metal-organic compounds

1-Propylquinolinium triiodidocuprate(I)

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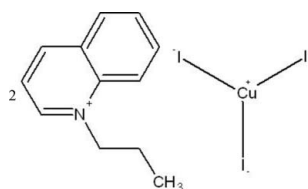Correspondence e-mail: zrchen@fzu.edu.cn

In the title compound, $(C_{12}H_{14}N)_2[CuI_3]$, the asymmetric unit contains two *N*-propylquinolinium cations which lie on opposite sides of the CuI_3^{2-} anion. In the anion, Cu—I bond distances lie in the range 2.5161 (13)–2.5529 (12) Å. All of the atoms in the anion are essentially coplanar, with an r.m.s. deviation from the $[CuI_3]^{2-}$ mean plane of 0.0001 Å. In the crystal structure, an extensive network of C—H···I hydrogen bonds links the cations and anions into an extended three-dimensional network, with the cations further aggregated through π–π stacking interactions [centroid–centroid distances 3.48 (7) and 3.43 (5) Å].

Related literature

For information on C—H···I hydrogen bonds, see Horn *et al.* (2003), and on π–π stacking, see Robin & Fromm (2006). For related literature, see: Huang & Xie (1988).

Experimental

Crystal data

$(C_{12}H_{14}N)_2[CuI]$
$M_r = 788.73$
Triclinic, $P\bar{1}$
$a = 9.4373$ (19) Å
$b = 9.5500$ (19) Å

$c = 16.175$ (3) Å
$\alpha = 81.27$ (3)°
$\beta = 76.03$ (3)°
$\gamma = 72.82$ (3)°
$V = 1346.4$ (5) Å^3

$Z = 2$
Mo $K\alpha$ radiation
$\mu = 4.26$ mm^{-1}

T = 293 (2) K
$0.20 \times 0.18 \times 0.16$ mm

Data collection

Rigaku R-AXIS RAPID Imaging Plate diffractometer
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
$T_{min} = 0.443$, $T_{max} = 0.506$

12812 measured reflections
6176 independent reflections
4121 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.149$
$S = 0.87$
6176 reflections

273 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.69$ e Å^{-3}
$\Delta\rho_{min} = -1.16$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···I2^i	0.97	3.09	4.046 (6)	167
C13—H13···I3^{ii}	0.93	3.04	3.871 (6)	150
C18—H18···I1^{iii}	0.93	3.08	3.986 (6)	165
C2—H2···I3^{iv}	0.93	3.16	3.852 (6)	133

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

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

References

Horn, C. J., Blake, A. J., Champness, N. R., Garau, A., Lippolis, V., Wilson, C. & Schröder, M. (2003). *Chem Commun.* pp. 312–313.
Huang, S. & Xie, R. G. (1988). *Preparation Manual of Organic Synthesis Reagents*, pp. 3498–3502. Chen Du: Sichuan University Press.
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supplementary materials

1-Propylquinolinium triiodidocuprate(I)

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Comment

In the title compound, (I) Fig. 1, the asymmetric unit contains two N-propylquinolinium cations which lie on opposite sides of the $CuI_3{}^{2-}$ anion. In the anion cluster, Cu—I bond distances lie in the range from 2.5161 (13) Å to 2.5529 (12)Å and the I1—Cu—I2, I2—Cu—I3 and I1—Cu—I3 bond angles are 124.29°, 117.02° and 118.69°, respectively. All of the atoms in the anion are essentially coplanar with an r.m.s. deviation from the $[CuI_3]^{2-}$ mean plane of 0.0001|%A. The inorganic and organic components are linked via C—H···I hydrogen bonds to give a three-dimensional network, Table 1. The cations are further aggregated through π-π stacking interactions with centroid to centroid distances of 3.48 (7)Å and 3.43 (5)Å respectively between the quinolinium rings, Fig 2.

Experimental

1-propylquinolinium iodide was prepared as reported in literature (Huang *et al.*, 1988). 1-propylquinolinium iodide (0.30 g, 1.0 mmol) and CuI (0.19 g, 1 mmol) were dissolved in 15 mL DMF and stirred for 20 min to give a clear red solution which was filtered and allowed to evaporate at room temperature. Red block-like crystals formed over one, week in 65% yield. (0.32 g). Calcd. For $C_{24}H_{28}CuI_3N_2$ (788.73): C, 36.40 H, 3.52 N, 3.53% Found: C, 36.51 H, 3.55 N, 3.55%.

Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for aromatic H atoms 0.97 Å for methylene H atoms and 0.96 Å for methyl H atoms, respectively, and with $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic and methylene H atoms, $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms.
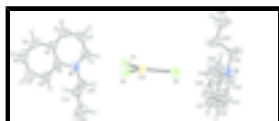
Figures

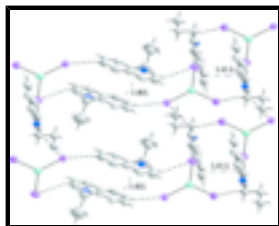Fig. 1. The structure of (I) showing the atom numbering with ellipsoids drawn at the 50% probability level.

Fig. 2. Crystal packing for (I) with hydrogen bonds drawn as dashed lines.

supplementary materials

1-Propylquinolinium triiodidocuprate(I)

Crystal data

$(C_{12}H_{14}N)_2[CuI_3]$	$Z = 2$
$M_r = 788.73$	$F_{000} = 748.0$
Triclinic, $P\bar{1}$	$D_x = 1.945$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.4373$ (19) Å	Cell parameters from 18 reflections
$b = 9.5500$ (19) Å	$\theta = 12–15°$
$c = 16.175$ (3) Å	$\mu = 4.26$ mm^{-1}
$\alpha = 81.27$ (3)°	$T = 293$ (2) K
$\beta = 76.03$ (3)°	Block, red
$\gamma = 72.82$ (3)°	$0.20 \times 0.18 \times 0.16$ mm
$V = 1346.4$ (5) Å^3	

Data collection

Rigaku R-AXIS RAPID Imaging Plate diffractometer	6176 independent reflections
Radiation source: rotor target	4121 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.052$
$T = 293(2)$ K	$\theta_{max} = 27.5°$
ω scans	$\theta_{min} = 3.1°$
Absorption correction: multi-scan (TEXRAY; Molecular Structure Corporation, 1999)	$h = -12 \rightarrow 12$
$T_{min} = 0.443$, $T_{max} = 0.506$	$k = -12 \rightarrow 12$
12812 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.149$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.87$	$\Delta\rho_{max} = 0.69$ e Å^{-3}
6176 reflections	$\Delta\rho_{min} = -1.16$ e Å^{-3}
273 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0010 (2)
Secondary atom site location: difference Fourier map	

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\AA^2$)

	x	y	z	$U_{iso}*/U_{eq}$
I1	0.55819 (5)	−0.00607 (5)	0.24539 (3)	0.05558 (16)
I2	0.40382 (5)	0.46869 (5)	0.18593 (3)	0.05692 (16)
I3	0.09917 (5)	0.25384 (6)	0.36757 (3)	0.06252 (17)
Cu1	0.35344 (9)	0.23210 (9)	0.26816 (5)	0.0511 (2)
N2	−0.2782 (5)	0.2353 (6)	0.5522 (3)	0.0471 (12)
N1	0.8453 (5)	0.2573 (6)	0.0483 (3)	0.0459 (11)
C1	0.8245 (8)	0.2374 (8)	0.1316 (5)	0.0577 (17)
H1	0.7371	0.2131	0.1627	0.069*
C2	0.9279 (9)	0.2515 (10)	0.1745 (5)	0.067 (2)
H2	0.9104	0.2371	0.2338	0.081*
C3	1.0563 (9)	0.2868 (9)	0.1292 (5)	0.0648 (19)
H3	1.1266	0.2971	0.1578	0.078*
C4	1.0827 (7)	0.3074 (7)	0.0405 (5)	0.0508 (15)
C5	1.2143 (8)	0.3423 (8)	−0.0111 (6)	0.0625 (19)
H5	1.2860	0.3564	0.0150	0.075*
C6	1.2376 (9)	0.3554 (9)	−0.0963 (6)	0.073 (2)
H6	1.3282	0.3712	−0.1287	0.087*
C7	1.1263 (9)	0.3454 (9)	−0.1371 (5)	0.067 (2)
H7	1.1419	0.3597	−0.1964	0.080*
C8	0.9949 (8)	0.3150 (8)	−0.0912 (5)	0.0538 (16)
H8	0.9211	0.3096	−0.1188	0.065*
C9	0.9736 (6)	0.2920 (6)	−0.0016 (4)	0.0422 (13)
C10	0.7275 (7)	0.2378 (7)	0.0078 (4)	0.0498 (15)
H10A	0.7120	0.3132	−0.0391	0.060*
H10B	0.6325	0.2504	0.0494	0.060*
C11	0.7708 (8)	0.0875 (8)	−0.0257 (5)	0.0581 (17)
H11A	0.8718	0.0690	−0.0617	0.070*
H11B	0.7723	0.0122	0.0219	0.070*
C12	0.6596 (10)	0.0795 (10)	−0.0766 (7)	0.080 (3)
H12A	0.6887	−0.0160	−0.0973	0.119*
H12B	0.6591	0.1532	−0.1241	0.119*
H12C	0.5600	0.0963	−0.0407	0.119*
C13	−0.3068 (8)	0.1201 (8)	0.5292 (5)	0.0596 (18)
H13	−0.2979	0.0339	0.5655	0.071*
C14	−0.3501 (9)	0.1256 (9)	0.4519 (6)	0.069 (2)
H14	−0.3675	0.0432	0.4364	0.083*
C15	−0.3662 (8)	0.2494 (9)	0.4005 (5)	0.0636 (19)
H15	−0.3962	0.2535	0.3493	0.076*

C16	−0.3382 (7)	0.3746 (8)	0.4227 (4)	0.0539 (16)
C17	−0.3528 (8)	0.5081 (11)	0.3699 (5)	0.070 (2)
H17	−0.3844	0.5166	0.3188	0.084*
C18	−0.3207 (9)	0.6242 (9)	0.3934 (6)	0.071 (2)
H18	−0.3310	0.7119	0.3585	0.085*
C19	−0.2729 (9)	0.6120 (9)	0.4690 (6)	0.070 (2)
H19	−0.2492	0.6920	0.4832	0.084*
C20	−0.2590 (7)	0.4888 (8)	0.5234 (5)	0.0540 (16)
H20	−0.2290	0.4847	0.5746	0.065*
C21	−0.2914 (6)	0.3660 (7)	0.5004 (4)	0.0405 (12)
C22	−0.2312 (8)	0.2202 (9)	0.6344 (4)	0.0589 (18)
H22A	−0.2700	0.1451	0.6725	0.071*
H22B	−0.2744	0.3124	0.6607	0.071*
C23	−0.0588 (8)	0.1787 (10)	0.6223 (5)	0.068 (2)
H23A	−0.0150	0.0869	0.5955	0.082*
H23B	−0.0196	0.2543	0.5850	0.082*
C24	−0.0146 (11)	0.1621 (15)	0.7068 (7)	0.104 (4)
H24A	0.0939	0.1359	0.6984	0.157*
H24B	−0.0524	0.0863	0.7433	0.157*
H24C	−0.0569	0.2534	0.7328	0.157*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0505 (3)	0.0452 (3)	0.0663 (3)	−0.01132 (19)	−0.0080 (2)	−0.0006 (2)
I2	0.0560 (3)	0.0485 (3)	0.0628 (3)	−0.0133 (2)	−0.0149 (2)	0.0082 (2)
I3	0.0488 (3)	0.0813 (4)	0.0485 (3)	−0.0122 (2)	−0.00168 (19)	−0.0029 (2)
Cu1	0.0473 (4)	0.0574 (5)	0.0480 (5)	−0.0128 (4)	−0.0118 (3)	−0.0015 (4)
N2	0.037 (2)	0.055 (3)	0.046 (3)	−0.012 (2)	−0.005 (2)	−0.001 (2)
N1	0.039 (2)	0.051 (3)	0.046 (3)	−0.012 (2)	−0.008 (2)	−0.003 (2)
C1	0.061 (4)	0.064 (5)	0.047 (4)	−0.020 (3)	−0.009 (3)	0.004 (3)
C2	0.075 (5)	0.088 (6)	0.040 (4)	−0.027 (4)	−0.016 (3)	0.010 (4)
C3	0.071 (5)	0.066 (5)	0.065 (5)	−0.018 (4)	−0.033 (4)	0.001 (4)
C4	0.051 (3)	0.049 (4)	0.055 (4)	−0.013 (3)	−0.016 (3)	−0.006 (3)
C5	0.043 (3)	0.061 (5)	0.086 (6)	−0.018 (3)	−0.010 (3)	−0.011 (4)
C6	0.056 (4)	0.068 (5)	0.089 (7)	−0.028 (4)	0.016 (4)	−0.018 (4)
C7	0.076 (5)	0.070 (5)	0.047 (4)	−0.025 (4)	0.011 (4)	−0.010 (4)
C8	0.055 (4)	0.055 (4)	0.052 (4)	−0.020 (3)	−0.003 (3)	−0.007 (3)
C9	0.043 (3)	0.035 (3)	0.046 (4)	−0.007 (2)	−0.008 (2)	−0.006 (3)
C10	0.040 (3)	0.057 (4)	0.054 (4)	−0.014 (3)	−0.015 (3)	0.003 (3)
C11	0.057 (4)	0.050 (4)	0.072 (5)	−0.014 (3)	−0.020 (3)	−0.010 (4)
C12	0.074 (5)	0.068 (5)	0.108 (8)	−0.022 (4)	−0.030 (5)	−0.016 (5)
C13	0.055 (4)	0.048 (4)	0.071 (5)	−0.013 (3)	−0.011 (3)	0.006 (3)
C14	0.066 (5)	0.068 (5)	0.087 (6)	−0.023 (4)	−0.028 (4)	−0.018 (5)
C15	0.055 (4)	0.082 (6)	0.058 (5)	−0.017 (4)	−0.013 (3)	−0.021 (4)
C16	0.036 (3)	0.076 (5)	0.045 (4)	−0.013 (3)	−0.004 (2)	−0.006 (3)
C17	0.042 (3)	0.103 (7)	0.052 (5)	−0.014 (4)	−0.011 (3)	0.019 (4)
C18	0.056 (4)	0.064 (5)	0.076 (6)	−0.010 (4)	−0.008 (4)	0.025 (4)

C19	0.053 (4)	0.053 (4)	0.094 (7)	−0.017 (3)	−0.001 (4)	0.003 (4)
C20	0.047 (3)	0.055 (4)	0.060 (4)	−0.014 (3)	−0.006 (3)	−0.011 (3)
C21	0.032 (3)	0.049 (3)	0.039 (3)	−0.014 (2)	−0.003 (2)	−0.001 (3)
C22	0.063 (4)	0.084 (5)	0.032 (3)	−0.024 (4)	−0.014 (3)	0.001 (3)
C23	0.058 (4)	0.085 (6)	0.062 (5)	−0.016 (4)	−0.020 (3)	−0.001 (4)
C24	0.078 (6)	0.161 (11)	0.074 (7)	−0.018 (6)	−0.040 (5)	0.003 (7)

Geometric parameters (Å, °)

I1—Cu1	2.5213 (14)	C11—H11B	0.9700
I2—Cu1	2.5529 (12)	C12—H12A	0.9600
I3—Cu1	2.5161 (13)	C12—H12B	0.9600
N2—C13	1.331 (9)	C12—H12C	0.9600
N2—C21	1.385 (8)	C13—C14	1.396 (11)
N2—C22	1.474 (8)	C13—H13	0.9300
N1—C1	1.306 (9)	C14—C15	1.330 (12)
N1—C9	1.382 (8)	C14—H14	0.9300
N1—C10	1.487 (7)	C15—C16	1.411 (10)
C1—C2	1.373 (10)	C15—H15	0.9300
C1—H1	0.9300	C16—C21	1.413 (9)
C2—C3	1.362 (11)	C16—C17	1.414 (11)
C2—H2	0.9300	C17—C18	1.358 (12)
C3—C4	1.390 (11)	C17—H17	0.9300
C3—H3	0.9300	C18—C19	1.381 (12)
C4—C9	1.414 (8)	C18—H18	0.9300
C4—C5	1.418 (10)	C19—C20	1.351 (11)
C5—C6	1.333 (13)	C19—H19	0.9300
C5—H5	0.9300	C20—C21	1.416 (9)
C6—C7	1.400 (12)	C20—H20	0.9300
C6—H6	0.9300	C22—C23	1.527 (10)
C7—C8	1.370 (10)	C22—H22A	0.9700
C7—H7	0.9300	C22—H22B	0.9700
C8—C9	1.407 (9)	C23—C24	1.496 (11)
C8—H8	0.9300	C23—H23A	0.9700
C10—C11	1.518 (9)	C23—H23B	0.9700
C10—H10A	0.9700	C24—H24A	0.9600
C10—H10B	0.9700	C24—H24B	0.9600
C11—C12	1.506 (10)	C24—H24C	0.9600
C11—H11A	0.9700		
I3—Cu1—I1	124.29 (5)	H12A—C12—H12B	109.5
I3—Cu1—I2	117.02 (5)	C11—C12—H12C	109.5
I1—Cu1—I2	118.69 (4)	H12A—C12—H12C	109.5
C13—N2—C21	121.1 (6)	H12B—C12—H12C	109.5
C13—N2—C22	118.3 (6)	N2—C13—C14	121.5 (7)
C21—N2—C22	120.6 (6)	N2—C13—H13	119.3
C1—N1—C9	121.8 (5)	C14—C13—H13	119.3
C1—N1—C10	117.8 (5)	C15—C14—C13	119.6 (7)
C9—N1—C10	120.4 (5)	C15—C14—H14	120.2
N1—C1—C2	121.9 (6)	C13—C14—H14	120.2

N1—C1—H1	119.1	C14—C15—C16	120.8 (7)
C2—C1—H1	119.1	C14—C15—H15	119.6
C3—C2—C1	119.3 (7)	C16—C15—H15	119.6
C3—C2—H2	120.3	C15—C16—C21	118.9 (7)
C1—C2—H2	120.3	C15—C16—C17	122.8 (7)
C2—C3—C4	120.3 (6)	C21—C16—C17	118.3 (7)
C2—C3—H3	119.9	C18—C17—C16	120.4 (7)
C4—C3—H3	119.9	C18—C17—H17	119.8
C3—C4—C9	118.8 (6)	C16—C17—H17	119.8
C3—C4—C5	123.6 (6)	C17—C18—C19	120.1 (7)
C9—C4—C5	117.6 (7)	C17—C18—H18	120.0
C6—C5—C4	121.5 (7)	C19—C18—H18	120.0
C6—C5—H5	119.2	C20—C19—C18	122.8 (8)
C4—C5—H5	119.2	C20—C19—H19	118.6
C5—C6—C7	120.3 (7)	C18—C19—H19	118.6
C5—C6—H6	119.8	C19—C20—C21	118.3 (7)
C7—C6—H6	119.8	C19—C20—H20	120.8
C8—C7—C6	121.2 (8)	C21—C20—H20	120.8
C8—C7—H7	119.4	N2—C21—C16	118.2 (6)
C6—C7—H7	119.4	N2—C21—C20	121.8 (6)
C7—C8—C9	118.8 (7)	C16—C21—C20	120.1 (6)
C7—C8—H8	120.6	N2—C22—C23	111.4 (6)
C9—C8—H8	120.6	N2—C22—H22A	109.3
N1—C9—C8	121.6 (5)	C23—C22—H22A	109.3
N1—C9—C4	117.9 (6)	N2—C22—H22B	109.3
C8—C9—C4	120.5 (6)	C23—C22—H22B	109.3
N1—C10—C11	112.3 (5)	H22A—C22—H22B	108.0
N1—C10—H10A	109.2	C24—C23—C22	110.2 (7)
C11—C10—H10A	109.2	C24—C23—H23A	109.6
N1—C10—H10B	109.2	C22—C23—H23A	109.6
C11—C10—H10B	109.2	C24—C23—H23B	109.6
H10A—C10—H10B	107.9	C22—C23—H23B	109.6
C12—C11—C10	110.6 (6)	H23A—C23—H23B	108.1
C12—C11—H11A	109.5	C23—C24—H24A	109.5
C10—C11—H11A	109.5	C23—C24—H24B	109.5
C12—C11—H11B	109.5	H24A—C24—H24B	109.5
C10—C11—H11B	109.5	C23—C24—H24C	109.5
H11A—C11—H11B	108.1	H24A—C24—H24C	109.5
C11—C12—H12A	109.5	H24B—C24—H24C	109.5
C11—C12—H12B	109.5		

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···I2[i]	0.97	3.09	4.046 (6)	167
C13—H13···I3[ii]	0.93	3.04	3.871 (6)	150
C18—H18···I1[iii]	0.93	3.08	3.986 (6)	165
C2—H2···I3[iv]	0.93	3.16	3.852 (6)	133

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

Fig. 1

Fig. 2