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## Structure Reports

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[2-Amino-4,6-bis(2-pyridyl)-1,3,5-triazine- $\kappa^3 N^4, N^5, N^6$ ]dichloridocadmium(II)

Man-Li Cao\* and Lei Shi

Department of Chemistry, Guangdong University of Education, Guangzhou 510303, People's Republic of China

Correspondence e-mail: caoml@mail3.sysu.edu.cn

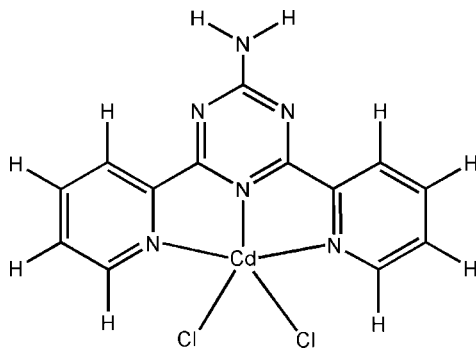
Received 8 March 2011; accepted 4 April 2011

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.020;  $wR$  factor = 0.056; data-to-parameter ratio = 13.0.

In the title compound,  $[\text{CdCl}_2(\text{C}_{13}\text{H}_{10}\text{N}_6)]$ , the 2-amino-4,6-bis(pyridin-2-yl)-1,3,5-triazine (HABPT) ligand adopts a tridentate tripyridyl coordination mode. The  $\text{Cd}^{\text{II}}$  atom is five-coordinated by three N atoms from the HABPT ligand and two chloride ions. In the crystal, molecules are linked *via*  $\text{N}-\text{H}\cdots\text{N}$ ,  $\text{N}-\text{H}\cdots\text{Cl}$  and  $\text{C}-\text{H}\cdots\text{Cl}$  hydrogen bonds into a supramolecular network.

## Related literature

For asymmetric ligands containing a triazine ring, see: Drew *et al.* (2000); Boubals *et al.* (2002); Medlycott *et al.* (2007); Chi *et al.* (2006); Cao *et al.* (2008, 2009). For the synthesis of the HABPT ligand, see: Case & Koft (1959). For metal complexes of the HABPT ligand, see: Drew *et al.* (2000); Boubals *et al.* (2002); Cao *et al.* (2009). For the diverse coordination modes of rigid multidentate polypyridyl ligands containing a triazine ring as a bridge, see: Zhou, Li, Wu & Zhang (2006); Zhou, Li, Zheng, Zhang & Wu (2006).



## Experimental

## Crystal data

$[\text{CdCl}_2(\text{C}_{13}\text{H}_{10}\text{N}_6)]$   
 $M_r = 433.58$   
 Triclinic,  $P\bar{1}$

$a = 8.8750$  (6) Å  
 $b = 9.2010$  (7) Å  
 $c = 10.2677$  (7) Å

$\alpha = 82.5151$  (9)°  
 $\beta = 65.636$  (1)°  
 $\gamma = 82.798$  (1)°  
 $V = 754.89$  (9) Å<sup>3</sup>  
 $Z = 2$

Mo  $K\alpha$  radiation  
 $\mu = 1.80$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.34 \times 0.31 \times 0.28$  mm

## Data collection

Bruker SMART APEX CCD  
 detector diffractometer  
 Absorption correction: multi-scan  
 (*SADABS*; Bruker, 2005)  
 $T_{\min} = 0.581$ ,  $T_{\max} = 0.636$

5102 measured reflections  
 2588 independent reflections  
 2499 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.014$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.020$   
 $wR(F^2) = 0.056$   
 $S = 1.01$   
 2588 reflections

199 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.28$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.30$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$                                         | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|-------------------------------------------------------|-------|-------------|-------------|---------------|
| $\text{N6}-\text{H6A}\cdots\text{N3}^{\text{i}}$      | 0.91  | 2.31        | 3.183 (3)   | 162           |
| $\text{N6}-\text{H6B}\cdots\text{Cl2}^{\text{ii}}$    | 0.91  | 2.45        | 3.334 (2)   | 165           |
| $\text{C12}-\text{H12A}\cdots\text{Cl1}^{\text{iii}}$ | 0.97  | 2.76        | 3.671 (2)   | 158           |
| $\text{C2}-\text{H2A}\cdots\text{Cl1}^{\text{iv}}$    | 0.97  | 2.75        | 3.705 (3)   | 166           |
| $\text{C11}-\text{H11A}\cdots\text{Cl2}^{\text{v}}$   | 0.97  | 2.82        | 3.596 (2)   | 138           |

Symmetry codes: (i)  $-x, -y + 2, -z + 1$ ; (ii)  $-x, -y + 1, -z + 1$ ; (iii)  $-x, -y, -z + 2$ ; (iv)  $-x + 1, -y + 1, -z + 2$ ; (v)  $x - 1, y, z$ .

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: ZQ2094).

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## supporting information

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**[2-Amino-4,6-bis(2-pyridyl)-1,3,5-triazine- $\kappa^3N^4,N^5,N^6$ ]dichloridocadmium(II)****Man-Li Cao and Lei Shi****S1. Comment**

The rigid multidentate polypyridyl ligands containing a triazine ring as a bridge have attracted greatly our attention due to their coordination diversity (Zhou, Li, Wu & Zhang, 2006; Zhou, Li, Zheng, Zhang & Wu, 2006). Although coordination chemistry of the symmetrical ligands like tri(2-pyridyl)-1,3,5-triazine (TPT) has been well explored, the observations on the asymmetric ligands containing triazine ring are still rare (Drew *et al.*, 2000; Boubals *et al.*, 2002; Medlycott *et al.*, 2007; Chi *et al.*, 2006; Cao *et al.*, 2008, 2009).

The ligand 2-amino-4,6-bis(2-pyridyl)-1,3,5-triazine (HABPT) has five potential coordinate sites, it may offer a tridentate chelating mode or bis-bidentate binding mode with the capability of bridging two metal ions in chelating way (Drew *et al.* 2000; Boubals *et al.*, 2002; Cao *et al.*, 2009). As a contribution to the synthesis and structural studies of coordination abilities of the ligand (Case *et al.*, 1959; Drew *et al.*, 2000; Boubals *et al.*, 2002 and Cao *et al.*, 2009), we present here the crystal structure of the title compound, a new cadmium(II) complex with the HABPT ligand.

Within the title compound,  $C_{13}H_{10}CdCl_2N_6$ , the  $Cd^{II}$  center is five-coordinated respectively by three N atoms [Cd—N1 2.387 (2), Cd—N2 2.2679 (18), Cd—N5 2.433 (2) Å] from the HABPT ligand and two Cl atoms [Cd—Cl1 2.4176 (7) and Cd—Cl2 2.4431 (7) Å]. The ligand adopts a tridentate tripyridyl mode to coordinate to the  $Cd^{II}$  ion. Two chloride ligands are posited up and down the plane of the ligand that further accept hydrogen bonds from other ligands, the deviations values of Cd, Cl1 and Cl2 from the least-squares plane (rms deviation 0.122 Å for all non-H atoms of the planar tridentate ligand) are -0.603 (1), 0.540 (2) and -2.997 (1) Å, respectively. Viewed from the whole crystal structure, molecules are linked by intermolecular N—H $\cdots$ N, N—H $\cdots$ Cl and C—H $\cdots$ Cl hydrogen bonds to form a supramolecular structure. A weak intermolecular  $\pi$ – $\pi$  interaction between the triazine ring and one pyridyl ring is also observed with a centroid-centroid distance of 3.976 (1) Å.

**S2. Experimental**

The ligand HABPT was prepared according to previously reported procedures (F.H. Case *et al.*, 1959). To a suspension of HABPT (0.025 g, 0.1 mmol) in 7 ml of ethanol was added the solution of  $CdCl_2$  (0.018 g, 0.1 mmol) in 7 ml distilled water. The resulting mixture was vibrated under ultrasonic condition for 20 min and then filtered. The obtained colorless filtrate was allowed to stay at ambient temperature for one week giving 0.026 g (60% yield, based on the ligand) of colourless crystals suitable for a structural determination.

Anal. Calcd. for  $C_{13}H_{10}Cl_2N_6Cd$  (%): C 36.01, H 2.31, N 19.38; found (%): C 36.12, H 2.40, N 19.31.

**S3. Refinement**

All H atoms were fixed geometrically and treated as riding with C—H = 0.96–0.99 Å and N—H = 0.90–0.91 Å with  $U_{iso}(H) = 1.2 U_{eq}(C \text{ or } N)$ .

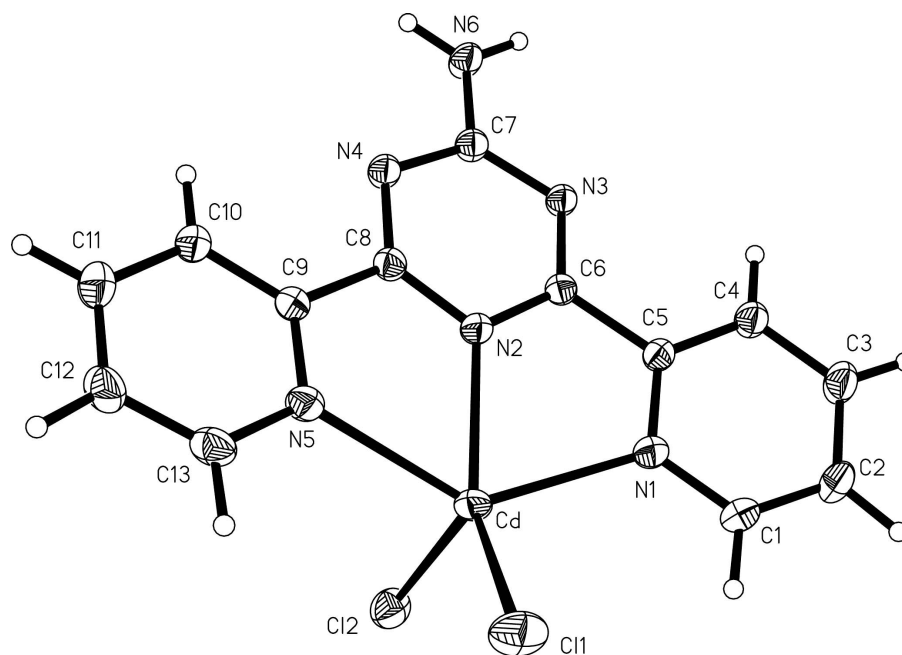


Figure 1

View of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

**[2-Amino-4,6-bis(2-pyridyl)-1,3,5-triazine-  $\kappa^3 N^4, N^5, N^6$ ]dichloridocadmium(II)**

*Crystal data*

$[\text{CdCl}_2(\text{C}_{13}\text{H}_{10}\text{N}_6)]$

$M_r = 433.58$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 8.8750\ (6)\ \text{\AA}$

$b = 9.2010\ (7)\ \text{\AA}$

$c = 10.2677\ (7)\ \text{\AA}$

$\alpha = 82.5151\ (9)^\circ$

$\beta = 65.636\ (1)^\circ$

$\gamma = 82.798\ (1)^\circ$

$V = 754.89\ (9)\ \text{\AA}^3$

$Z = 2$

$F(000) = 424$

$D_x = 1.908\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2588 reflections

$\theta = 2.2\text{--}25.0^\circ$

$\mu = 1.80\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, colourless

$0.34 \times 0.31 \times 0.28\ \text{mm}$

*Data collection*

Bruker SMART APEX CCD detector  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2005)

$T_{\min} = 0.581$ ,  $T_{\max} = 0.636$

5102 measured reflections

2588 independent reflections

2499 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.014$

$\theta_{\max} = 25.0^\circ$ ,  $\theta_{\min} = 2.2^\circ$

$h = -10 \rightarrow 10$

$k = -10 \rightarrow 10$

$l = -12 \rightarrow 12$

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.020$  $wR(F^2) = 0.056$  $S = 1.01$ 

2588 reflections

199 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0354P)^2 + 0.2818P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.001$  $\Delta\rho_{\max} = 0.28 \text{ e } \text{\AA}^{-3}$  $\Delta\rho_{\min} = -0.30 \text{ e } \text{\AA}^{-3}$ *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 ( $\text{\AA}^2$ )*

|     | <i>x</i>     | <i>y</i>      | <i>z</i>      | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|---------------|---------------|----------------------------------|
| Cd  | 0.21372 (2)  | 0.386656 (17) | 0.788019 (17) | 0.03420 (8)                      |
| Cl1 | 0.22830 (10) | 0.26193 (9)   | 1.00530 (7)   | 0.05660 (19)                     |
| Cl2 | 0.41551 (8)  | 0.26525 (8)   | 0.58040 (7)   | 0.04683 (16)                     |
| N1  | 0.2999 (2)   | 0.6218 (2)    | 0.7893 (2)    | 0.0354 (4)                       |
| N2  | 0.0652 (2)   | 0.5692 (2)    | 0.7109 (2)    | 0.0316 (4)                       |
| N3  | 0.0354 (2)   | 0.8157 (2)    | 0.6236 (2)    | 0.0307 (4)                       |
| N4  | −0.1444 (2)  | 0.6385 (2)    | 0.6264 (2)    | 0.0332 (4)                       |
| N5  | −0.0378 (2)  | 0.2992 (2)    | 0.7962 (2)    | 0.0352 (4)                       |
| N6  | −0.1636 (3)  | 0.8735 (2)    | 0.5305 (2)    | 0.0404 (5)                       |
| H6A | −0.1322      | 0.9668        | 0.5070        | 0.048*                           |
| H6B | −0.2468      | 0.8494        | 0.5095        | 0.048*                           |
| C1  | 0.4108 (3)   | 0.6446 (3)    | 0.8398 (3)    | 0.0444 (6)                       |
| H1A | 0.4555       | 0.5567        | 0.8820        | 0.053*                           |
| C2  | 0.4571 (3)   | 0.7822 (3)    | 0.8394 (3)    | 0.0472 (6)                       |
| H2A | 0.5370       | 0.7896        | 0.8800        | 0.057*                           |
| C3  | 0.3859 (3)   | 0.9019 (3)    | 0.7847 (3)    | 0.0467 (6)                       |
| H3A | 0.4194       | 0.9989        | 0.7835        | 0.056*                           |
| C4  | 0.2714 (3)   | 0.8806 (3)    | 0.7307 (3)    | 0.0377 (5)                       |
| H4A | 0.2264       | 0.9664        | 0.6864        | 0.045*                           |
| C5  | 0.2318 (3)   | 0.7398 (3)    | 0.7343 (2)    | 0.0303 (5)                       |
| C6  | 0.1044 (3)   | 0.7081 (2)    | 0.6848 (2)    | 0.0290 (5)                       |
| C7  | −0.0883 (3)  | 0.7746 (3)    | 0.5937 (2)    | 0.0321 (5)                       |
| C8  | −0.0629 (3)  | 0.5416 (2)    | 0.6838 (2)    | 0.0303 (5)                       |
| C9  | −0.1177 (3)  | 0.3903 (2)    | 0.7273 (2)    | 0.0311 (5)                       |
| C10 | −0.2455 (3)  | 0.3474 (3)    | 0.7005 (3)    | 0.0381 (5)                       |

|      |             |            |            |            |
|------|-------------|------------|------------|------------|
| H10A | −0.3033     | 0.4136     | 0.6498     | 0.046*     |
| C11  | −0.2923 (3) | 0.2053 (3) | 0.7456 (3) | 0.0481 (6) |
| H11A | −0.3814     | 0.1696     | 0.7309     | 0.058*     |
| C12  | −0.2127 (3) | 0.1126 (3) | 0.8178 (3) | 0.0478 (6) |
| H12A | −0.2415     | 0.0132     | 0.8551     | 0.057*     |
| C13  | −0.0864 (3) | 0.1634 (3) | 0.8405 (3) | 0.0427 (6) |
| H13A | −0.0270     | 0.0998     | 0.8914     | 0.051*     |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Cd  | 0.03892 (12) | 0.02984 (12) | 0.03786 (12) | 0.00290 (8)  | −0.02185 (9) | −0.00009 (8) |
| Cl1 | 0.0672 (4)   | 0.0623 (5)   | 0.0399 (3)   | 0.0064 (4)   | −0.0279 (3)  | 0.0077 (3)   |
| Cl2 | 0.0430 (3)   | 0.0568 (4)   | 0.0433 (3)   | 0.0013 (3)   | −0.0188 (3)  | −0.0137 (3)  |
| N1  | 0.0387 (10)  | 0.0315 (11)  | 0.0427 (11)  | 0.0007 (8)   | −0.0245 (9)  | −0.0014 (8)  |
| N2  | 0.0321 (10)  | 0.0272 (10)  | 0.0403 (10)  | −0.0013 (8)  | −0.0199 (8)  | −0.0015 (8)  |
| N3  | 0.0352 (10)  | 0.0268 (10)  | 0.0355 (10)  | −0.0027 (8)  | −0.0204 (8)  | 0.0005 (8)   |
| N4  | 0.0390 (10)  | 0.0284 (10)  | 0.0389 (10)  | −0.0042 (8)  | −0.0236 (9)  | 0.0023 (8)   |
| N5  | 0.0368 (10)  | 0.0294 (11)  | 0.0401 (11)  | −0.0015 (8)  | −0.0180 (9)  | 0.0021 (8)   |
| N6  | 0.0485 (12)  | 0.0314 (11)  | 0.0551 (13)  | −0.0068 (9)  | −0.0372 (11) | 0.0088 (9)   |
| C1  | 0.0432 (14)  | 0.0467 (16)  | 0.0534 (16)  | 0.0046 (12)  | −0.0312 (13) | −0.0062 (12) |
| C2  | 0.0435 (14)  | 0.0562 (18)  | 0.0551 (16)  | −0.0070 (12) | −0.0313 (13) | −0.0081 (13) |
| C3  | 0.0494 (15)  | 0.0447 (16)  | 0.0565 (16)  | −0.0134 (12) | −0.0295 (13) | −0.0030 (12) |
| C4  | 0.0429 (13)  | 0.0329 (13)  | 0.0436 (13)  | −0.0066 (10) | −0.0237 (11) | 0.0003 (10)  |
| C5  | 0.0294 (11)  | 0.0331 (13)  | 0.0303 (11)  | −0.0029 (9)  | −0.0141 (9)  | −0.0025 (9)  |
| C6  | 0.0315 (11)  | 0.0275 (12)  | 0.0300 (11)  | −0.0012 (9)  | −0.0147 (9)  | −0.0026 (9)  |
| C7  | 0.0358 (12)  | 0.0307 (12)  | 0.0325 (11)  | −0.0027 (9)  | −0.0172 (10) | −0.0001 (9)  |
| C8  | 0.0328 (11)  | 0.0278 (12)  | 0.0317 (11)  | −0.0017 (9)  | −0.0149 (9)  | −0.0017 (9)  |
| C9  | 0.0323 (11)  | 0.0279 (12)  | 0.0333 (11)  | −0.0016 (9)  | −0.0136 (9)  | −0.0024 (9)  |
| C10 | 0.0375 (12)  | 0.0340 (13)  | 0.0467 (14)  | −0.0033 (10) | −0.0211 (11) | −0.0027 (10) |
| C11 | 0.0459 (15)  | 0.0414 (15)  | 0.0608 (17)  | −0.0142 (12) | −0.0233 (13) | −0.0007 (13) |
| C12 | 0.0489 (15)  | 0.0310 (14)  | 0.0585 (17)  | −0.0117 (11) | −0.0168 (13) | 0.0048 (12)  |
| C13 | 0.0440 (14)  | 0.0315 (13)  | 0.0474 (14)  | −0.0008 (11) | −0.0166 (12) | 0.0065 (11)  |

*Geometric parameters (Å, °)*

|        |             |         |           |
|--------|-------------|---------|-----------|
| Cd—N2  | 2.2679 (18) | C1—C2   | 1.378 (4) |
| Cd—N1  | 2.387 (2)   | C1—H1A  | 0.9845    |
| Cd—Cl1 | 2.4176 (7)  | C2—C3   | 1.373 (4) |
| Cd—N5  | 2.433 (2)   | C2—H2A  | 0.9723    |
| Cd—Cl2 | 2.4431 (7)  | C3—C4   | 1.386 (3) |
| N1—C1  | 1.336 (3)   | C3—H3A  | 0.9727    |
| N1—C5  | 1.349 (3)   | C4—C5   | 1.376 (3) |
| N2—C6  | 1.331 (3)   | C4—H4A  | 0.9838    |
| N2—C8  | 1.337 (3)   | C5—C6   | 1.489 (3) |
| N3—C6  | 1.324 (3)   | C8—C9   | 1.485 (3) |
| N3—C7  | 1.362 (3)   | C9—C10  | 1.384 (3) |
| N4—C8  | 1.311 (3)   | C10—C11 | 1.385 (4) |

|              |              |              |             |
|--------------|--------------|--------------|-------------|
| N4—C7        | 1.356 (3)    | C10—H10A     | 0.9818      |
| N5—C13       | 1.333 (3)    | C11—C12      | 1.375 (4)   |
| N5—C9        | 1.348 (3)    | C11—H11A     | 0.9664      |
| N6—C7        | 1.321 (3)    | C12—C13      | 1.381 (4)   |
| N6—H6A       | 0.9078       | C12—H12A     | 0.9670      |
| N6—H6B       | 0.9080       | C13—H13A     | 0.9815      |
| N2—Cd—N1     | 68.97 (6)    | C4—C3—H3A    | 122.2       |
| N2—Cd—Cl1    | 141.58 (5)   | C5—C4—C3     | 118.9 (2)   |
| N1—Cd—Cl1    | 100.97 (5)   | C5—C4—H4A    | 122.6       |
| N2—Cd—N5     | 69.07 (7)    | C3—C4—H4A    | 118.4       |
| N1—Cd—N5     | 134.84 (7)   | N1—C5—C4     | 122.3 (2)   |
| Cl1—Cd—N5    | 101.44 (5)   | N1—C5—C6     | 115.38 (19) |
| N2—Cd—Cl2    | 108.57 (5)   | C4—C5—C6     | 122.3 (2)   |
| N1—Cd—Cl2    | 109.67 (5)   | N3—C6—N2     | 124.7 (2)   |
| Cl1—Cd—Cl2   | 109.69 (3)   | N3—C6—C5     | 120.0 (2)   |
| N5—Cd—Cl2    | 98.80 (5)    | N2—C6—C5     | 115.24 (19) |
| C1—N1—C5     | 117.9 (2)    | N6—C7—N4     | 116.1 (2)   |
| C1—N1—Cd     | 124.73 (17)  | N6—C7—N3     | 118.9 (2)   |
| C5—N1—Cd     | 117.40 (14)  | N4—C7—N3     | 124.9 (2)   |
| C6—N2—C8     | 116.34 (19)  | N4—C8—N2     | 124.9 (2)   |
| C6—N2—Cd     | 122.13 (14)  | N4—C8—C9     | 118.8 (2)   |
| C8—N2—Cd     | 121.48 (15)  | N2—C8—C9     | 116.28 (19) |
| C6—N3—C7     | 114.17 (19)  | N5—C9—C10    | 122.5 (2)   |
| C8—N4—C7     | 114.62 (19)  | N5—C9—C8     | 116.0 (2)   |
| C13—N5—C9    | 117.9 (2)    | C10—C9—C8    | 121.5 (2)   |
| C13—N5—Cd    | 125.93 (16)  | C9—C10—C11   | 118.7 (2)   |
| C9—N5—Cd     | 115.21 (15)  | C9—C10—H10A  | 122.5       |
| C7—N6—H6A    | 120.1        | C11—C10—H10A | 118.8       |
| C7—N6—H6B    | 120.9        | C12—C11—C10  | 119.0 (2)   |
| H6A—N6—H6B   | 119.0        | C12—C11—H11A | 118.6       |
| N1—C1—C2     | 123.1 (2)    | C10—C11—H11A | 122.4       |
| N1—C1—H1A    | 115.9        | C11—C12—C13  | 118.9 (2)   |
| C2—C1—H1A    | 121.0        | C11—C12—H12A | 123.4       |
| C3—C2—C1     | 118.6 (2)    | C13—C12—H12A | 117.7       |
| C3—C2—H2A    | 123.3        | N5—C13—C12   | 123.0 (2)   |
| C1—C2—H2A    | 118.0        | N5—C13—H13A  | 116.2       |
| C2—C3—C4     | 119.2 (2)    | C12—C13—H13A | 120.8       |
| C2—C3—H3A    | 118.6        |              |             |
| N2—Cd—N1—C1  | 174.8 (2)    | C7—N3—C6—N2  | 2.9 (3)     |
| Cl1—Cd—N1—C1 | 33.5 (2)     | C7—N3—C6—C5  | −175.0 (2)  |
| N5—Cd—N1—C1  | 152.02 (19)  | C8—N2—C6—N3  | −6.0 (3)    |
| Cl2—Cd—N1—C1 | −82.2 (2)    | Cd—N2—C6—N3  | 171.45 (17) |
| N2—Cd—N1—C5  | −5.55 (16)   | C8—N2—C6—C5  | 172.00 (19) |
| Cl1—Cd—N1—C5 | −146.86 (16) | Cd—N2—C6—C5  | −10.6 (3)   |
| N5—Cd—N1—C5  | −28.3 (2)    | N1—C5—C6—N3  | −177.2 (2)  |
| Cl2—Cd—N1—C5 | 97.44 (16)   | C4—C5—C6—N3  | 5.9 (3)     |

|               |              |                 |              |
|---------------|--------------|-----------------|--------------|
| N1—Cd—N2—C6   | 8.74 (16)    | N1—C5—C6—N2     | 4.8 (3)      |
| Cl1—Cd—N2—C6  | 89.73 (18)   | C4—C5—C6—N2     | −172.2 (2)   |
| N5—Cd—N2—C6   | 171.65 (19)  | C8—N4—C7—N6     | 177.5 (2)    |
| Cl2—Cd—N2—C6  | −95.81 (17)  | C8—N4—C7—N3     | −3.8 (3)     |
| N1—Cd—N2—C8   | −173.96 (19) | C6—N3—C7—N6     | −179.0 (2)   |
| Cl1—Cd—N2—C8  | −92.97 (18)  | C6—N3—C7—N4     | 2.3 (3)      |
| N5—Cd—N2—C8   | −11.05 (17)  | C7—N4—C8—N2     | 0.3 (3)      |
| Cl2—Cd—N2—C8  | 81.49 (17)   | C7—N4—C8—C9     | 178.3 (2)    |
| N2—Cd—N5—C13  | −179.5 (2)   | C6—N2—C8—N4     | 4.2 (3)      |
| N1—Cd—N5—C13  | −156.69 (19) | Cd—N2—C8—N4     | −173.20 (17) |
| Cl1—Cd—N5—C13 | −38.3 (2)    | C6—N2—C8—C9     | −173.76 (19) |
| Cl2—Cd—N5—C13 | 73.9 (2)     | Cd—N2—C8—C9     | 8.8 (3)      |
| N2—Cd—N5—C9   | 12.20 (16)   | C13—N5—C9—C10   | −0.6 (4)     |
| N1—Cd—N5—C9   | 35.0 (2)     | Cd—N5—C9—C10    | 168.70 (18)  |
| Cl1—Cd—N5—C9  | 153.32 (16)  | C13—N5—C9—C8    | 178.2 (2)    |
| Cl2—Cd—N5—C9  | −94.40 (16)  | Cd—N5—C9—C8     | −12.4 (3)    |
| C5—N1—C1—C2   | 0.6 (4)      | N4—C8—C9—N5     | −174.8 (2)   |
| Cd—N1—C1—C2   | −179.7 (2)   | N2—C8—C9—N5     | 3.3 (3)      |
| N1—C1—C2—C3   | 0.1 (4)      | N4—C8—C9—C10    | 4.0 (3)      |
| C1—C2—C3—C4   | −0.6 (4)     | N2—C8—C9—C10    | −177.8 (2)   |
| C2—C3—C4—C5   | 0.4 (4)      | N5—C9—C10—C11   | −0.3 (4)     |
| C1—N1—C5—C4   | −0.9 (3)     | C8—C9—C10—C11   | −179.1 (2)   |
| Cd—N1—C5—C4   | 179.46 (18)  | C9—C10—C11—C12  | 1.2 (4)      |
| C1—N1—C5—C6   | −177.8 (2)   | C10—C11—C12—C13 | −1.2 (4)     |
| Cd—N1—C5—C6   | 2.5 (3)      | C9—N5—C13—C12   | 0.6 (4)      |
| C3—C4—C5—N1   | 0.3 (4)      | Cd—N5—C13—C12   | −167.4 (2)   |
| C3—C4—C5—C6   | 177.1 (2)    | C11—C12—C13—N5  | 0.3 (4)      |

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

| $D\cdots H\cdots A$                  | $D\cdots H$ | $H\cdots A$ | $D\cdots A$ | $D\cdots H\cdots A$ |
|--------------------------------------|-------------|-------------|-------------|---------------------|
| N6—H6A $\cdots$ N3 <sup>i</sup>      | 0.91        | 2.31        | 3.183 (3)   | 162                 |
| N6—H6B $\cdots$ Cl2 <sup>ii</sup>    | 0.91        | 2.45        | 3.334 (2)   | 165                 |
| C12—H12A $\cdots$ Cl1 <sup>iii</sup> | 0.97        | 2.76        | 3.671 (2)   | 158                 |
| C2—H2A $\cdots$ Cl1 <sup>iv</sup>    | 0.97        | 2.75        | 3.705 (3)   | 166                 |
| C11—H11A $\cdots$ Cl2 <sup>v</sup>   | 0.97        | 2.82        | 3.596 (2)   | 138                 |

Symmetry codes: (i)  $-x, -y+2, -z+1$ ; (ii)  $-x, -y+1, -z+1$ ; (iii)  $-x, -y, -z+2$ ; (iv)  $-x+1, -y+1, -z+2$ ; (v)  $x-1, y, z$ .