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Bis(cyclohexylammonium) tetrabromidocuprate(II)

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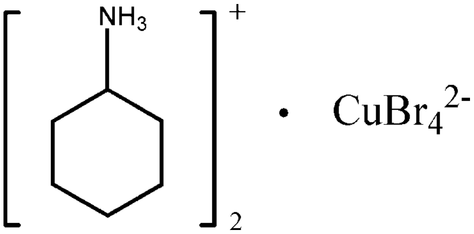
Key indicators: single-crystal X-ray study; *T* = 293 K; mean σ(C–C) = 0.008 Å; *R* factor = 0.047; *wR* factor = 0.095; data-to-parameter ratio = 25.0.

The structure of the title salt, $(C_6H_{14}N)_2[CuBr_4]$, is built up from cyclohexylammonium cations and tetrabromidocuprate anions, the latter being located on an inversion center. In the crystal, anions and cations are interconnected by N—H⋯Br hydrogen bonds, forming ribbons parallel to $[0\overline{1}\overline{1}]$.

Related literature

For background to the development of ferroelectric pure organic or inorganic compounds, see: Haertling (1999); Homes *et al.* (2001). For the synthesis of a variety of compounds with potential piezoelectric and ferroelectric properties, see: Fu *et al.* (2009); Hang *et al.* (2009). For the synthesis of the title compound, see: Willett (2004).



Experimental

Crystal data

$(C_6H_{14}N)_2[CuBr_4]$
M_r = 583.51
Monoclinic, $P2_1/c$
a = 14.372 (3) Å
b = 7.6483 (15) Å
c = 9.1561 (18) Å
β = 106.89 (3)°
V = 963.0 (3) Å^3
Z = 2
Mo *K*α radiation
μ = 9.42 mm^{-1}
T = 293 K
0.33 × 0.28 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.056, T_{max} = 0.152
9579 measured reflections
2199 independent reflections
1468 reflections with $I > 2\sigma(I)$
R_{int} = 0.092
2 standard reflections every 150 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.095
S = 1.03
2199 reflections
88 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N1—H1*D*⋯Br2^{i}	0.89	2.60	3.474 (4)	166
N1—H1*C*⋯Br2^{ii}	0.89	2.56	3.445 (4)	174
N1—H1*E*⋯Br3^{iii}	0.89	2.62	3.341 (4)	138

Symmetry codes: (i) $x, y+1, z-1$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

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: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2418).

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supporting information

Acta Cryst. (2012). E**68**, m448 [https://doi.org/10.1107/S1600536812011117]

Bis(cyclohexylammonium) tetrabromidocuprate(II)

Meng Ting Han

S1. Comment

At present, much attention in ferroelectric material field is focused on developing ferroelectric pure organic or inorganic compounds (Haertling, 1999; Homes *et al.* 2001). Recently we have reported the synthesis of a variety of compounds (Fu *et al.*, 2009; Hang *et al.*, 2009), which have potential piezoelectric and ferroelectric properties. In order to find more dielectric ferroelectric materials, we investigated the physical properties of the title compound (Fig. 1). The dielectric constant of the title compound as a function of temperature indicates that the permittivity is basically temperature-independent (dielectric constant equaling to 0.42 to 6.6), suggesting that this compound should be not a real ferroelectrics or that no phase transition occurs within the measured temperature range. Similarly, below the melting point (443 K) of the compound, the dielectric constant as a function of temperature also goes smoothly, and there is no dielectric anomaly observed. Herein, we report the synthesis and crystal structure of the title compound.

The structure of the title compound is shown in Fig. 1. There are one half $CuBr_4^{2-}$ anion and one cyclohexylammonium cation in the asymmetric unit. The cyclohexyl ring has the chair conformation. As it can be seen from the packing diagram (Fig. 2), ions are connected *via* intermolecular N—H···Br hydrogen bonds to form a one dimensional chain in the crystal. Dipole–dipole and van der Waals interactions are effective in the molecular packing.

S2. Experimental

Crystals of the title compound were grown by evaporation of an aqueous solution containing a 2:1 ratio of cyclohexylammonium bromide and copper(II) bromide. A few drops of hydrobromic acid were added to the solution to avoid hydrolysis of the Cu(II) ion (Willett, 2004).

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.97–0.98 Å, N—H = 0.89 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 1.5U_{eq}(N)$.

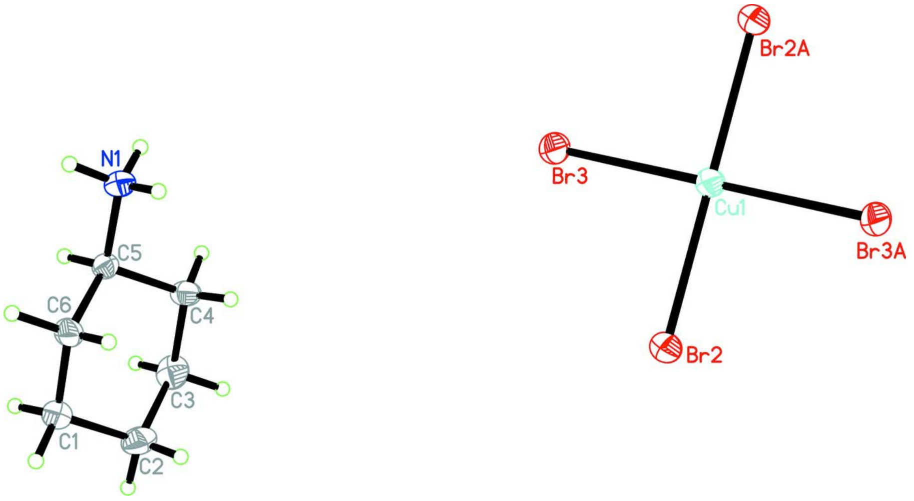

Figure 1

Perspective structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

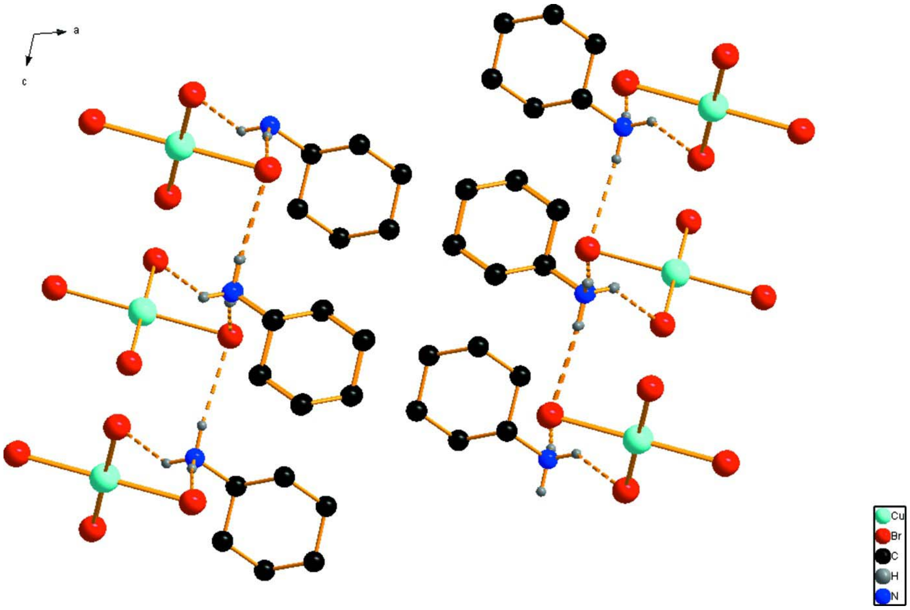

Figure 2

The crystal packing of the title compound viewed along the *b* axis showing the hydrogen bonds network. Some of the H atoms have been omitted for clarity.

Bis(cyclohexylammonium) tetrabromidocuprate(II)

Crystal data

$(C_6H_{14}N)_2[CuBr_4]$	$V = 963.0\ (3)$ Å^3
$M_r = 583.51$	$Z = 2$
Monoclinic, $P2_1/c$	$F(000) = 566$
Hall symbol: -P 2ybc	$D_x = 2.012$ Mg m^{-3}
$a = 14.372\ (3)$ Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 7.6483\ (15)$ Å	Cell parameters from 2203 reflections
$c = 9.1561\ (18)$ Å	$\theta = 2.3$–$27.5°$
$\beta = 106.89\ (3)°$	$\mu = 9.42$ mm^{-1}

T = 293 K
Block, sepia

0.33 × 0.28 × 0.20 mm

Data collection

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.056, T_{max} = 0.152
9579 measured reflections

2199 independent reflections
1468 reflections with $I > 2\sigma(I)$
R_{int} = 0.092
θ_{max} = 27.5°, θ_{min} = 3.1°
$h = -18 \rightarrow 18$
$k = -9 \rightarrow 9$
$l = -11 \rightarrow 11$
2 standard reflections every 150 reflections
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.095$
S = 1.03
2199 reflections
88 parameters
0 restraints
0 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.024P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.62 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cu1	0.0000	0.0000	1.0000	0.0342 (2)
Br2	0.17788 (4)	0.00282 (7)	1.09313 (6)	0.03796 (18)
Br3	0.00212 (4)	0.25662 (7)	0.84636 (6)	0.04466 (19)
N1	0.1634 (3)	0.9201 (6)	0.4590 (4)	0.0399 (11)
H1E	0.1113	0.9760	0.4690	0.060*
H1C	0.1627	0.8100	0.4898	0.060*
H1D	0.1627	0.9216	0.3615	0.060*
C1	0.4344 (4)	1.0010 (7)	0.6360 (6)	0.0484 (16)
H1A	0.4396	1.1186	0.5994	0.058*
H1B	0.4905	0.9351	0.6282	0.058*
C2	0.4348 (5)	1.0087 (7)	0.8026 (6)	0.0525 (17)
H2A	0.4376	0.8909	0.8429	0.063*
H2B	0.4923	1.0709	0.8618	0.063*
C3	0.3442 (4)	1.1006 (8)	0.8188 (6)	0.0497 (16)
H3A	0.3442	1.0960	0.9247	0.060*
H3B	0.3459	1.2225	0.7906	0.060*
C4	0.2518 (4)	1.0177 (7)	0.7197 (5)	0.0389 (14)
H4A	0.1961	1.0857	0.7260	0.047*
H4B	0.2453	0.9006	0.7563	0.047*
C5	0.2537 (4)	1.0092 (6)	0.5542 (5)	0.0309 (12)
H5A	0.2542	1.1290	0.5166	0.037*
C6	0.3421 (4)	0.9158 (8)	0.5364 (5)	0.0400 (14)

H6A	0.3419	0.9197	0.4304	0.048*
H6B	0.3403	0.7941	0.5654	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0304 (6)	0.0312 (5)	0.0383 (5)	−0.0027 (4)	0.0055 (4)	0.0048 (4)
Br2	0.0322 (4)	0.0389 (3)	0.0412 (3)	−0.0035 (3)	0.0082 (3)	0.0022 (2)
Br3	0.0428 (4)	0.0384 (3)	0.0463 (3)	−0.0101 (3)	0.0026 (3)	0.0103 (3)
N1	0.031 (3)	0.046 (3)	0.039 (2)	0.005 (2)	0.004 (2)	0.006 (2)
C1	0.035 (4)	0.066 (4)	0.044 (3)	0.004 (3)	0.011 (3)	0.008 (3)
C2	0.043 (4)	0.066 (4)	0.039 (3)	−0.001 (3)	−0.002 (3)	−0.001 (3)
C3	0.060 (5)	0.052 (4)	0.037 (3)	−0.008 (3)	0.012 (3)	−0.015 (3)
C4	0.030 (4)	0.048 (4)	0.036 (3)	0.004 (3)	0.006 (3)	−0.004 (3)
C5	0.030 (3)	0.029 (3)	0.031 (3)	−0.001 (3)	0.006 (2)	0.001 (2)
C6	0.032 (4)	0.058 (4)	0.032 (3)	0.002 (3)	0.013 (3)	−0.005 (3)

Geometric parameters (Å, º)

Cu1—Br3$^{\rm i}$	2.4201 (6)	C2—H2A	0.9700
Cu1—Br3	2.4201 (6)	C2—H2B	0.9700
Cu1—Br2	2.4488 (9)	C3—C4	1.513 (7)
Cu1—Br2$^{\rm i}$	2.4488 (9)	C3—H3A	0.9700
N1—C5	1.500 (6)	C3—H3B	0.9700
N1—H1E	0.8900	C4—C5	1.525 (6)
N1—H1C	0.8900	C4—H4A	0.9700
N1—H1D	0.8900	C4—H4B	0.9700
C1—C6	1.521 (7)	C5—C6	1.507 (7)
C1—C2	1.525 (6)	C5—H5A	0.9800
C1—H1A	0.9700	C6—H6A	0.9700
C1—H1B	0.9700	C6—H6B	0.9700
C2—C3	1.525 (7)		
Br3$^{\rm i}$—Cu1—Br3	180.0	C4—C3—C2	112.0 (4)
Br3$^{\rm i}$—Cu1—Br2	89.59 (3)	C4—C3—H3A	109.2
Br3—Cu1—Br2	90.41 (3)	C2—C3—H3A	109.2
Br3$^{\rm i}$—Cu1—Br2$^{\rm i}$	90.41 (3)	C4—C3—H3B	109.2
Br3—Cu1—Br2$^{\rm i}$	89.59 (3)	C2—C3—H3B	109.2
Br2—Cu1—Br2$^{\rm i}$	180.000 (9)	H3A—C3—H3B	107.9
C5—N1—H1E	109.5	C3—C4—C5	110.3 (5)
C5—N1—H1C	109.5	C3—C4—H4A	109.6
H1E—N1—H1C	109.5	C5—C4—H4A	109.6
C5—N1—H1D	109.5	C3—C4—H4B	109.6
H1E—N1—H1D	109.5	C5—C4—H4B	109.6
H1C—N1—H1D	109.5	H4A—C4—H4B	108.1
C6—C1—C2	111.4 (5)	N1—C5—C6	109.6 (4)
C6—C1—H1A	109.3	N1—C5—C4	109.6 (4)
C2—C1—H1A	109.3	C6—C5—C4	112.8 (4)

C6—C1—H1B	109.3	N1—C5—H5A	108.3
C2—C1—H1B	109.3	C6—C5—H5A	108.3
H1A—C1—H1B	108.0	C4—C5—H5A	108.3
C3—C2—C1	111.1 (5)	C5—C6—C1	110.4 (4)
C3—C2—H2A	109.4	C5—C6—H6A	109.6
C1—C2—H2A	109.4	C1—C6—H6A	109.6
C3—C2—H2B	109.4	C5—C6—H6B	109.6
C1—C2—H2B	109.4	C1—C6—H6B	109.6
H2A—C2—H2B	108.0	H6A—C6—H6B	108.1

Symmetry code: (i) −*x*, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*D*···Br2^{ii}	0.89	2.60	3.474 (4)	166
N1—H1*C*···Br2^{iii}	0.89	2.56	3.445 (4)	174
N1—H1*E*···Br3^{iv}	0.89	2.62	3.341 (4)	138

Symmetry codes: (ii) *x*, *y*+1, *z*−1; (iii) *x*, −*y*+1/2, *z*−1/2; (iv) *x*, −*y*+3/2, *z*−1/2.