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Bis[iododibis(1,10-phenanthroline-κ^2N,N')copper(II)] tetraiodidocadmate(II)

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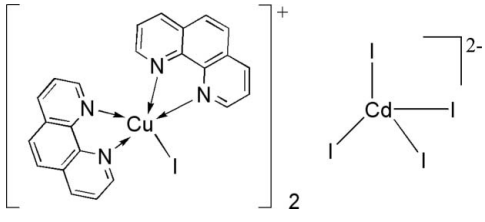
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.006 Å; R factor = 0.033; wR factor = 0.085; data-to-parameter ratio = 19.7.

A new mixed-metal complex, $[CuI(C_{12}H_8N_2)_2]_2[CdI_4]$, with an asymmetric unit consisting of one $[CuI(phen)_2]^+$ cation (phen = 1,10-phenanthroline) and half of a $[CdI_4]^{2-}$ anion lying on a twofold rotation axis, has been synthesized. The Cu^{2+} ion in the $[CuI(phen)_2]^+$ cation is five-coordinated by two bidentate phenanthroline ligands and an iodide ligand. The crystal packing is stabilized by intermolecular C—H···I hydrogen bonds.

Related literature

For related literature see: Chesnut *et al.* (1999); Ferbinteanu *et al.* (1998); Shiren *et al.* (2002); Bowmaker *et al.* (1973); Boys (1988); Boys *et al.* (1981); Healy *et al.* (1985); Pallenberg *et al.* (1995); Yang *et al.* (2004).



Experimental

Crystal data

$[CuI(C_{12}H_8N_2)_2]_2[CdI_4]$
M_r = 1721.70
Monoclinic, $C2/c$
a = 21.0726 (5) Å
b = 15.4727 (5) Å
c = 15.5907 (4) Å
β = 90.991 (1)°
V = 5082.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.93 mm^{-1}
T = 173 (2) K
0.66 × 0.41 × 0.36 mm

Data collection

Rigaku R-AXIS SPIDER diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.10, T_{max} = 0.16
(expected range = 0.106–0.170)
24621 measured reflections
5821 independent reflections
5537 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.085
S = 1.11
5821 reflections
295 parameters
Only H-atom displacement parameters refined
$\Delta\rho_{max}$ = 2.18 e Å^{-3}
$\Delta\rho_{min}$ = −1.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···I2	0.93	3.16	3.916 (4)	140
C5—H5···I1^{i}	0.93	3.15	3.884 (4)	138

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2017).

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supplementary materials

Acta Cryst. (2007). E**63**, m1782 [**doi:10.1107/S1600536807025329**]

Bis[iodidobis(1,10-phenanthroline-κ^2N,N')copper(II)] tetraiodidocadmate(II)

M.-L. Cao, X. Fang, Y.-J. Zhang, H.-Y. Yu and J.-D. Wang

Comment

Considerable attention has been paid to heteronuclear metal complexes. At present, a variety of mixed metal complexes have been reported. (Chesnut *et al.*, 1999. Ferbinteanu *et al.*, 1998. Shiren *et al.*, 2002.). Here, a new mixed metal complex is obtained under low temperature conditions. The asymmetric unit of the title compound, (I), contains one $[CuI(phen)_2]^+$ cation and a CdI_2 subunit of the CdI_4 dianion with the cadmium atom observed on a crystallographic twofold axis. In the cation, four N atoms of two bidentate phenanthroline ligands and one iodo ligand form an approximately trigonal-bipyramidal arrangement around the Cu^{2+} ion, with atoms I3, N1 and N4 occupying equatorial positions whereas N2 and N3 occupy the axial positions (Fig. 1). The equatorial plane (Table 1) is distorted with angles of 124.07 (9)° (N1—Cu1—I3), 125.98 (9)° (N4—Cu1—I3), and 109.94 (13)° (N1—Cu1—N4). In the crystal structure of (I), the crystal packing is stabilized by intermolecular I—H interactions between I atoms of the anion and H atoms of the phenanthroline ligands with distances of 3.15 Å, as listed in Table 1. In addition, one of the iodine atoms of the anion (I1) is positioned over the adjacent ring of one of the phenanthroline ligands (C13—C17—C24) with a distance of 3.535 Å.

Experimental

The title compound was prepared at room temperature. Firstly, CdI_2 (0.0366 g, 0.1 mmol) and phen (0.018 g, 0.1 mmol) were slowly added to 5 ml DMF and stirred for 30 min. Meanwhile, CuI (0.0191 g, 0.1 mmol) was added to another 5 ml of DMF, followed by slow addition of KI (0.0116 g,0.1 mmol) in 10 ml DMF until the solution became clear, and stirred for 30 min. Then the two solutions were mixed, stirred for 20 min, and filtered. After the solvent was slowly evaporated at −5°C, dark-purple crystals of the title compound weres obtained.

Refinement

All H atoms were located at calculated positions where U parameters were refined.

Figures

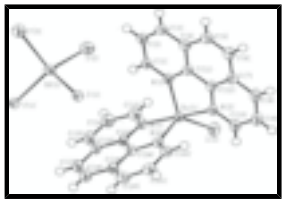

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

Bis[iodidobis(1,10-phenanthroline-κ^2*N*,*N*')copper(II)] tetraiodidocadmate(II)

Crystal data

$[CuI(C_{12}H_8N_2)_2]_2[CdI_4]$	F_{000} = 3200
M_r = 1721.70	D_x = 2.250 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C2yc	Cell parameters from 24621 reflections
a = 21.0726 (5) Å	θ = 6.1–55.0º
b = 15.4727 (5) Å	μ = 4.93 mm^{-1}
c = 15.5907 (4) Å	*T* = 173 (2) K
β = 90.991 (1)º	Block, black
V = 5082.6 (2) Å^3	0.66 × 0.41 × 0.36 mm
Z = 4	

Data collection

Rigaku R-AXIS SPIDER diffractometer	5821 independent reflections
Radiation source: fine-focus sealed tube	5537 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.061
Detector resolution: 10 pixels mm^{-1}	θ_{max} = 27.5º
T = 173(2) K	θ_{min} = 3.1º
ω oscillation scans	*h* = −27→27
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*k* = −20→18
T_{min} = 0.10, T_{max} = 0.16	*l* = −20→20
24621 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	Only H-atom displacement parameters refined
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$w = 1/[\sigma^2(F_o^2) + (0.0235P)^2 + 27.9995P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.085	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.11	$\Delta\rho_{max}$ = 2.18 e Å^{-3}
5821 reflections	$\Delta\rho_{min}$ = −1.31 e Å^{-3}
295 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00044 (4)
Secondary atom site location: difference Fourier map	

Special details

Experimental. collimator diameter: 0.800000 mm

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}
I1	0.423976 (12)	0.574827 (17)	0.144226 (16)	0.02418 (9)
I2	0.564820 (16)	0.78122 (2)	0.13363 (3)	0.05017 (13)
I3	0.851339 (13)	0.54118 (2)	0.092126 (18)	0.03378 (10)
Cd1	0.5000	0.67667 (3)	0.2500	0.03004 (12)
Cu1	0.78535 (2)	0.55003 (3)	0.23361 (3)	0.02163 (12)
N3	0.70292 (15)	0.5289 (2)	0.1721 (2)	0.0233 (7)
N4	0.75284 (15)	0.4442 (2)	0.3055 (2)	0.0214 (6)
N2	0.86250 (15)	0.5681 (2)	0.3079 (2)	0.0239 (7)
N1	0.75895 (15)	0.6662 (2)	0.2927 (2)	0.0215 (6)
C1	0.70786 (18)	0.7152 (3)	0.2834 (3)	0.0240 (8)
H1	0.6774	0.6994	0.2425	0.029*
C2	0.69748 (19)	0.7896 (3)	0.3321 (3)	0.0261 (8)
H2	0.6609	0.8224	0.3233	0.031*
C3	0.7417 (2)	0.8138 (3)	0.3929 (3)	0.0264 (8)
H3	0.7354	0.8632	0.4257	0.032*
C4	0.79673 (19)	0.7635 (3)	0.4054 (2)	0.0242 (8)
C5	0.8465 (2)	0.7822 (3)	0.4664 (3)	0.0278 (8)
H5	0.8425	0.8302	0.5018	0.033*
C6	0.8982 (2)	0.7332 (3)	0.4742 (3)	0.0307 (9)
H6	0.9294	0.7476	0.5147	0.037*
C7	0.90659 (19)	0.6585 (3)	0.4211 (3)	0.0263 (8)
C8	0.9604 (2)	0.6047 (3)	0.4244 (3)	0.0334 (10)
H8	0.9934	0.6163	0.4629	0.040*
C9	0.9637 (2)	0.5352 (3)	0.3707 (3)	0.0353 (10)
H9	0.9990	0.4991	0.3728	0.042*
C10	0.9137 (2)	0.5183 (3)	0.3123 (3)	0.0315 (9)
H10	0.9166	0.4710	0.2758	0.038*
C11	0.80319 (18)	0.6898 (3)	0.3528 (2)	0.0211 (7)
C12	0.85850 (17)	0.6375 (3)	0.3612 (2)	0.0221 (7)
C13	0.6792 (2)	0.5724 (3)	0.1061 (3)	0.0315 (9)
H13	0.7019	0.6191	0.0851	0.038*

C14	0.6213 (2)	0.5511 (3)	0.0665 (3)	0.0359 (10)
H14	0.6060	0.5833	0.0203	0.043*
C15	0.5874 (2)	0.4826 (3)	0.0962 (3)	0.0340 (10)
H15	0.5491	0.4673	0.0699	0.041*
C16	0.61076 (18)	0.4357 (3)	0.1666 (3)	0.0270 (8)
C17	0.57891 (19)	0.3634 (3)	0.2041 (3)	0.0317 (9)
H17	0.5400	0.3457	0.1812	0.038*
C18	0.6040 (2)	0.3205 (3)	0.2716 (3)	0.0347 (10)
H18	0.5820	0.2737	0.2940	0.042*
C19	0.66377 (19)	0.3450 (3)	0.3098 (3)	0.0272 (8)
C20	0.6931 (2)	0.3022 (3)	0.3785 (3)	0.0344 (10)
H20	0.6738	0.2543	0.4029	0.041*
C21	0.7504 (2)	0.3312 (3)	0.4097 (3)	0.0329 (9)
H21	0.7703	0.3033	0.4556	0.039*
C22	0.7788 (2)	0.4031 (3)	0.3716 (3)	0.0259 (8)
H22	0.8174	0.4227	0.3937	0.031*
C23	0.66964 (18)	0.4619 (3)	0.2029 (2)	0.0223 (8)
C24	0.69596 (18)	0.4160 (3)	0.2747 (2)	0.0215 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.02396 (14)	0.02735 (15)	0.02109 (14)	−0.00515 (9)	−0.00331 (9)	0.00105 (10)
I2	0.04088 (19)	0.03983 (18)	0.0688 (3)	−0.01745 (14)	−0.02675 (17)	0.02747 (17)
I3	0.02672 (15)	0.04954 (19)	0.02509 (15)	0.00118 (11)	0.00064 (11)	0.00351 (12)
Cd1	0.0284 (2)	0.0233 (2)	0.0379 (2)	0.000	−0.01419 (18)	0.000
Cu1	0.0176 (2)	0.0273 (2)	0.0198 (2)	−0.00080 (17)	−0.00559 (17)	0.00044 (19)
N3	0.0210 (15)	0.0285 (17)	0.0203 (15)	0.0005 (13)	−0.0034 (12)	−0.0005 (14)
N4	0.0221 (15)	0.0256 (16)	0.0166 (14)	0.0007 (12)	−0.0001 (12)	−0.0032 (13)
N2	0.0191 (15)	0.0297 (17)	0.0227 (16)	−0.0014 (13)	−0.0051 (12)	0.0016 (14)
N1	0.0179 (15)	0.0276 (16)	0.0189 (15)	−0.0030 (12)	−0.0015 (12)	0.0052 (13)
C1	0.0188 (17)	0.029 (2)	0.0241 (18)	−0.0022 (14)	−0.0010 (14)	0.0052 (16)
C2	0.0236 (19)	0.029 (2)	0.026 (2)	0.0024 (15)	0.0033 (15)	0.0067 (17)
C3	0.033 (2)	0.0242 (19)	0.0220 (19)	−0.0041 (16)	0.0059 (16)	0.0006 (16)
C4	0.0267 (19)	0.0288 (19)	0.0170 (17)	−0.0076 (15)	0.0010 (14)	0.0035 (16)
C5	0.034 (2)	0.033 (2)	0.0168 (17)	−0.0085 (17)	−0.0023 (15)	−0.0005 (16)
C6	0.030 (2)	0.041 (2)	0.0210 (19)	−0.0128 (18)	−0.0066 (16)	0.0003 (18)
C7	0.0230 (19)	0.035 (2)	0.0206 (18)	−0.0070 (16)	−0.0058 (15)	0.0044 (17)
C8	0.023 (2)	0.047 (3)	0.030 (2)	−0.0036 (18)	−0.0103 (16)	0.004 (2)
C9	0.022 (2)	0.048 (3)	0.036 (2)	0.0061 (18)	−0.0071 (17)	0.005 (2)
C10	0.025 (2)	0.037 (2)	0.032 (2)	0.0023 (17)	−0.0036 (17)	−0.0007 (19)
C11	0.0214 (18)	0.0264 (18)	0.0156 (16)	−0.0062 (14)	−0.0002 (13)	0.0029 (15)
C12	0.0202 (17)	0.0293 (19)	0.0167 (16)	−0.0047 (14)	−0.0030 (14)	0.0044 (15)
C13	0.032 (2)	0.037 (2)	0.025 (2)	−0.0009 (17)	−0.0080 (17)	0.0003 (18)
C14	0.029 (2)	0.047 (3)	0.031 (2)	0.0085 (19)	−0.0121 (18)	0.000 (2)
C15	0.023 (2)	0.047 (3)	0.032 (2)	0.0059 (18)	−0.0073 (17)	−0.013 (2)
C16	0.0177 (18)	0.036 (2)	0.027 (2)	0.0021 (15)	0.0010 (15)	−0.0142 (18)
C17	0.0190 (18)	0.041 (2)	0.035 (2)	−0.0043 (17)	0.0045 (16)	−0.014 (2)

C18	0.029 (2)	0.039 (2)	0.036 (2)	−0.0108 (18)	0.0109 (18)	−0.012 (2)
C19	0.0259 (19)	0.030 (2)	0.026 (2)	−0.0023 (16)	0.0066 (15)	−0.0067 (17)
C20	0.042 (3)	0.030 (2)	0.032 (2)	−0.0050 (18)	0.0096 (19)	−0.0002 (19)
C21	0.043 (3)	0.033 (2)	0.022 (2)	0.0033 (19)	−0.0035 (17)	0.0037 (18)
C22	0.028 (2)	0.030 (2)	0.0200 (18)	0.0020 (16)	−0.0019 (15)	−0.0018 (16)
C23	0.0176 (17)	0.032 (2)	0.0179 (17)	0.0024 (14)	0.0024 (13)	−0.0083 (15)
C24	0.0204 (17)	0.0261 (18)	0.0181 (17)	0.0019 (14)	0.0039 (14)	−0.0068 (15)

Geometric parameters (Å, °)

I1—Cd1	2.7709 (3)	C7—C12	1.404 (5)
I2—Cd1	2.8036 (4)	C7—C8	1.407 (6)
I3—Cu1	2.6314 (6)	C8—C9	1.365 (7)
Cd1—I1^{i}	2.7708 (3)	C8—H8	0.9300
Cd1—I2^{i}	2.8036 (4)	C9—C10	1.405 (6)
Cu1—N3	1.996 (3)	C9—H9	0.9300
Cu1—N2	1.999 (3)	C10—H10	0.9300
Cu1—N1	2.099 (3)	C11—C12	1.424 (5)
Cu1—N4	2.105 (3)	C13—C14	1.397 (6)
N3—C13	1.321 (5)	C13—H13	0.9300
N3—C23	1.346 (5)	C14—C15	1.362 (7)
N4—C22	1.321 (5)	C14—H14	0.9300
N4—C24	1.356 (5)	C15—C16	1.397 (6)
N2—C10	1.327 (5)	C15—H15	0.9300
N2—C12	1.362 (5)	C16—C23	1.414 (5)
N1—C1	1.323 (5)	C16—C17	1.435 (6)
N1—C11	1.360 (5)	C17—C18	1.344 (7)
C1—C2	1.399 (6)	C17—H17	0.9300
C1—H1	0.9300	C18—C19	1.436 (6)
C2—C3	1.370 (6)	C18—H18	0.9300
C2—H2	0.9300	C19—C20	1.394 (7)
C3—C4	1.407 (6)	C19—C24	1.407 (6)
C3—H3	0.9300	C20—C21	1.370 (7)
C4—C11	1.413 (6)	C20—H20	0.9300
C4—C5	1.433 (5)	C21—C22	1.401 (6)
C5—C6	1.331 (6)	C21—H21	0.9300
C5—H5	0.9300	C22—H22	0.9300
C6—C7	1.434 (6)	C23—C24	1.429 (6)
C6—H6	0.9300		
I1—Cd1—I1^{i}	110.681 (18)	C9—C8—H8	120.2
I1—Cd1—I2^{i}	115.477 (9)	C7—C8—H8	120.2
I1^{i}—Cd1—I2^{i}	103.070 (9)	C8—C9—C10	119.8 (4)
I1—Cd1—I2	103.070 (9)	C8—C9—H9	120.1
I1^{i}—Cd1—I2	115.477 (9)	C10—C9—H9	120.1
I2^{i}—Cd1—I2	109.52 (2)	N2—C10—C9	121.8 (4)
N3—Cu1—N2	173.27 (14)	N2—C10—H10	119.1
N3—Cu1—N1	96.64 (13)	C9—C10—H10	119.1

N2—Cu1—N1	81.10 (13)	N1—C11—C4	123.0 (4)
N3—Cu1—N4	80.80 (13)	N1—C11—C12	117.5 (3)
N2—Cu1—N4	93.96 (13)	C4—C11—C12	119.5 (3)
N1—Cu1—N4	109.94 (13)	N2—C12—C7	122.5 (4)
N3—Cu1—I3	93.26 (10)	N2—C12—C11	116.8 (3)
N2—Cu1—I3	93.24 (10)	C7—C12—C11	120.6 (4)
N1—Cu1—I3	124.07 (9)	N3—C13—C14	122.7 (4)
N4—Cu1—I3	125.98 (9)	N3—C13—H13	118.7
C13—N3—C23	118.5 (4)	C14—C13—H13	118.7
C13—N3—Cu1	127.3 (3)	C15—C14—C13	119.4 (4)
C23—N3—Cu1	114.2 (3)	C15—C14—H14	120.3
C22—N4—C24	118.2 (4)	C13—C14—H14	120.3
C22—N4—Cu1	131.0 (3)	C14—C15—C16	119.4 (4)
C24—N4—Cu1	110.8 (3)	C14—C15—H15	120.3
C10—N2—C12	119.0 (3)	C16—C15—H15	120.3
C10—N2—Cu1	127.0 (3)	C15—C16—C23	117.4 (4)
C12—N2—Cu1	113.9 (3)	C15—C16—C17	124.4 (4)
C1—N1—C11	117.9 (4)	C23—C16—C17	118.2 (4)
C1—N1—Cu1	131.6 (3)	C18—C17—C16	121.6 (4)
C11—N1—Cu1	110.4 (3)	C18—C17—H17	119.2
N1—C1—C2	123.2 (4)	C16—C17—H17	119.2
N1—C1—H1	118.4	C17—C18—C19	121.6 (4)
C2—C1—H1	118.4	C17—C18—H18	119.2
C3—C2—C1	119.3 (4)	C19—C18—H18	119.2
C3—C2—H2	120.3	C20—C19—C24	117.4 (4)
C1—C2—H2	120.3	C20—C19—C18	124.6 (4)
C2—C3—C4	119.6 (4)	C24—C19—C18	118.0 (4)
C2—C3—H3	120.2	C21—C20—C19	119.6 (4)
C4—C3—H3	120.2	C21—C20—H20	120.2
C3—C4—C11	116.9 (3)	C19—C20—H20	120.2
C3—C4—C5	125.0 (4)	C20—C21—C22	119.4 (4)
C11—C4—C5	118.1 (4)	C20—C21—H21	120.3
C6—C5—C4	122.3 (4)	C22—C21—H21	120.3
C6—C5—H5	118.8	N4—C22—C21	122.6 (4)
C4—C5—H5	118.8	N4—C22—H22	118.7
C5—C6—C7	121.0 (4)	C21—C22—H22	118.7
C5—C6—H6	119.5	N3—C23—C16	122.5 (4)
C7—C6—H6	119.5	N3—C23—C24	117.7 (3)
C12—C7—C8	117.3 (4)	C16—C23—C24	119.8 (4)
C12—C7—C6	118.4 (4)	N4—C24—C19	122.9 (4)
C8—C7—C6	124.3 (4)	N4—C24—C23	116.5 (4)
C9—C8—C7	119.7 (4)	C19—C24—C23	120.6 (4)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···I2	0.93	3.16	3.916 (4)	140
C5—H5···I1^{ii}	0.93	3.15	3.884 (4)	138

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

Fig. 1