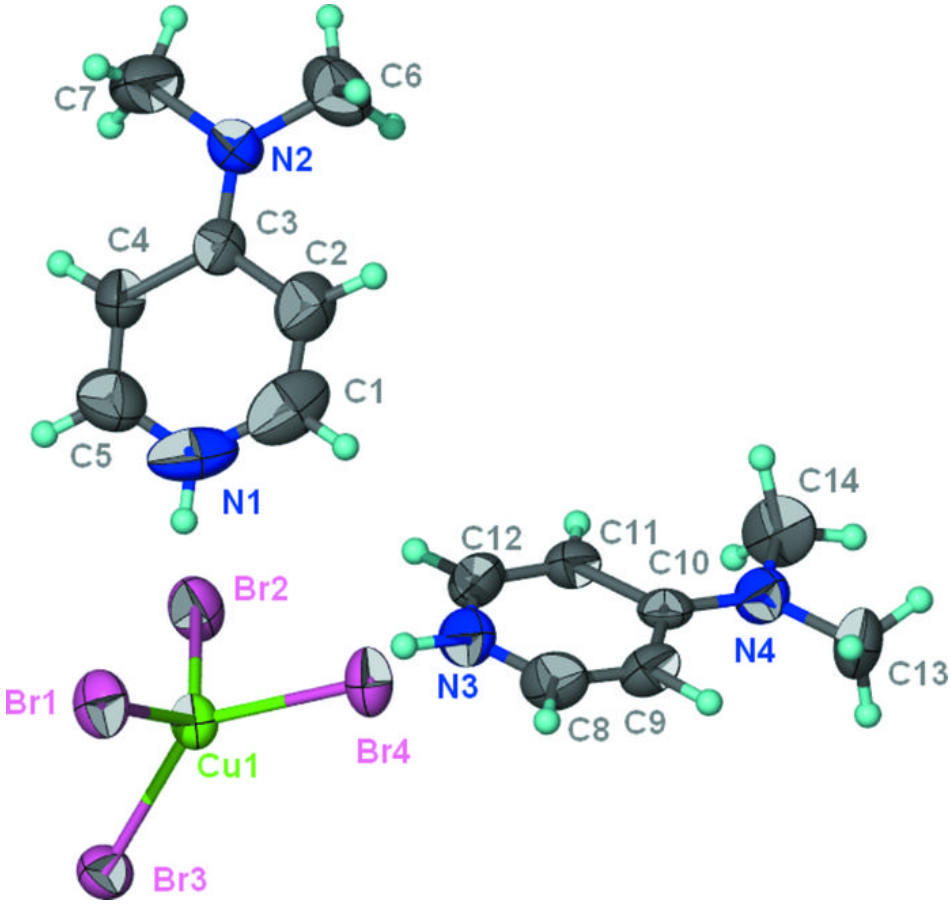
Br1—Cu1	2.4164 (9)	C4—H4	0.9400
Br2—Cu1	2.4039 (9)	C5—H5	0.9400
Br3—Cu1	2.3544 (9)	C6—H6A	0.9700
Br4—Cu1	2.3662 (9)	C6—H6B	0.9700
N1—C5	1.320 (10)	C6—H6C	0.9700
N1—C1	1.330 (11)	C7—H7A	0.9700
N1—H1	0.8800	C7—H7B	0.9700
N2—C3	1.339 (7)	C7—H7C	0.9700
N2—C6	1.458 (9)	C8—C9	1.314 (9)
N2—C7	1.463 (8)	C8—H8	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, °)

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

Fig. 1


C7
C6
N2
C4
C3
C2
C1
C5
N1
C14
C12
C11
C10
Br2
N4
Br1
N3
C13
C8
C9
Cu1
Br4
Br3