Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis{4-[4-(dimethylamino)styryl]-1-ethylpyridinium} di-μ-iodido-bis[iodidocuprate(II)]

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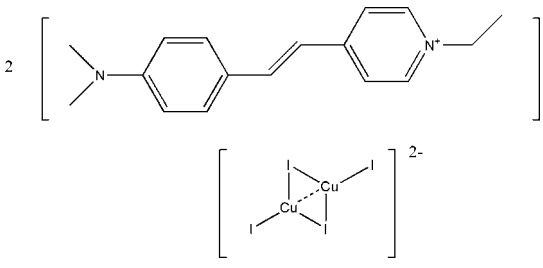
Received 6 September 2007; accepted 15 October 2007

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.080; data-to-parameter ratio = 21.9.

The title compound, $(C_{17}H_{21}N_2)_2[Cu_2I_4]$, consists of an organic cation, 4-[4-(dimethylamino)styryl]-1-ethylpyrdinium, and an inorganic anion, $[Cu_2I_4]^{2-}$. The Cu(I) atom exhibits a trigonal coordination. The anions form discrete centrosymmetric dimers about inversion centers and are surrounded by the cations.

Related literature

For related literature, see: Asplund *et al.* (1982); Cariati *et al.* (2001); Guloy *et al.* (2001); Mehrotra & Hoffmann (1978).



Experimental

Crystal data

$(C_{17}H_{21}N_2)_2[Cu_2I_4]$
M_r = 1141.42
Monoclinic, $P2_1/c$
a = 10.707 (4) Å
b = 7.367 (4) Å
c = 24.127 (9) Å
β = 90.908 (14)°
V = 1902.9 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.39 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID imaging plate diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.645, T_{max} = 0.651
18111 measured reflections
4356 independent reflections
3506 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.081
S = 1.05
4356 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

Table 1
Selected geometric parameters (Å, °) .

Cu1—I2	2.5019 (9)	Cu1—I1^{i}	2.5800 (10)
Cu1—I1	2.5731 (9)		
I2—Cu1—I1	124.42 (3)	I1—Cu1—Cu1^{i}	57.15 (2)
I2—Cu1—I1^{i}	121.38 (3)	I1^{i}—Cu1—Cu1^{i}	56.91 (3)
I1—Cu1—I1^{i}	114.05 (3)	Cu1—I1—Cu1^{i}	65.95 (3)
I2—Cu1—Cu1^{i}	176.04 (4)		

Symmetry code: (i) $-x, -y+2, -z+1$.

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*.

We are grateful for financial support from the National Natural Science Foundation of China (No. 0041814161).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2032).

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supplementary materials

Acta Cryst. (2007). E**63**, m2957 [**doi:10.1107/S160053680705074X**]

Bis{4-[4-(dimethylamino)styryl]-1-ethylpyridinium} di-μ-iodido-bis[iodidocuprate(II)]

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Comment

Organic-inorganic complex materials have received extensive attention in recent years owing to their interesting crystal structure and some special properties, such as nonlinear optical response (Cariati *et al.*, 2001) and luminescence (Guloy *et al.*, 2001). 4-(4-(Dimethylamino) stryl)-1-ethylpyrdinium iodide possesses large conjugation system, which will be beneficial to the nonlinera optical response. In order to understand this phenomenon better, we present here the synthesis and the structure of the title compound, (I).

As shown in Fig. 1, the crystal structure of (I) consists of an organic cation, 4-(4-(dimethylmino)stryl)-1-ethylpridinium and an in-organic anion, $[Cu_2I_4]^{2-}$. The configuration of the anion is similar to that of $[Cu_2I_4]^{2-}$ anion reported in the tetrabutylammonium salt (Asplund *et al.*, 1982). There are, however, somewhat smaller differences between the Cu—$I_{terminal}$ and Cu—$I_{bridging}$ ligand distances in the anion reported in tetrabutylammonium salt and in (I), *i.e.* Cu—$I_{terminal}$ = 2.514 (2) Å, Cu—$I_{bridging}$ = 2.566 (2) and 2.592 (2)Å in the tetrabutylammonium salt compared to 2.5019 (9), 2.5731 (9) and 2.5800 (10) Å, respectively, in (I). Moreover, the distance d(Cu—Cu) in (I), 2.8046 (13) Å, is slightly longer than that in the tetrabutylammonium salt. It seems that the Cu···Cu distance is longer than the shortest possible distance for the given coordination, but that the value 2.8046 (13) Å in (I) indicates a weak attractive Cu(I)—Cu(I) interaction (Mehrotra *et al.*, 1978). In the crystal structure, the organic cations are surround by the anions which form centrosymmetric dimers about inversion centers resulting in the organic-inorganic complex structure.

Experimental

All chemicals and reagents were analytical grade available commercially and were used without further purfication. The title compound was prepared by self-assembling reaction of CuI with 4-(4-(dimethylmino)stryl)-1-ethyl- pridinium iodide. 4-(4-(Dimethylmino)stryl)-1-ethylpridinium iodide (0.19 g, 0.5 mmol) and CuI (0.095 g, 0.5 mmol) were dissolved in 8 ml dimethylformamide (DMF). The mixed solution was stirred still clear, with the pH value being adjusted to 6 by the addition of 10% HI/DMF solution and then filtered. The resulting solution was kept at room temperature for five days to obtain brown block crystals.

Figures

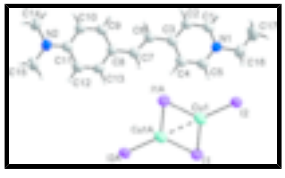


Fig. 1. The molecular structure of (I), with atomic labels and 50% probability displacement ellipsoids for non-H atoms. The codes A in the symmetry related atoms of the anions is generatd by the symmertry operation (−*x*, −*y* + 2, −*z* + 1)

Bis{4-[4-(dimethylamino)styryl]-1-ethylpyridinium} di-μ-iodido-bis[iodidocuprate(II)]

Crystal data

$(C_{17}H_{21}N_2)_2[Cu_2I_4]$	F_{000} = 1088.0
M_r = 1141.42	D_x = 1.992 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 14979 reflections
a = 10.707 (4) Å	θ = 3.2–27.5º
b = 7.367 (4) Å	μ = 4.39 mm^{-1}
c = 24.127 (9) Å	T = 293 (2) K
β = 90.908 (14)º	Block, brown
V = 1902.9 (14) Å^3	0.10 × 0.10 × 0.10 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID Imaging Plate diffractometer	4356 independent reflections
Radiation source: fine-focus sealed tube	3506 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.079
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan (Higash, 1995)	h = −13→13
T_{min} = 0.645, T_{max} = 0.651	k = −9→9
18111 measured reflections	l = −31→31

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.034	H-atom parameters constrained
$wR(F^2)$ = 0.081	$w = 1/[\sigma^2(F_o^2) + 0.277P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.002
4356 reflections	$\Delta\rho_{max}$ = 0.57 e Å^{-3}
199 parameters	$\Delta\rho_{min}$ = −0.68 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	−0.02181 (5)	0.88384 (8)	0.54486 (2)	0.06562 (15)
N1	0.2231 (2)	0.2381 (5)	0.60271 (12)	0.0512 (7)
N2	0.7093 (3)	0.3834 (5)	0.22097 (13)	0.0654 (9)
I1	0.16416 (2)	0.84431 (4)	0.479695 (11)	0.06287 (10)
I2	−0.05789 (2)	0.69481 (4)	0.629255 (10)	0.06314 (10)
C1	0.3368 (3)	0.1598 (6)	0.60262 (15)	0.0605 (10)
H1A	0.3621	0.0889	0.6326	0.073*
C2	0.4154 (3)	0.1826 (6)	0.55930 (15)	0.0594 (10)
H2A	0.4945	0.1308	0.5608	0.071*
C3	0.3792 (3)	0.2816 (5)	0.51307 (13)	0.0465 (7)
C4	0.2609 (3)	0.3617 (5)	0.51481 (14)	0.0497 (8)
H4A	0.2329	0.4322	0.4851	0.060*
C5	0.1864 (3)	0.3379 (5)	0.55932 (14)	0.0536 (9)
H5A	0.1081	0.3924	0.5595	0.064*
C6	0.4607 (3)	0.2970 (5)	0.46644 (14)	0.0505 (8)
H6A	0.5424	0.2567	0.4714	0.061*
C7	0.4299 (3)	0.3635 (5)	0.41694 (14)	0.0517 (8)
H7A	0.3492	0.4092	0.4133	0.062*
C8	0.5049 (3)	0.3738 (5)	0.36851 (14)	0.0478 (8)
C9	0.6319 (3)	0.3220 (5)	0.36681 (14)	0.0501 (8)
H9A	0.6717	0.2850	0.3994	0.060*
C10	0.6976 (3)	0.3246 (5)	0.31940 (14)	0.0534 (9)
H10A	0.7807	0.2876	0.3204	0.064*
C11	0.6443 (3)	0.3813 (5)	0.26860 (14)	0.0493 (8)
C12	0.5181 (3)	0.4374 (6)	0.27021 (14)	0.0591 (10)
H12A	0.4786	0.4786	0.2380	0.071*
C13	0.4540 (3)	0.4320 (6)	0.31796 (15)	0.0605 (10)
H13A	0.3711	0.4694	0.3171	0.073*
C14	0.8395 (4)	0.3222 (7)	0.21911 (19)	0.0844 (15)
H14A	0.8681	0.2915	0.2558	0.127*
H14B	0.8906	0.4177	0.2046	0.127*
H14C	0.8451	0.2174	0.1956	0.127*
C15	0.6530 (4)	0.4375 (8)	0.16883 (16)	0.0840 (15)

H15A	0.5687	0.4767	0.1748	0.126*
H15B	0.6526	0.3364	0.1437	0.126*
H15C	0.7001	0.5354	0.1533	0.126*
C16	0.1340 (4)	0.2066 (7)	0.64840 (17)	0.0749 (13)
H16A	0.0757	0.3074	0.6492	0.090*
H16B	0.0863	0.0978	0.6400	0.090*
C17	0.1902 (4)	0.1865 (8)	0.70363 (17)	0.0846 (15)
H17A	0.1257	0.1675	0.7302	0.127*
H17B	0.2360	0.2946	0.7130	0.127*
H17C	0.2459	0.0844	0.7039	0.127*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0730 (3)	0.0628 (4)	0.0608 (3)	0.0051 (3)	−0.0046 (2)	0.0030 (2)
N1	0.0456 (14)	0.057 (2)	0.0505 (15)	−0.0001 (14)	0.0014 (13)	0.0024 (14)
N2	0.0533 (16)	0.095 (3)	0.0483 (16)	−0.0006 (17)	0.0045 (15)	0.0059 (16)
I1	0.06111 (15)	0.05589 (18)	0.07167 (17)	0.01157 (12)	0.00291 (13)	0.00773 (12)
I2	0.05782 (15)	0.0763 (2)	0.05521 (15)	0.01122 (12)	−0.00368 (12)	0.00891 (12)
C1	0.0540 (19)	0.073 (3)	0.054 (2)	0.0093 (19)	−0.0013 (17)	0.0118 (18)
C2	0.0445 (17)	0.079 (3)	0.055 (2)	0.0116 (18)	−0.0008 (16)	0.0060 (19)
C3	0.0469 (16)	0.046 (2)	0.0466 (17)	−0.0033 (15)	−0.0019 (15)	−0.0040 (15)
C4	0.0581 (19)	0.047 (2)	0.0437 (16)	0.0083 (16)	−0.0016 (15)	−0.0035 (14)
C5	0.0477 (17)	0.060 (3)	0.0528 (19)	0.0081 (16)	−0.0018 (16)	−0.0072 (17)
C6	0.0432 (15)	0.058 (2)	0.0501 (18)	0.0031 (16)	−0.0001 (15)	−0.0037 (16)
C7	0.0489 (17)	0.054 (2)	0.0524 (18)	−0.0021 (16)	−0.0045 (16)	−0.0025 (16)
C8	0.0448 (16)	0.051 (2)	0.0471 (17)	−0.0007 (15)	0.0027 (15)	−0.0022 (15)
C9	0.0481 (16)	0.057 (2)	0.0456 (17)	−0.0023 (16)	−0.0063 (15)	0.0036 (15)
C10	0.0418 (15)	0.062 (3)	0.056 (2)	−0.0006 (16)	−0.0014 (16)	−0.0009 (17)
C11	0.0454 (16)	0.053 (2)	0.0499 (18)	−0.0024 (15)	0.0001 (15)	0.0000 (15)
C12	0.0528 (19)	0.078 (3)	0.0458 (17)	0.0059 (19)	−0.0044 (16)	0.0065 (17)
C13	0.0400 (16)	0.082 (3)	0.060 (2)	0.0109 (18)	−0.0017 (16)	0.005 (2)
C14	0.061 (2)	0.121 (5)	0.072 (3)	0.014 (3)	0.021 (2)	0.011 (3)
C15	0.078 (3)	0.121 (5)	0.053 (2)	0.003 (3)	0.007 (2)	0.016 (2)
C16	0.056 (2)	0.097 (4)	0.072 (3)	−0.007 (2)	0.017 (2)	0.012 (2)
C17	0.085 (3)	0.115 (5)	0.054 (2)	−0.020 (3)	0.015 (2)	−0.006 (2)

Geometric parameters (Å, °)

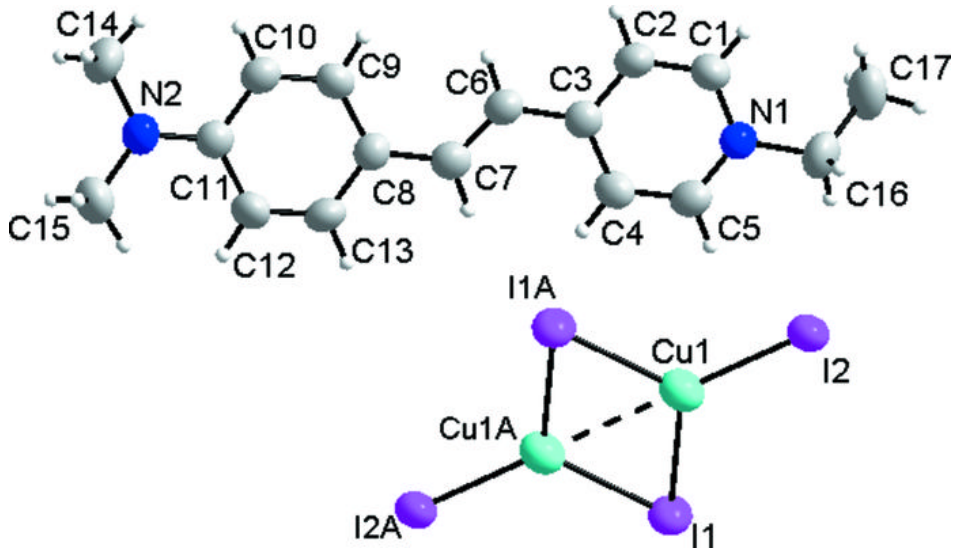
Cu1—I2	2.5019 (9)	C7—H7A	0.9300
Cu1—I1	2.5731 (9)	C8—C13	1.395 (5)
Cu1—I1^{i}	2.5800 (10)	C8—C9	1.414 (5)
Cu1—Cu1^{i}	2.8046 (13)	C9—C10	1.352 (4)
N1—C5	1.333 (5)	C9—H9A	0.9300
N1—C1	1.347 (4)	C10—C11	1.407 (5)
N1—C16	1.488 (4)	C10—H10A	0.9300
N2—C11	1.353 (4)	C11—C12	1.414 (5)
N2—C15	1.443 (5)	C12—C13	1.351 (5)

N2—C14	1.466 (5)	C12—H12A	0.9300
I1—Cu1^{i}	2.5800 (10)	C13—H13A	0.9300
C1—C2	1.362 (5)	C14—H14A	0.9600
C1—H1A	0.9300	C14—H14B	0.9600
C2—C3	1.383 (5)	C14—H14C	0.9600
C2—H2A	0.9300	C15—H15A	0.9600
C3—C4	1.398 (5)	C15—H15B	0.9600
C3—C6	1.439 (4)	C15—H15C	0.9600
C4—C5	1.359 (5)	C16—C17	1.461 (6)
C4—H4A	0.9300	C16—H16A	0.9700
C5—H5A	0.9300	C16—H16B	0.9700
C6—C7	1.328 (5)	C17—H17A	0.9600
C6—H6A	0.9300	C17—H17B	0.9600
C7—C8	1.430 (4)	C17—H17C	0.9600
I2—Cu1—I1	124.42 (3)	C10—C9—H9A	118.9
I2—Cu1—I1^{i}	121.38 (3)	C8—C9—H9A	118.9
I1—Cu1—I1^{i}	114.05 (3)	C9—C10—C11	122.1 (3)
I2—Cu1—Cu1^{i}	176.04 (4)	C9—C10—H10A	118.9
I1—Cu1—Cu1^{i}	57.15 (2)	C11—C10—H10A	118.9
I1^{i}—Cu1—Cu1^{i}	56.91 (3)	N2—C11—C10	122.4 (3)
C5—N1—C1	119.3 (3)	N2—C11—C12	121.7 (3)
C5—N1—C16	118.9 (3)	C10—C11—C12	116.0 (3)
C1—N1—C16	121.7 (3)	C13—C12—C11	120.9 (3)
C11—N2—C15	122.0 (3)	C13—C12—H12A	119.6
C11—N2—C14	121.7 (3)	C11—C12—H12A	119.6
C15—N2—C14	116.3 (3)	C12—C13—C8	123.9 (3)
Cu1—I1—Cu1^{i}	65.95 (3)	C12—C13—H13A	118.0
N1—C1—C2	121.2 (3)	C8—C13—H13A	118.0
N1—C1—H1A	119.4	N2—C14—H14A	109.5
C2—C1—H1A	119.4	N2—C14—H14B	109.5
C1—C2—C3	121.0 (3)	H14A—C14—H14B	109.5
C1—C2—H2A	119.5	N2—C14—H14C	109.5
C3—C2—H2A	119.5	H14A—C14—H14C	109.5
C2—C3—C4	116.2 (3)	H14B—C14—H14C	109.5
C2—C3—C6	120.4 (3)	N2—C15—H15A	109.5
C4—C3—C6	123.4 (3)	N2—C15—H15B	109.5
C5—C4—C3	120.8 (3)	H15A—C15—H15B	109.5
C5—C4—H4A	119.6	N2—C15—H15C	109.5
C3—C4—H4A	119.6	H15A—C15—H15C	109.5
N1—C5—C4	121.5 (3)	H15B—C15—H15C	109.5
N1—C5—H5A	119.3	C17—C16—N1	115.6 (3)
C4—C5—H5A	119.3	C17—C16—H16A	108.4
C7—C6—C3	126.0 (3)	N1—C16—H16A	108.4
C7—C6—H6A	117.0	C17—C16—H16B	108.4
C3—C6—H6A	117.0	N1—C16—H16B	108.4
C6—C7—C8	128.3 (3)	H16A—C16—H16B	107.5
C6—C7—H7A	115.9	C16—C17—H17A	109.5

C8—C7—H7A	115.9	C16—C17—H17B	109.5
C13—C8—C9	114.8 (3)	H17A—C17—H17B	109.5
C13—C8—C7	120.9 (3)	C16—C17—H17C	109.5
C9—C8—C7	124.2 (3)	H17A—C17—H17C	109.5
C10—C9—C8	122.3 (3)	H17B—C17—H17C	109.5
I2—Cu1—I1—Cu1^{i}	−175.63 (4)	C13—C8—C9—C10	−1.7 (6)
I1^{i}—Cu1—I1—Cu1^{i}	0.0	C7—C8—C9—C10	176.3 (4)
C5—N1—C1—C2	0.8 (6)	C8—C9—C10—C11	0.9 (6)
C16—N1—C1—C2	176.8 (4)	C15—N2—C11—C10	178.4 (4)
N1—C1—C2—C3	−2.4 (7)	C14—N2—C11—C10	1.4 (6)
C1—C2—C3—C4	2.6 (6)	C15—N2—C11—C12	−1.9 (6)
C1—C2—C3—C6	−176.9 (4)	C14—N2—C11—C12	−178.9 (4)
C2—C3—C4—C5	−1.5 (5)	C9—C10—C11—N2	−179.7 (4)
C6—C3—C4—C5	178.0 (3)	C9—C10—C11—C12	0.6 (6)
C1—N1—C5—C4	0.3 (6)	N2—C11—C12—C13	179.1 (4)
C16—N1—C5—C4	−175.8 (4)	C10—C11—C12—C13	−1.3 (6)
C3—C4—C5—N1	0.1 (6)	C11—C12—C13—C8	0.4 (7)
C2—C3—C6—C7	169.0 (4)	C9—C8—C13—C12	1.0 (6)
C4—C3—C6—C7	−10.5 (6)	C7—C8—C13—C12	−177.0 (4)
C3—C6—C7—C8	−176.6 (4)	C5—N1—C16—C17	−148.8 (4)
C6—C7—C8—C13	173.7 (4)	C1—N1—C16—C17	35.2 (6)
C6—C7—C8—C9	−4.1 (6)		

Symmetry codes: (i) −*x*, −*y*+2, −*z*+1.

Fig. 1


C14
C10
C9
N2
C6
C3
C2
C1
C17
N1
C11
C8
C7
C16
C15
C12
C13
C4
C5
I1A
Cu1
I2
Cu1A
I2A
I1