

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(4,4'-Dimethyl-2,2'-bipyridine- κ^2N,N')-(dimethylformamide- κO)diiodido-cadmium

 Sadif A. Shirvan,^{a*} Sara Haydari Dezfuli,^a Fereydoon Khazali^a and Ali Borsalani^b
^aDepartment of Chemistry, Omidieh Branch, Islamic Azad University, Omidieh, Iran, and ^bDepartment of Petroleum Engineering, Omidieh Branch, Islamic Azad University, Omidieh, Iran

Correspondence e-mail: sadifchemist@hotmail.com

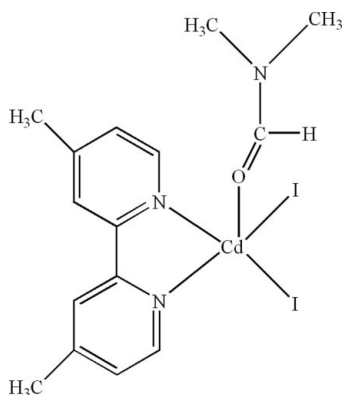
Received 11 November 2012; accepted 12 November 2012

 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.008$ Å; R factor = 0.040; wR factor = 0.084; data-to-parameter ratio = 19.6.

In the title compound, $[CdI_2(C_{12}H_{12}N_2)(C_3H_7NO)]$, the Cd^{II} cation is five-coordinated in a distorted trigonal-bipyramidal configuration by two N atoms from a 4,4'-dimethyl-2,2'-bipyridine ligand, one O atom from a dimethylformamide ligand and two I^- anions. π - π stacking between pyridine rings of adjacent molecules [centroid-centroid distance = 3.666 (3) and 3.709 (4) Å] stabilizes the three-dimensional structure

Related literature

For related structures, see: Ahmadi *et al.* (2008); Alizadeh *et al.* (2010); Amani *et al.* (2009); Bellusci *et al.* (2008); Hojjat Kashani *et al.* (2008); Kalateh *et al.* (2008, 2010); Shirvan & Haydari Dezfuli (2012); Sofetis *et al.* (2006); Willett *et al.* (2001); Yousefi *et al.* (2008).



Experimental

Crystal data

 $[CdI_2(C_{12}H_{12}N_2)(C_3H_7NO)]$
 $M_r = 623.54$

 Monoclinic, $P2_1/c$
 $a = 8.6103$ (6) Å
 $b = 15.1325$ (8) Å
 $c = 15.4263$ (10) Å
 $\beta = 98.347$ (5)°
 $V = 1988.7$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 4.21$ mm⁻¹
 $T = 298$ K
 $0.45 \times 0.40 \times 0.35$ mm

Data collection

 Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{min} = 0.188$, $T_{max} = 0.223$

 12059 measured reflections
 3907 independent reflections
 2859 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.052$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.084$
 $S = 0.98$
 3907 reflections

 199 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.85$ e Å⁻³
 $\Delta\rho_{min} = -1.08$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cd1—N1	2.327 (4)	Cd1—I1	2.7523 (7)
Cd1—N2	2.365 (5)	Cd1—I2	2.7635 (6)
Cd1—O1	2.345 (5)		

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

We are grateful to the Islamic Azad University, Omidieh Branch, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5650).

References

- Ahmadi, R., Kalateh, K., Abedi, A., Amani, V. & Khavasi, H. R. (2008). *Acta Cryst. E* **64**, m1306–m1307.
- Alizadeh, R., Mohammadi Eshlaghi, P. & Amani, V. (2010). *Acta Cryst. E* **66**, m996.
- Amani, V., Safari, N., Notash, B. & Khavasi, H. R. (2009). *J. Coord. Chem.* **62**, 1939–1950.
- Bellusci, A., Crispini, A., Pucci, D., Szerb, E. I. & Ghedini, M. (2008). *Cryst. Growth Des.* **8**, 3114–3122.
- Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2007). *APEX2* and *S SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Hojjat Kashani, L., Amani, V., Yousefi, M. & Khavasi, H. R. (2008). *Acta Cryst. E* **64**, m905–m906.
- Kalateh, K., Ahmadi, R. & Amani, V. (2010). *Acta Cryst. E* **66**, m512.
- Kalateh, K., Ebadi, A., Ahmadi, R., Amani, V. & Khavasi, H. R. (2008). *Acta Cryst. E* **64**, m1397–m1398.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Shirvan, S. A. & Haydari Dezfuli, S. (2012). *Acta Cryst. E* **68**, m1006–m1007.
- Sofetis, A., Raptopoulou, C. P., Terzis, A. & Zafropoulos, T. F. (2006). *Inorg. Chim. Acta.* **359**, 3389–3395.
- Willett, R. D., Pon, G. & Nagy, C. (2001). *Inorg. Chem.* **40**, 4342–4352.
- Yousefi, M., Tadayon Pour, N., Amani, V. & Khavasi, H. R. (2008). *Acta Cryst. E* **64**, m1259.

supporting information

Acta Cryst. (2012). E68, m1495 [doi:10.1107/S1600536812046648]

(4,4'-Dimethyl-2,2'-bipyridine- κ^2N,N')(dimethylformamide- κO)diiodidocadmium

Sadif A. Shirvan, Sara Haydari Dezfuli, Fereydoon Khazali and Ali Borsalani

S1. Comment

Recently, we reported the synthesis and crystal structure of [CdBr₂(4,4'-dmbpy)(DMSO)] (Shirvan & Haydari Dezfuli, 2012) [where 4,4'-dmbpy is 4,4'-dimethyl-2,2'-bipyridine and DMSO is dimethyl sulfoxide]. 4,4'-Dimethyl-2,2'-bipyridine is a good bidentate ligand, and numerous complexes with 4,4'-dmbpy have been prepared, such as that of mercury (Kalateh *et al.*, 2008; Yousefi *et al.*, 2008), indium (Ahmadi *et al.*, 2008), iron (Amani *et al.*, 2009), platinum (Hojjat Kashani *et al.*, 2008), silver (Bellusci *et al.*, 2008), gallium (Sofetis *et al.*, 2006), copper (Willett *et al.*, 2001), cadmium (Kalateh *et al.*, 2010) and zinc (Alizadeh *et al.*, 2010). Here, we report the synthesis and structure of the title compound.

In the title compound, (Fig. 1), the Cd^{II} atom is five-coordinated in a distorted trigonal-bipyramidal configuration by two N atoms from one 4,4'-dimethyl-2,2'-bipyridine, one O atom from one dimethylformamide and two I atoms. The Cd—N, Cd—I and Cd—O bond lengths and angles are collected in Table 1.

In the crystal structure, π - π contacts (Fig. 2) between the pyridine rings, Cg2—Cg2ⁱ and Cg2—Cg3ⁱⁱ [symmetry cods: (i) 1-X,-Y,-Z and (ii) 2-X,-Y,-Z, where Cg2 and Cg3 are centroids of the rings (N1/C1—C3/C5—C6) and (N2/C7—C9/C11—C12), respectively] stabilize the structure, with centroid-centroid distance of 3.666 (3) and 3.709 (4) Å.

S2. Experimental

For the preparation of the title compound, a solution of 4,4'-dimethyl-2,2'-bipyridine (0.15 g, 0.80 mmol) in methanol (10 ml) was added to a solution of CdI₂ (0.29 g, 0.80 mmol) in methanol (5 ml) at room temperature. The suitable crystals for X-ray diffraction experiment were obtained by methanol diffusion to a colorless solution in dimethylformamide. Suitable crystals were isolated after one week (yield; 0.37 g, 74.2%).

S3. Refinement

H atoms were positioned geometrically with C—H = 0.93–0.96 Å and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

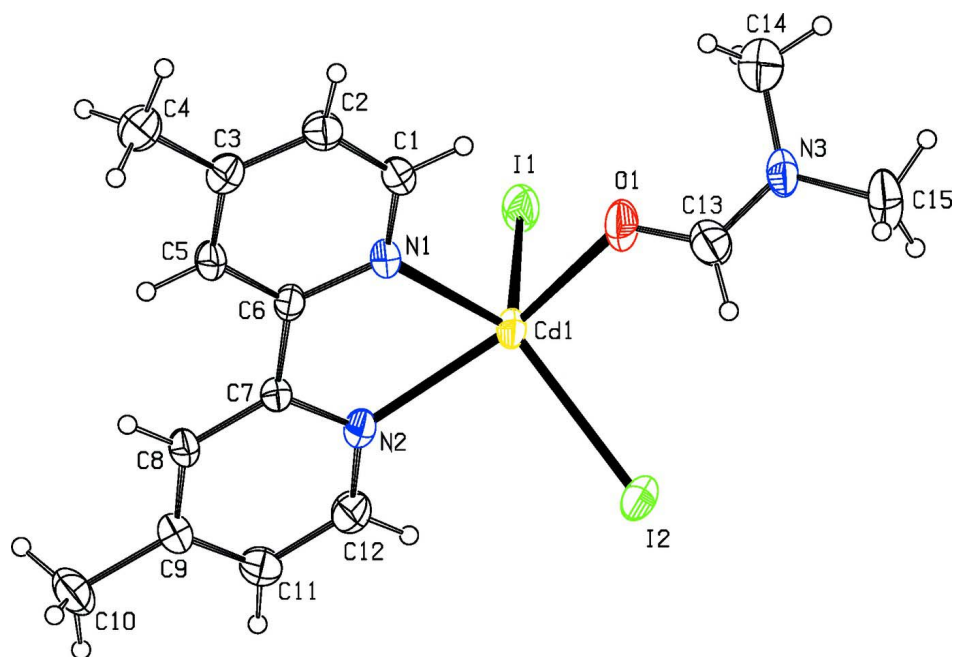
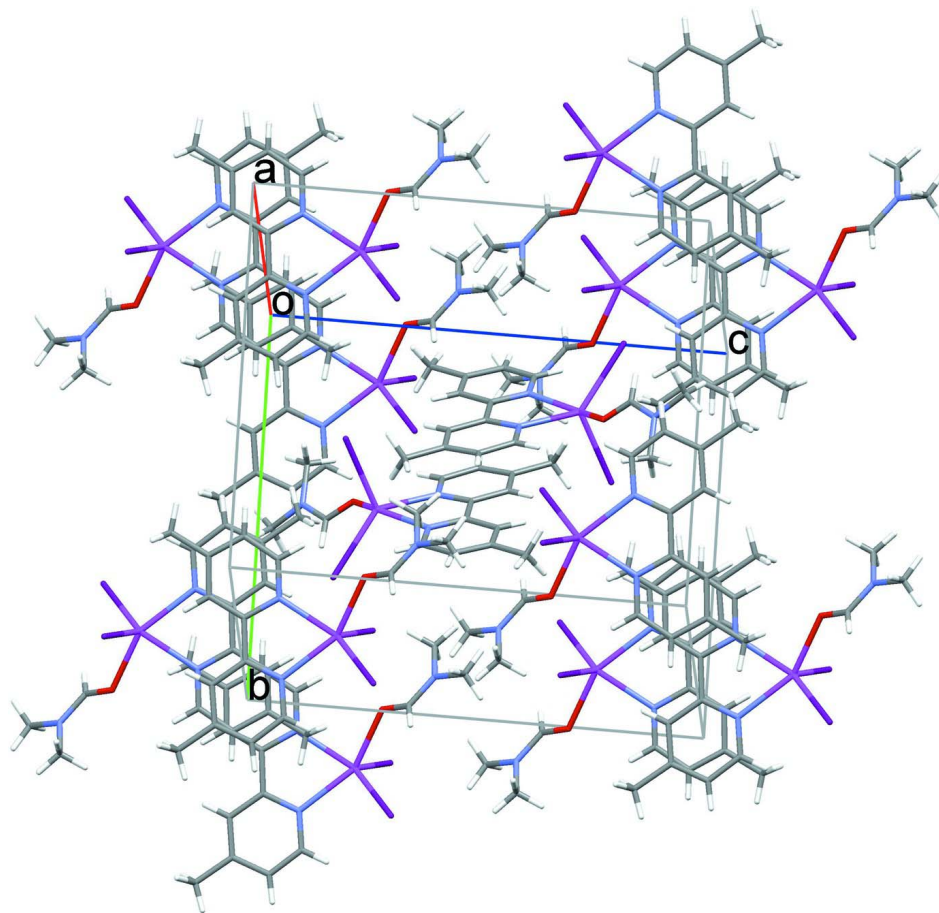


Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

**Figure 2**

Unit-cell packing diagram for title molecule.

(4,4'-Dimethyl-2,2'-bipyridine- κ^2N,N')(dimethylformamide- κO)diiodidocadmium

Crystal data

[CdI₂(C₁₂H₁₂N₂)(C₃H₇NO)]

$M_r = 623.54$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 8.6103$ (6) Å

$b = 15.1325$ (8) Å

$c = 15.4263$ (10) Å

$\beta = 98.347$ (5)°

$V = 1988.7$ (2) Å³

$Z = 4$

$F(000) = 1168$

$D_x = 2.083$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 12059 reflections

$\theta = 2.4$ – 26.0°

$\mu = 4.21$ mm⁻¹

$T = 298$ K

Prism, colorless

$0.45 \times 0.40 \times 0.35$ mm

Data collection

Bruker APEXII CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.188$, $T_{\max} = 0.223$

12059 measured reflections

3907 independent reflections

2859 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$
 $\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 2.4^\circ$
 $h = -10 \rightarrow 9$

$k = -18 \rightarrow 17$
 $l = -19 \rightarrow 19$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.084$
 $S = 0.98$
 3907 reflections
 199 parameters
 0 restraints
 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
 $w = 1/[\sigma^2(F_o^2) + (0.0426P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.007$
 $\Delta\rho_{\text{max}} = 0.85 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -1.08 \text{ e } \text{\AA}^{-3}$

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	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.8789 (8)	-0.0736 (4)	0.0980 (3)	0.0488 (15)
H1	0.9275	-0.0965	0.1510	0.059*
C2	0.9026 (7)	-0.1170 (4)	0.0221 (4)	0.0477 (15)
H2	0.9664	-0.1668	0.0242	0.057*
C3	0.8286 (7)	-0.0843 (4)	-0.0571 (3)	0.0444 (14)
C4	0.8494 (9)	-0.1285 (5)	-0.1415 (4)	0.0619 (19)
H4A	0.8981	-0.0881	-0.1774	0.074*
H4B	0.7488	-0.1460	-0.1719	0.074*
H4C	0.9147	-0.1797	-0.1295	0.074*
C5	0.7387 (7)	-0.0090 (4)	-0.0555 (3)	0.0404 (14)
H5	0.6901	0.0149	-0.1080	0.049*
C6	0.7189 (7)	0.0318 (4)	0.0225 (3)	0.0353 (12)
C7	0.6243 (6)	0.1118 (4)	0.0260 (3)	0.0346 (12)
C8	0.5479 (7)	0.1536 (4)	-0.0481 (3)	0.0412 (14)
H8	0.5560	0.1305	-0.1031	0.049*
C9	0.4610 (8)	0.2282 (4)	-0.0416 (4)	0.0500 (16)
C10	0.3786 (10)	0.2740 (5)	-0.1238 (4)	0.070 (2)
H10A	0.3051	0.2340	-0.1559	0.083*
H10B	0.4550	0.2917	-0.1600	0.083*
H10C	0.3238	0.3252	-0.1074	0.083*
C11	0.4523 (8)	0.2614 (5)	0.0406 (4)	0.0552 (17)
H11	0.3936	0.3118	0.0477	0.066*

C12	0.5324 (8)	0.2183 (5)	0.1124 (4)	0.0546 (17)
H12	0.5279	0.2417	0.1677	0.066*
C13	1.0539 (9)	-0.0020 (5)	0.3557 (4)	0.0620 (19)
H13	1.0829	0.0570	0.3635	0.074*
C14	1.0840 (14)	-0.1519 (7)	0.4055 (6)	0.116 (4)
H14A	1.1070	-0.1741	0.3504	0.140*
H14B	0.9743	-0.1597	0.4087	0.140*
H14C	1.1450	-0.1836	0.4525	0.140*
C15	1.2436 (9)	-0.0323 (6)	0.4837 (4)	0.077 (3)
H15A	1.2016	0.0111	0.5193	0.092*
H15B	1.3308	-0.0074	0.4597	0.092*
H15C	1.2782	-0.0828	0.5188	0.092*
N1	0.7921 (6)	-0.0018 (3)	0.1005 (3)	0.0413 (12)
N2	0.6153 (6)	0.1455 (3)	0.1065 (3)	0.0408 (12)
N3	1.1228 (6)	-0.0590 (4)	0.4127 (3)	0.0526 (14)
O1	0.9541 (6)	-0.0201 (4)	0.2930 (3)	0.0708 (15)
Cd1	0.74180 (5)	0.06619 (3)	0.22889 (2)	0.04265 (13)
I1	0.51473 (6)	-0.03208 (3)	0.29304 (2)	0.05923 (15)
I2	0.84760 (6)	0.21673 (3)	0.32035 (3)	0.06213 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.066 (4)	0.042 (4)	0.035 (3)	0.010 (3)	-0.003 (3)	0.003 (2)
C2	0.051 (4)	0.045 (4)	0.047 (3)	0.010 (3)	0.006 (3)	-0.002 (3)
C3	0.046 (3)	0.047 (4)	0.041 (3)	-0.004 (3)	0.008 (2)	-0.006 (2)
C4	0.082 (5)	0.059 (5)	0.047 (3)	0.011 (4)	0.016 (3)	-0.012 (3)
C5	0.049 (4)	0.046 (4)	0.025 (2)	0.001 (3)	0.004 (2)	0.001 (2)
C6	0.038 (3)	0.039 (3)	0.028 (2)	-0.006 (3)	0.001 (2)	-0.001 (2)
C7	0.040 (3)	0.034 (3)	0.029 (2)	-0.002 (3)	0.001 (2)	0.001 (2)
C8	0.052 (4)	0.043 (4)	0.026 (2)	0.004 (3)	0.000 (2)	0.002 (2)
C9	0.062 (4)	0.047 (4)	0.038 (3)	0.002 (3)	-0.003 (3)	0.007 (2)
C10	0.090 (6)	0.066 (5)	0.050 (3)	0.028 (4)	0.000 (3)	0.015 (3)
C11	0.063 (4)	0.044 (4)	0.057 (4)	0.015 (3)	0.000 (3)	-0.001 (3)
C12	0.069 (5)	0.052 (4)	0.043 (3)	0.008 (4)	0.007 (3)	-0.009 (3)
C13	0.063 (5)	0.062 (5)	0.057 (4)	-0.001 (4)	-0.004 (3)	0.011 (3)
C14	0.162 (11)	0.083 (7)	0.085 (6)	-0.012 (7)	-0.044 (7)	0.003 (5)
C15	0.067 (5)	0.115 (7)	0.042 (3)	-0.008 (5)	-0.012 (3)	0.009 (4)
N1	0.048 (3)	0.044 (3)	0.029 (2)	0.001 (2)	-0.0041 (19)	0.0007 (19)
N2	0.047 (3)	0.044 (3)	0.031 (2)	0.000 (2)	0.0004 (19)	-0.0054 (19)
N3	0.058 (3)	0.067 (4)	0.029 (2)	0.004 (3)	-0.003 (2)	0.000 (2)
O1	0.077 (4)	0.077 (4)	0.048 (2)	0.011 (3)	-0.025 (2)	-0.007 (2)
Cd1	0.0527 (3)	0.0474 (3)	0.02556 (18)	-0.0051 (2)	-0.00212 (15)	-0.00121 (16)
I1	0.0755 (3)	0.0669 (3)	0.03425 (19)	-0.0214 (2)	0.00443 (18)	0.00662 (17)
I2	0.0806 (3)	0.0571 (3)	0.0446 (2)	-0.0157 (2)	-0.0047 (2)	-0.01291 (18)

Geometric parameters (Å, °)

C1—N1	1.322 (8)	C10—H10C	0.9600
C1—C2	1.383 (8)	C11—C12	1.380 (8)
C1—H1	0.9300	C11—H11	0.9300
C2—C3	1.385 (8)	C12—N2	1.323 (8)
C2—H2	0.9300	C12—H12	0.9300
C3—C5	1.379 (9)	C13—O1	1.229 (8)
C3—C4	1.498 (8)	C13—N3	1.310 (8)
C4—H4A	0.9600	C13—H13	0.9300
C4—H4B	0.9600	C14—N3	1.445 (11)
C4—H4C	0.9600	C14—H14A	0.9600
C5—C6	1.384 (7)	C14—H14B	0.9600
C5—H5	0.9300	C14—H14C	0.9600
C6—N1	1.373 (6)	C15—N3	1.454 (8)
C6—C7	1.464 (8)	C15—H15A	0.9600
C7—N2	1.355 (6)	C15—H15B	0.9600
C7—C8	1.386 (7)	C15—H15C	0.9600
C8—C9	1.367 (9)	Cd1—N1	2.327 (4)
C8—H8	0.9300	Cd1—N2	2.365 (4)
C9—C11	1.377 (9)	Cd1—O1	2.345 (5)
C9—C10	1.527 (8)	Cd1—I1	2.7523 (7)
C10—H10A	0.9600	Cd1—I2	2.7635 (6)
C10—H10B	0.9600		
N1—C1—C2	124.6 (5)	N2—C12—C11	123.4 (5)
N1—C1—H1	117.7	N2—C12—H12	118.3
C2—C1—H1	117.7	C11—C12—H12	118.3
C1—C2—C3	118.1 (6)	O1—C13—N3	125.3 (7)
C1—C2—H2	120.9	O1—C13—H13	117.3
C3—C2—H2	120.9	N3—C13—H13	117.3
C5—C3—C2	117.8 (5)	N3—C14—H14A	109.5
C5—C3—C4	121.6 (5)	N3—C14—H14B	109.5
C2—C3—C4	120.6 (6)	H14A—C14—H14B	109.5
C3—C4—H4A	109.5	N3—C14—H14C	109.5
C3—C4—H4B	109.5	H14A—C14—H14C	109.5
H4A—C4—H4B	109.5	H14B—C14—H14C	109.5
C3—C4—H4C	109.5	N3—C15—H15A	109.5
H4A—C4—H4C	109.5	N3—C15—H15B	109.5
H4B—C4—H4C	109.5	H15A—C15—H15B	109.5
C3—C5—C6	121.7 (5)	N3—C15—H15C	109.5
C3—C5—H5	119.2	H15A—C15—H15C	109.5
C6—C5—H5	119.2	H15B—C15—H15C	109.5
N1—C6—C5	119.9 (5)	C1—N1—C6	117.9 (5)
N1—C6—C7	117.4 (4)	C1—N1—Cd1	124.4 (3)
C5—C6—C7	122.7 (5)	C6—N1—Cd1	117.6 (4)
N2—C7—C8	120.0 (5)	C12—N2—C7	118.7 (5)
N2—C7—C6	116.8 (4)	C12—N2—Cd1	123.9 (4)

C8—C7—C6	123.1 (5)	C7—N2—Cd1	117.4 (4)
C9—C8—C7	121.1 (5)	C13—N3—C14	120.8 (6)
C9—C8—H8	119.5	C13—N3—C15	121.7 (7)
C7—C8—H8	119.5	C14—N3—C15	117.4 (6)
C8—C9—C11	118.2 (5)	C13—O1—Cd1	128.4 (5)
C8—C9—C10	120.5 (5)	N1—Cd1—O1	83.23 (16)
C11—C9—C10	121.3 (6)	N1—Cd1—N2	70.51 (16)
C9—C10—H10A	109.5	O1—Cd1—N2	149.27 (18)
C9—C10—H10B	109.5	N1—Cd1—I1	107.25 (13)
H10A—C10—H10B	109.5	O1—Cd1—I1	95.65 (14)
C9—C10—H10C	109.5	N2—Cd1—I1	106.98 (12)
H10A—C10—H10C	109.5	N1—Cd1—I2	135.29 (13)
H10B—C10—H10C	109.5	O1—Cd1—I2	93.72 (12)
C9—C11—C12	118.7 (6)	N2—Cd1—I2	93.95 (12)
C9—C11—H11	120.7	I1—Cd1—I2	117.42 (2)
C12—C11—H11	120.7		
N1—C1—C2—C3	-1.1 (11)	C6—C7—N2—C12	179.2 (6)
C1—C2—C3—C5	1.5 (9)	C8—C7—N2—Cd1	177.8 (4)
C1—C2—C3—C4	-179.9 (6)	C6—C7—N2—Cd1	-3.2 (6)
C2—C3—C5—C6	-1.6 (9)	O1—C13—N3—C14	-0.2 (13)
C4—C3—C5—C6	179.8 (6)	O1—C13—N3—C15	178.0 (7)
C3—C5—C6—N1	1.1 (9)	N3—C13—O1—Cd1	147.5 (6)
C3—C5—C6—C7	179.9 (6)	C1—N1—Cd1—O1	16.0 (5)
N1—C6—C7—N2	-0.8 (8)	C6—N1—Cd1—O1	-168.1 (4)
C5—C6—C7—N2	-179.6 (5)	C1—N1—Cd1—N2	179.8 (6)
N1—C6—C7—C8	178.2 (5)	C6—N1—Cd1—N2	-4.4 (4)
C5—C6—C7—C8	-0.6 (9)	C1—N1—Cd1—I1	-77.8 (5)
N2—C7—C8—C9	-0.9 (9)	C6—N1—Cd1—I1	98.0 (4)
C6—C7—C8—C9	-179.9 (6)	C1—N1—Cd1—I2	104.5 (5)
C7—C8—C9—C11	0.6 (10)	C6—N1—Cd1—I2	-79.7 (4)
C7—C8—C9—C10	179.5 (6)	C13—O1—Cd1—N1	146.2 (7)
C8—C9—C11—C12	0.5 (11)	C13—O1—Cd1—N2	115.2 (6)
C10—C9—C11—C12	-178.4 (7)	C13—O1—Cd1—I1	-107.0 (6)
C9—C11—C12—N2	-1.3 (11)	C13—O1—Cd1—I2	11.0 (6)
C2—C1—N1—C6	0.6 (10)	C12—N2—Cd1—N1	-178.6 (6)
C2—C1—N1—Cd1	176.4 (5)	C7—N2—Cd1—N1	4.0 (4)
C5—C6—N1—C1	-0.6 (8)	C12—N2—Cd1—O1	-145.7 (5)
C7—C6—N1—C1	-179.4 (6)	C7—N2—Cd1—O1	36.9 (6)
C5—C6—N1—Cd1	-176.7 (4)	C12—N2—Cd1—I1	78.7 (5)
C7—C6—N1—Cd1	4.5 (6)	C7—N2—Cd1—I1	-98.8 (4)
C11—C12—N2—C7	0.9 (10)	C12—N2—Cd1—I2	-41.6 (5)
C11—C12—N2—Cd1	-176.5 (5)	C7—N2—Cd1—I2	140.9 (4)
C8—C7—N2—C12	0.2 (9)		