

Tetrakis(2,2'-bipyridine)-1κ⁴N,N';-4κ⁴N,N'-hexa-μ-iodido-1:2κ⁴I:I;-2:3κ⁴I:I;3:4κ⁴I:I-1,4-dicadmium(II)-2,3-disilver(I)

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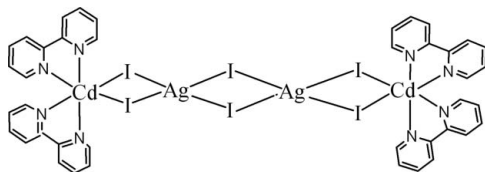
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.013$ Å; R factor = 0.044; wR factor = 0.121; data-to-parameter ratio = 23.5.

The centrosymmetric title compound, $[\text{Ag}_2\text{Cd}_2\text{I}_6(\text{C}_{10}\text{H}_8\text{N}_2)_4]$, was synthesized by the reaction of CdI_2 , KAgI_2 and 2,2'-bipyridine in dimethylformamide. The crystal structure contains an Ag_2I_6 chain and $\text{Cd}(2,2'\text{-bipyridine})_2$ units; the four 2,2'-bipyridine ligands are positioned at the ends of the molecule and μ_2 -iodo bridges link two $\text{Cd}(2,2'\text{-bipyridine})\text{-I}_2\text{Ag}$ units. The Cd atom exhibits a distorted octahedral geometry.

Related literature

For related literature, see: Li *et al.* (2006); Cheetham (1994); Estienne (1986); Helgsson & Jagner (1991); Jones (1992); Meyer (1963); Niu *et al.* (2004); Rutherford (1998); Wu *et al.* (2003); Yaghi *et al.* (1998).



Experimental

Crystal data

$[\text{Ag}_2\text{Cd}_2\text{I}_6(\text{C}_{10}\text{H}_8\text{N}_2)_4]$	$V = 2458.0$ (3) Å ³
$M_r = 1826.68$	$Z = 2$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 8.9170$ (6) Å	$\mu = 5.44$ mm ⁻¹
$b = 21.5098$ (15) Å	$T = 293$ (2) K
$c = 12.8527$ (9) Å	$0.20 \times 0.15 \times 0.15$ mm
$\beta = 94.374$ (4)°	

Data collection

Bruker SMART APEX CCD diffractometer	6188 independent reflections
Absorption correction: none	4890 reflections with $I > 2\sigma(I)$
14678 measured reflections	$R_{\text{int}} = 0.045$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$	263 parameters
$wR(F^2) = 0.121$	H-atom parameters constrained
$S = 1.00$	$\Delta\rho_{\text{max}} = 1.19$ e Å ⁻³
6188 reflections	$\Delta\rho_{\text{min}} = -1.02$ e Å ⁻³

Table 1

Selected geometric parameters (Å, °).

Cd1—N1	2.407 (6)	Cd1—I1	2.9368 (6)
Cd1—N2	2.331 (5)	I2—Ag1	2.9058 (8)
Cd1—N3	2.339 (4)	I3—Ag1	2.8036 (7)
Cd1—N4	2.399 (5)	I1—Ag1	2.8784 (7)
Cd1—I2	2.8352 (6)		
N2—Cd1—N3	155.03 (18)	N4—Cd1—I1	86.86 (12)
N2—Cd1—N4	90.75 (18)	I2—Cd1—I1	96.217 (17)
N3—Cd1—N4	69.61 (17)	Ag1—I3—Ag1 ⁱ	70.08 (2)
N2—Cd1—N1	69.7 (2)	I3—Ag1—I1	109.69 (2)
N3—Cd1—N1	92.37 (19)	I3—Ag1—I2	118.40 (2)
N4—Cd1—N1	84.32 (17)	I1—Ag1—I2	95.96 (2)
N4—Cd1—I2	171.04 (13)		

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); 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: KP2139).

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supplementary materials

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Tetrakis(2,2'-bipyridine)-1 κ^4 N,N';4 κ^4 N,N'-hexa- μ -iodido-1:2 κ^4 I:I;2:3 κ^4 I:I;3:4 κ^4 I:I-1,4-dicadmium(II)-2,3-disilver(I)

Y.-S. Jiang, H.-G. Yao, L.-J. Zou and Y.-L. An

Comment

Divers and useful physical properties as well as large structural variety have prompted the recent surge in design and synthesis of new hybrid organic-inorganic materials. These materials have attracted much attention of chemists and physicists, not due to variety of intriguing structure topologies, but also for their potential application in catalysis, materials science, medicine, magntochemistry, and optical materials (Cheetham, 1994; Yaghi *et al.*, 1998; Wu *et al.*, 2003; Niu *et al.*, 2004). Among the various families of hybrid functional materials, silver(I) halides occupy an important role (Li *et al.*, 2006; Rutherford, 1998). Up to now the structure of silver(I) halides containing Ag₂I₄, Ag₃I₆, Ag₄I₆, and Ag₄I₈ anions exhibit isolated anions, one-dimensional infinite chains, two- and three-dimensional frameworks (Meyer, 1963; Estienne, 1986; Helgsson & Jagner, 1991; Jones, 1992). In this paper we report the synthesis and structure of a new one-dimensional organic-inorganic hybrid compound Ag₂I₆[Cd(2,2'-bipyridine)₂]₂.

The structure of the compound contains an one-dimensional Ag₂I₆ chain: the six iodide atoms acting as bridges between the silver atoms (Fig. 1). Ag atoms are in a tetrahedral arrangement where AgI₄ tetrahedra share all corners with the neighbouring metal atoms (Figs. 1 and 2). The Ag—I distances range from 2.8036 (7) Å to 2.9058 (8) Å, while the Ag—I—Ag angle is 70.08 (2)°, and the I—Ag—I angles range from 95.96 (2)° to 118.40 (2)° (Table 1). In Ag₂I₆ the Ag...Ag separation is 3.2260 (11) Å. Cd(II) reveals a distorted octahedral geometry with two 2,2'-bipyridine ligands and two iodide atoms (Fig. 1). The Cd—I distances range from 2.8352 (6) Å to 2.9368 (6) Å, whereas Cd—N are in the range from 2.331 (5) Å to 2.407 (6) Å. The N—Cd—N angles range from 69.61 (17)° to 155.03 (18)°, I—Cd—I is 96.217 (17)°, and the N—Cd—I angles are from 86.86 (12)° to 171.04 (13)° (Table 1). Ag₂I₆ links adjacent Cd centres into the chains.

Experimental

KAgI₂ was prepared by dropping excessive KI/DMF solution into AgNO₃/DMF solution. The title compound was synthesized by CdI₂ (0.074 g) and 2,2'-bipyridine (0.015 g) dissolved in DMF (2.5 ml) followed by dropping the KAgI₂ (4 ml) solution. The mixture was stirred for 2 m and then filtered off. The filtrate was kept at room temperature for five days and the deep-brown block crystals were obtained. Crystals were washed with ethanol and then with water.

Refinement

H atoms were positioned geometrically with C—H = 0.93 Å and allowed to ride during subsequent refinement with $U_{iso}(H)=1.2U_{eq}(C)$.

Figures

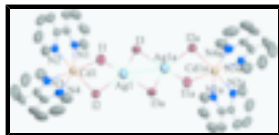


Fig. 1. The molecular structure of (I) with the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level. Symmetry codes: (i) $-x + 2, -y, -z + 1$. H atoms have been omitted.

Tetrakis(2,2-bipyridine)-1 κ^4 N,N';4 κ^4 N,N'- hexa- μ -iodido-1:2 κ^4 I:I;2:3 κ^4 I:I;3:4 κ^4 I:I- 1,4-dicadmium(II)-2,3-disilver(I)(Ag—Ag)

Crystal data

[Ag₂Cd₂I₆(C₁₀H₈N₂)₄]

$M_r = 1826.68$

Monoclinic, $P2_1/n$

$a = 8.9170$ (6) Å

$b = 21.5098$ (15) Å

$c = 12.8527$ (9) Å

$\beta = 94.374$ (4)°

$V = 2458.0$ (3) Å³

$Z = 2$

$F_{000} = 1672$

$D_x = 2.468$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 6188 reflections

$\theta = 2.5$ – 26.3 °

$\mu = 5.44$ mm⁻¹

$T = 293$ (2) K

Block, brown

$0.20 \times 0.15 \times 0.15$ mm

Data collection

Bruker SMART APEXII CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293$ (2) K

φ and ω scans

Absorption correction: none

14678 measured reflections

6188 independent reflections

4890 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\text{max}} = 28.5$ °

$\theta_{\text{min}} = 2.5$ °

$h = -11 \rightarrow 11$

$k = -25 \rightarrow 28$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.121$

$S = 1.00$

6188 reflections

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 1.6703P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 1.19$ e Å⁻³

$\Delta\rho_{\text{min}} = -1.02$ e Å⁻³

263 parameters

Extinction correction: SHELXL97 (Sheldrick, 1997),

$$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.0073 (3)

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.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.82840 (5)	0.162316 (19)	0.20025 (3)	0.04285 (13)
I1	0.68673 (5)	0.04486 (2)	0.25574 (3)	0.06171 (15)
I2	0.98594 (5)	0.18259 (2)	0.39736 (3)	0.05907 (15)
I3	0.80925 (5)	0.01176 (2)	0.60922 (3)	0.05752 (15)
Ag1	0.92118 (7)	0.05126 (3)	0.42222 (4)	0.06661 (17)
N1	0.8859 (7)	0.2636 (3)	0.1342 (4)	0.0571 (13)
N2	0.6309 (6)	0.2308 (3)	0.2223 (4)	0.0583 (14)
N3	1.0127 (5)	0.1145 (2)	0.1076 (4)	0.0456 (11)
N4	0.7331 (6)	0.1421 (2)	0.0239 (4)	0.0494 (11)
C1	0.7836 (9)	0.3074 (3)	0.1394 (5)	0.0608 (18)
C2	0.8089 (12)	0.3669 (4)	0.1002 (7)	0.087 (3)
H2A	0.7350	0.3973	0.1027	0.104*
C3	0.9371 (15)	0.3803 (5)	0.0595 (9)	0.111 (4)
H3A	0.9542	0.4203	0.0354	0.134*
C4	1.0433 (14)	0.3358 (5)	0.0530 (8)	0.099 (3)
H4A	1.1337	0.3442	0.0243	0.118*
C5	1.0125 (10)	0.2774 (4)	0.0907 (6)	0.078 (2)
H5A	1.0838	0.2462	0.0854	0.094*
C6	0.6409 (8)	0.2892 (3)	0.1866 (5)	0.0616 (18)
C7	0.5247 (13)	0.3303 (5)	0.1890 (7)	0.095 (3)
H7A	0.5325	0.3705	0.1634	0.113*
C8	0.3968 (15)	0.3105 (6)	0.2302 (9)	0.108 (4)
H8A	0.3153	0.3374	0.2310	0.129*
C9	0.3850 (10)	0.2524 (7)	0.2702 (8)	0.106 (4)
H9A	0.2980	0.2396	0.2996	0.128*
C10	0.5080 (9)	0.2125 (5)	0.2658 (7)	0.080 (2)
H10A	0.5037	0.1727	0.2937	0.096*
C11	0.5951 (8)	0.1549 (4)	-0.0136 (5)	0.0624 (17)

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H11A	0.5384	0.1823	0.0234	0.075*
C12	0.5298 (9)	0.1296 (4)	-0.1058 (6)	0.072 (2)
H12A	0.4315	0.1392	-0.1297	0.086*
C13	0.6148 (10)	0.0904 (4)	-0.1598 (5)	0.073 (2)
H13A	0.5751	0.0727	-0.2219	0.087*
C14	0.7597 (9)	0.0772 (4)	-0.1222 (5)	0.0649 (18)
H14A	0.8182	0.0499	-0.1579	0.078*
C15	0.8172 (7)	0.1048 (3)	-0.0312 (4)	0.0465 (13)
C16	1.1535 (7)	0.1061 (3)	0.1497 (6)	0.0584 (15)
H16A	1.1784	0.1189	0.2179	0.070*
C17	1.2614 (9)	0.0791 (4)	0.0943 (7)	0.071 (2)
H17A	1.3587	0.0741	0.1247	0.086*
C18	1.2264 (9)	0.0599 (4)	-0.0041 (7)	0.074 (2)
H18A	1.2998	0.0416	-0.0417	0.089*
C19	1.0838 (9)	0.0669 (3)	-0.0490 (6)	0.068 (2)
H19A	1.0582	0.0532	-0.1167	0.081*
C20	0.9763 (7)	0.0957 (3)	0.0103 (4)	0.0483 (13)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.0466 (2)	0.0396 (2)	0.0428 (2)	0.00666 (17)	0.00627 (16)	-0.00090 (15)
I2	0.0791 (3)	0.0469 (3)	0.0492 (2)	-0.0079 (2)	-0.00834 (19)	-0.00098 (16)
I3	0.0673 (3)	0.0548 (3)	0.0524 (2)	0.0105 (2)	0.01750 (19)	-0.00039 (17)
I1	0.0624 (3)	0.0576 (3)	0.0635 (3)	-0.0183 (2)	-0.0058 (2)	0.00984 (19)
Ag1	0.0715 (4)	0.0658 (4)	0.0631 (3)	0.0075 (3)	0.0083 (3)	0.0091 (2)
N3	0.048 (3)	0.041 (3)	0.050 (2)	0.006 (2)	0.016 (2)	0.0011 (19)
N4	0.058 (3)	0.048 (3)	0.043 (2)	0.002 (2)	0.006 (2)	0.005 (2)
N2	0.045 (3)	0.072 (4)	0.057 (3)	0.015 (3)	0.000 (2)	-0.011 (3)
N1	0.070 (3)	0.044 (3)	0.056 (3)	0.002 (3)	-0.004 (3)	0.002 (2)
C15	0.063 (4)	0.036 (3)	0.041 (2)	-0.011 (3)	0.010 (2)	0.002 (2)
C6	0.074 (4)	0.051 (4)	0.056 (3)	0.025 (3)	-0.017 (3)	-0.021 (3)
C20	0.059 (3)	0.037 (3)	0.052 (3)	-0.003 (3)	0.024 (3)	0.003 (2)
C1	0.084 (5)	0.037 (3)	0.056 (3)	0.008 (3)	-0.028 (3)	-0.004 (3)
C16	0.048 (3)	0.052 (4)	0.076 (4)	0.004 (3)	0.003 (3)	0.000 (3)
C14	0.083 (5)	0.066 (5)	0.047 (3)	-0.015 (4)	0.011 (3)	-0.001 (3)
C19	0.090 (6)	0.052 (4)	0.066 (4)	-0.001 (4)	0.037 (4)	-0.005 (3)
C11	0.063 (4)	0.064 (4)	0.059 (3)	-0.001 (3)	-0.004 (3)	0.007 (3)
C18	0.066 (5)	0.060 (5)	0.103 (6)	0.007 (4)	0.044 (4)	-0.003 (4)
C17	0.058 (4)	0.054 (4)	0.104 (6)	0.007 (3)	0.022 (4)	-0.003 (4)
C12	0.068 (4)	0.086 (6)	0.060 (4)	-0.029 (4)	-0.004 (3)	0.015 (4)
C5	0.084 (5)	0.071 (5)	0.082 (5)	-0.020 (4)	0.017 (4)	0.003 (4)
C13	0.098 (6)	0.077 (5)	0.043 (3)	-0.036 (5)	0.002 (4)	-0.002 (3)
C10	0.060 (4)	0.094 (7)	0.089 (5)	0.014 (4)	0.019 (4)	-0.018 (5)
C7	0.106 (7)	0.079 (6)	0.093 (6)	0.053 (6)	-0.027 (6)	-0.036 (5)
C2	0.104 (7)	0.039 (4)	0.107 (6)	0.011 (4)	-0.051 (6)	0.003 (4)
C9	0.054 (5)	0.160 (12)	0.107 (7)	0.014 (6)	0.018 (5)	-0.053 (8)
C8	0.114 (9)	0.102 (9)	0.106 (7)	0.049 (7)	0.007 (6)	-0.035 (6)

C3	0.129 (9)	0.072 (7)	0.124 (8)	-0.042 (7)	-0.056 (7)	0.032 (6)
C4	0.125 (9)	0.081 (7)	0.086 (6)	-0.036 (6)	-0.011 (6)	0.027 (5)

Geometric parameters (Å, °)

Cd1—N1	2.407 (6)	C11—C12	1.391 (10)
Cd1—N2	2.331 (5)	C18—C17	1.344 (12)
Cd1—N3	2.339 (4)	C12—C13	1.359 (12)
Cd1—N4	2.399 (5)	C5—C4	1.381 (12)
Cd1—I2	2.8352 (6)	C10—C9	1.397 (12)
Cd1—I1	2.9368 (6)	C7—C8	1.362 (16)
I2—Ag1	2.9058 (8)	C2—C3	1.325 (15)
I3—Ag1	2.8036 (7)	C9—C8	1.358 (17)
I3—Ag1 ⁱ	2.8155 (7)	C3—C4	1.353 (17)
I1—Ag1	2.8784 (7)	C1—H1A	0.930
Ag1—I3 ⁱ	2.8155 (7)	C2—H2A	0.930
Ag1—Ag1 ⁱ	3.2260 (11)	C3—H3A	0.930
N3—C20	1.332 (7)	C4—H4A	0.930
N3—C16	1.341 (8)	C5—H5A	0.930
N4—C11	1.317 (8)	C6—H6A	0.930
N4—C15	1.337 (8)	C7—H7A	0.930
N2—C10	1.328 (9)	C8—H8A	0.930
N2—C6	1.341 (9)	C9—H9A	0.930
N1—C1	1.316 (9)	C10—H10A	0.930
N1—C5	1.332 (9)	C11—H11A	0.930
C15—C14	1.376 (9)	C12—H12A	0.930
C15—C20	1.489 (9)	C13—H13A	0.930
C6—C7	1.365 (10)	C14—H14A	0.930
C6—C1	1.503 (11)	C15—H15A	0.930
C20—C19	1.412 (9)	C16—H16A	0.930
C1—C2	1.400 (11)	C17—H17A	0.930
C16—C17	1.369 (10)	C18—H18A	0.930
C14—C13	1.374 (11)	C19—H19A	0.930
C19—C18	1.364 (12)	C20—H20A	0.930
N2—Cd1—N3	155.03 (18)	N1—C1—C6	116.4 (6)
N2—Cd1—N4	90.75 (18)	C2—C1—C6	123.2 (7)
N3—Cd1—N4	69.61 (17)	N3—C16—C17	121.4 (7)
N2—Cd1—N1	69.7 (2)	C13—C14—C15	119.3 (7)
N3—Cd1—N1	92.37 (19)	C18—C19—C20	118.0 (7)
N4—Cd1—N1	84.32 (17)	N4—C11—C12	123.3 (8)
N2—Cd1—I2	96.99 (13)	C17—C18—C19	120.4 (7)
N3—Cd1—I2	101.70 (12)	C18—C17—C16	119.8 (8)
N4—Cd1—I2	171.04 (13)	C13—C12—C11	117.7 (8)
N1—Cd1—I2	94.10 (13)	N1—C5—C4	123.2 (10)
N2—Cd1—I1	99.88 (16)	C12—C13—C14	119.6 (6)
N3—Cd1—I1	94.44 (12)	N2—C10—C9	120.7 (10)
N4—Cd1—I1	86.86 (12)	C8—C7—C6	117.7 (11)
N1—Cd1—I1	166.23 (14)	C3—C2—C1	120.5 (9)

supplementary materials

I2—Cd1—I1	96.217 (17)	C8—C9—C10	117.8 (10)
Cd1—I2—Ag1	81.934 (18)	C9—C8—C7	121.8 (10)
Ag1—I3—Ag1 ⁱ	70.08 (2)	C2—C3—C4	119.9 (9)
Ag1—I1—Cd1	80.672 (18)	C3—C4—C5	117.6 (11)
I3—Ag1—I3 ⁱ	109.92 (2)	H2A—C2—C1	118.70
I3—Ag1—I1	109.69 (2)	H2A—C2—C3	120.25
I3 ⁱ —Ag1—I1	116.74 (2)	H3A—C3—C2	118.67
I3—Ag1—I2	118.40 (2)	H3A—C3—C4	118.70
I3 ⁱ —Ag1—I2	105.86 (2)	H4A—C4—C3	120.25
I1—Ag1—I2	95.96 (2)	H4A—C4—C5	120.22
I3—Ag1—Ag1 ⁱ	55.135 (19)	H5A—C5—C4	120.69
I3 ⁱ —Ag1—Ag1 ⁱ	54.790 (19)	H5A—C5—N1	120.71
I1—Ag1—Ag1 ⁱ	133.27 (3)	H7A—C7—C6	118.22
I2—Ag1—Ag1 ⁱ	130.68 (3)	H7A—C7—C8	118.28
C20—N3—C16	119.5 (5)	H8A—C8—C7	118.38
C20—N3—Cd1	118.8 (4)	H8A—C8—C9	118.39
C16—N3—Cd1	121.8 (4)	H9A—C9—C8	120.51
C11—N4—C15	118.6 (6)	H9A—C9—C10	120.52
C11—N4—Cd1	124.2 (4)	H10A—C10—C9	120.59
C15—N4—Cd1	115.9 (4)	H10A—C10—N2	120.64
C10—N2—C6	120.0 (7)	H11A—C11—N4	120.53
C10—N2—Cd1	121.3 (6)	H11A—C11—C12	120.57
C6—N2—Cd1	118.7 (5)	H12A—C12—C11	118.34
C1—N1—C5	118.3 (7)	H12A—C12—C13	118.41
C1—N1—Cd1	117.6 (5)	H13A—C13—C12	118.67
C5—N1—Cd1	124.1 (5)	H13A—C13—C14	118.70
N4—C15—C14	121.4 (6)	H14A—C14—C13	120.25
N4—C15—C20	116.5 (5)	H14A—C14—C15	120.22
C14—C15—C20	122.1 (6)	H16A—C16—N3	120.69
N2—C6—C7	121.9 (9)	H16A—C16—C17	120.71
N2—C6—C1	117.5 (5)	H17A—C17—C16	118.22
C7—C6—C1	120.5 (9)	H17A—C17—C18	118.28
N3—C20—C19	120.9 (6)	H18A—C18—C17	118.38
N3—C20—C15	117.0 (5)	H18A—C18—C19	118.39
C19—C20—C15	122.1 (6)	H19A—C19—C18	120.51
N1—C1—C2	120.3 (8)	H19A—C19—C20	120.52

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

Fig. 1

