

## catena-Poly[[chloridocadmium(II)]bis[ $\mu$ -1-[(2-ethyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole][chloridocadmium(II)]di- $\mu$ -chlorido]

Xia Wang,<sup>a\*</sup> Xian-Ju Shi,<sup>b</sup> Huai-Xia Yang,<sup>a</sup> Hu Feng<sup>a</sup> and Pan Liu<sup>a</sup>

<sup>a</sup>Pharmacy College, Henan University of Traditional Chinese Medicine, Zhengzhou 450008, People's Republic of China, and <sup>b</sup>Department of Petroleum & Chemical Engineering, Puyang Vocational and Technical College, Puyang 457000, People's Republic of China

Correspondence e-mail: wangxiawx83@yahoo.com.cn

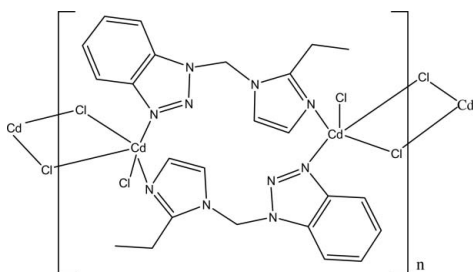
Received 12 May 2011; accepted 25 May 2011

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.035;  $wR$  factor = 0.069; data-to-parameter ratio = 16.3.

In the polymeric title complex,  $[\text{CdCl}_2(\text{C}_{12}\text{H}_{13}\text{N}_5)]_n$ , the  $\text{Cd}^{\text{II}}$  atom is five-coordinated by two N atoms from two bridging 1-[(2-ethyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole (bmei) ligands, two bridging Cl atoms and one terminal Cl atom in a distorted trigonal-bipyramidal geometry. The  $\text{Cd}^{\text{II}}$  atoms are connected alternately by the Cl atoms and bmei ligands, leading to a zigzag chain extending parallel to [011].  $\pi$ - $\pi$  interactions, with a centroid-centroid distance of 3.3016 (3) Å, help to stabilize the crystal packing.

### Related literature

For similar compounds with symmetric or asymmetric *N*-heterocyclic ligands, see: Li *et al.* (2011); Hu *et al.* (2009); Meng *et al.* (2009); Huang *et al.* (2006).



### Experimental

#### Crystal data

$[\text{CdCl}_2(\text{C}_{12}\text{H}_{13}\text{N}_5)]$   
 $M_r = 410.57$   
 Triclinic,  $P\bar{1}$   
 $a = 7.6055$  (6) Å  
 $b = 9.7027$  (11) Å  
 $c = 10.3144$  (10) Å  
 $\alpha = 74.431$  (9)°  
 $\beta = 81.609$  (7)°

$\gamma = 87.720$  (8)°  
 $V = 725.36$  (12) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.87$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.20 \times 0.20 \times 0.18$  mm

#### Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer  
 Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010)  
 $T_{\text{min}} = 0.993$ ,  $T_{\text{max}} = 1.000$

6082 measured reflections  
 2963 independent reflections  
 2534 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.069$   
 $S = 1.02$   
 2963 reflections

182 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.47$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.50$  e Å<sup>-3</sup>

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors thank the Department of Science and Technology of Henan Province for financial support (No. 082102330003), and Professors Hong-Wei Hou and Meng Xiang-Ru of Zhengzhou University for their help.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2490).

### References

- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.  
 Hu, M.-C., Wang, Y., Zhai, Q.-G., Li, S.-N., Jiang, Y.-C. & Zhang, Y. (2009). *Inorg. Chem.* **48**, 1449–1468.  
 Huang, M.-H., Liu, P., Wang, J., Chen, Y. & Liu, Q.-Y. (2006). *Inorg. Chem. Commun.* **9**, 952–954.  
 Li, B.-Y., Yang, F., Li, G.-H., Liu, D., Zhou, Q., Shi, Z. & Feng, S.-H. (2011). *Cryst. Growth Des.* **11**, 1475–1485.  
 Meng, X.-R., Jin, S.-Z., Hou, H.-W., Du, C.-X. & Ng, S. W. (2009). *Inorg. Chim. Acta*, **362**, 1519–1527.  
 Oxford Diffraction (2010). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, England.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

**supplementary materials**

*Acta Cryst.* (2011). E67, m846 [ doi:10.1107/S1600536811019908 ]

**catena-Poly[[chloridocadmium(II)]bis{ $\mu$ -1-[(2-ethyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole}[chloridocadmium(II)]di- $\mu$ -chlorido]**

**X. Wang, X.-J. Shi, H.-X. Yang, H. Feng and P. Liu**

**Comment**

In coordination and supramolecular chemistry many symmetric imidazole and benzotriazole ligands have been applied (Li *et al.*, 2011; Hu *et al.*, 2009). However, studies involving asymmetric imidazole and benzotriazole ligands are rather rare (Meng *et al.*, 2009; Huang *et al.*, 2006). We were thus engaged in the synthesis of asymmetric N-heterocyclic ligands and synthesized the compound 1-[(1*H*-benzotriazol-1-yl)methyl]-1*H*-1,3-(2-ethyl-imidazol) (bmei). In this work, we selected this compound as a ligand for generation of the new complex [Cd(C<sub>12</sub>H<sub>13</sub>N<sub>5</sub>)Cl<sub>2</sub>]<sub>n</sub> (I), that is reported here.

In the complex (I) the Cd<sup>II</sup> atom is five-coordinated by two N atoms from two bridging bmei ligands, two bridging Cl atoms and one terminal Cl atom in a distorted trigonal-bipyramidal geometry (Fig. 1). The two Cd<sup>II</sup> ions are connected by a pair of bridging Cl atoms, yielding a centrosymmetric Cd<sub>2</sub>Cl<sub>2</sub> binuclear unit with a Cd...Cd distance of 3.9657 (6) Å. The dimers are further linked by bmei ligands to give a zigzag chain extending parallel to [011] (Fig. 2). The distance between two Cd atoms bridged by the bmei ligand is 9.0727 (12) Å. In addition, the benzotriazole rings between adjacent chains are stacked in a face-to-face orientation with a centroid—centroid distance of 3.3016 (3) Å, so the crystal structure involves also  $\pi$ — $\pi$  interactions.

**Experimental**

The ligand 1-[(1*H*-benzotriazol-1-yl)methyl]-1*H*-1,3-(2-ethyl-imidazol) (0.04 mmol, 0.0096 g) in methanol (6 ml) was added dropwise to a methanol solution (5 ml) of CdCl<sub>2</sub> (0.04 mmol, 0.0074 g) in methanol. The resulting solution was allowed to stand at room temperature. After one week good quality colourless crystals were obtained and dried in air.

**Refinement**

H atoms were placed geometrically and refined as riding atoms with C-H = 0.93 Å and U<sub>iso</sub>(H) = 1.2U<sub>eq</sub>(C).

**Figures**

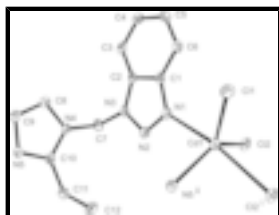


Fig. 1. A fragment of the title complex, showing the coordination of the Cd<sup>II</sup> atom with atom labelling of the non-H atoms and with 30% probability ellipsoids. [Symmetry codes: (i) -x + 1, -y + 1, -z + 1; (ii) -x + 1, -y + 2, -z.]

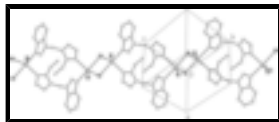


Fig. 2. View of the zigzag chain structure of the title complex.

**catena-Poly[[chloridocadmium(II)]bis{ $\mu$ -1-[(2-ethyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole}[chloridocadmium(II)]di- $\mu$ -chlorido]**

*Crystal data*

[CdCl <sub>2</sub> (C <sub>12</sub> H <sub>13</sub> N <sub>5</sub> )]	$Z = 2$
$M_r = 410.57$	$F(000) = 404$
Triclinic, $P\bar{1}$	$D_x = 1.880 \text{ Mg m}^{-3}$
$a = 7.6055 (6) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.7107 \text{ \AA}$
$b = 9.7027 (11) \text{ \AA}$	Cell parameters from 2806 reflections
$c = 10.3144 (10) \text{ \AA}$	$\theta = 3.2\text{--}26.3^\circ$
$\alpha = 74.431 (9)^\circ$	$\mu = 1.87 \text{ mm}^{-1}$
$\beta = 81.609 (7)^\circ$	$T = 293 \text{ K}$
$\gamma = 87.720 (8)^\circ$	Prismatic, colorless
$V = 725.36 (12) \text{ \AA}^3$	$0.20 \times 0.20 \times 0.18 \text{ mm}$

*Data collection*

Oxford Diffraction Xcalibur Eos Gemini diffractometer	2963 independent reflections
Radiation source: Enhance (Mo) X-ray Source graphite	2534 reflections with $I > 2\sigma(I)$
Detector resolution: 16.2312 pixels $\text{mm}^{-1}$	$R_{\text{int}} = 0.027$
$\omega$ scans	$\theta_{\text{max}} = 26.3^\circ$ , $\theta_{\text{min}} = 3.2^\circ$
Absorption correction: multi-scan ( <i>CrysAlis PRO</i> ; Oxford Diffraction, 2010)	$h = -9 \rightarrow 9$
$T_{\text{min}} = 0.993$ , $T_{\text{max}} = 1.000$	$k = -12 \rightarrow 11$
6082 measured reflections	$l = -12 \rightarrow 11$

*Refinement*

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.035$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.069$	H-atom parameters constrained
$S = 1.02$	$w = 1/[\sigma^2(F_o^2) + (0.0217P)^2]$
2963 reflections	where $P = (F_o^2 + 2F_c^2)/3$
182 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.47 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.50 \text{ e \AA}^{-3}$

*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>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.37119 (4)	0.60250 (3)	0.34830 (3)	0.02594 (10)
C11	0.10727 (13)	0.49171 (10)	0.30891 (11)	0.0366 (3)
C12	0.41293 (13)	0.62093 (9)	0.58398 (10)	0.0321 (2)
N1	0.2477 (4)	0.8391 (3)	0.3168 (3)	0.0266 (7)
N2	0.3564 (4)	0.9476 (3)	0.2763 (3)	0.0270 (7)
N3	0.2578 (4)	1.0677 (3)	0.2711 (3)	0.0240 (7)
N4	0.3531 (4)	1.2614 (3)	0.0745 (3)	0.0268 (7)
N5	0.4535 (4)	1.3280 (3)	-0.1440 (3)	0.0302 (8)
C1	0.0746 (5)	0.8865 (4)	0.3398 (4)	0.0241 (8)
C2	0.0805 (5)	1.0354 (4)	0.3106 (4)	0.0223 (8)
C3	-0.0701 (5)	1.1177 (4)	0.3322 (4)	0.0267 (8)
H3	-0.0656	1.2167	0.3151	0.032*
C4	-0.2255 (5)	1.0418 (4)	0.3806 (4)	0.0303 (9)
H4	-0.3299	1.0915	0.3969	0.036*
C5	-0.2333 (5)	0.8923 (4)	0.4064 (4)	0.0322 (9)
H5	-0.3426	0.8466	0.4374	0.039*
C6	-0.0851 (5)	0.8122 (4)	0.3874 (4)	0.0281 (9)
H6	-0.0904	0.7132	0.4052	0.034*
C7	0.3445 (5)	1.2069 (4)	0.2205 (4)	0.0294 (9)
H7B	0.2797	1.2742	0.2643	0.035*
H7A	0.4640	1.1987	0.2442	0.035*
C8	0.2094 (5)	1.3085 (4)	0.0082 (4)	0.0345 (10)
H8	0.0919	1.3119	0.0479	0.041*
C9	0.2719 (5)	1.3492 (4)	-0.1261 (4)	0.0382 (10)
H9	0.2035	1.3856	-0.1954	0.046*
C10	0.4998 (5)	1.2744 (4)	-0.0210 (4)	0.0266 (8)
C11	0.6844 (5)	1.2391 (4)	0.0090 (4)	0.0365 (10)
H11B	0.7009	1.2715	0.0876	0.044*
H11A	0.7665	1.2922	-0.0674	0.044*
C12	0.7329 (6)	1.0793 (4)	0.0370 (4)	0.0457 (11)
H12A	0.7140	1.0451	-0.0389	0.069*
H12B	0.6593	1.0264	0.1173	0.069*
H12C	0.8555	1.0668	0.0502	0.069*

## supplementary materials

---

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cd1	0.02975 (16)	0.02168 (16)	0.02519 (18)	0.00200 (11)	-0.00631 (12)	-0.00314 (12)
C11	0.0331 (5)	0.0287 (5)	0.0511 (7)	-0.0001 (4)	-0.0110 (5)	-0.0133 (5)
C12	0.0412 (6)	0.0275 (5)	0.0290 (6)	0.0108 (4)	-0.0100 (4)	-0.0087 (4)
N1	0.0333 (18)	0.0213 (16)	0.0227 (19)	0.0029 (14)	-0.0050 (14)	-0.0014 (13)
N2	0.0319 (18)	0.0236 (16)	0.0238 (19)	0.0048 (14)	-0.0044 (14)	-0.0038 (13)
N3	0.0314 (18)	0.0182 (15)	0.0197 (18)	0.0015 (13)	-0.0017 (14)	-0.0017 (13)
N4	0.0287 (17)	0.0235 (16)	0.0251 (19)	0.0018 (13)	-0.0074 (14)	0.0005 (13)
N5	0.0283 (18)	0.0332 (18)	0.0240 (19)	0.0025 (14)	-0.0036 (14)	0.0009 (14)
C1	0.031 (2)	0.0235 (19)	0.017 (2)	0.0042 (16)	-0.0018 (16)	-0.0045 (15)
C2	0.0267 (19)	0.0219 (19)	0.017 (2)	0.0004 (15)	-0.0028 (15)	-0.0036 (15)
C3	0.037 (2)	0.0228 (19)	0.021 (2)	0.0059 (17)	-0.0074 (17)	-0.0064 (16)
C4	0.027 (2)	0.036 (2)	0.028 (2)	0.0062 (17)	-0.0050 (17)	-0.0095 (18)
C5	0.029 (2)	0.036 (2)	0.029 (2)	-0.0055 (18)	-0.0010 (18)	-0.0051 (18)
C6	0.035 (2)	0.0225 (19)	0.025 (2)	-0.0036 (17)	-0.0068 (17)	-0.0011 (16)
C7	0.040 (2)	0.025 (2)	0.023 (2)	-0.0029 (17)	-0.0034 (18)	-0.0063 (17)
C8	0.027 (2)	0.036 (2)	0.035 (3)	0.0032 (18)	-0.0033 (18)	-0.0013 (19)
C9	0.030 (2)	0.045 (2)	0.032 (3)	0.0039 (19)	-0.0086 (19)	0.004 (2)
C10	0.030 (2)	0.0191 (18)	0.028 (2)	0.0003 (16)	-0.0031 (17)	-0.0019 (16)
C11	0.029 (2)	0.047 (3)	0.029 (2)	-0.0005 (19)	-0.0057 (18)	-0.002 (2)
C12	0.046 (3)	0.056 (3)	0.034 (3)	0.021 (2)	-0.012 (2)	-0.009 (2)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Cd1—C11	2.4482 (10)	C3—H3	0.9300
Cd1—C12 <sup>i</sup>	2.6687 (10)	C3—C4	1.374 (5)
Cd1—C12	2.5505 (10)	C4—H4	0.9300
Cd1—N1	2.403 (3)	C4—C5	1.405 (5)
Cd1—N5 <sup>ii</sup>	2.272 (3)	C5—H5	0.9300
C12—Cd1 <sup>i</sup>	2.6686 (10)	C5—C6	1.363 (5)
N1—N2	1.303 (4)	C6—H6	0.9300
N1—C1	1.386 (5)	C7—H7B	0.9700
N2—N3	1.353 (4)	C7—H7A	0.9700
N3—C2	1.374 (4)	C8—H8	0.9300
N3—C7	1.457 (4)	C8—C9	1.353 (5)
N4—C7	1.449 (5)	C9—H9	0.9300
N4—C8	1.371 (5)	C10—C11	1.488 (5)
N4—C10	1.362 (5)	C11—H11B	0.9700
N5—Cd1 <sup>ii</sup>	2.272 (3)	C11—H11A	0.9700
N5—C9	1.381 (5)	C11—C12	1.539 (5)
N5—C10	1.329 (5)	C12—H12A	0.9600
C1—C2	1.395 (5)	C12—H12B	0.9600
C1—C6	1.394 (5)	C12—H12C	0.9600
C2—C3	1.396 (5)		
Cd1—C12—Cd1 <sup>i</sup>	98.87 (3)	C3—C4—H4	118.6

C11—Cd1—C12 <sup>i</sup>	102.49 (3)	C3—C4—C5	122.8 (4)
C11—Cd1—C12	121.87 (4)	C4—C3—C2	115.1 (3)
C12—Cd1—C12 <sup>i</sup>	81.13 (3)	C4—C3—H3	122.5
N1—Cd1—C11	95.86 (8)	C4—C5—H5	119.1
N1—Cd1—C12	85.51 (8)	C5—C4—H4	118.6
N1—Cd1—C12 <sup>i</sup>	161.13 (8)	C5—C6—C1	116.5 (3)
N1—N2—N3	107.5 (3)	C5—C6—H6	121.7
N1—C1—C2	107.3 (3)	C6—C1—C2	121.3 (3)
N1—C1—C6	131.4 (3)	C6—C5—C4	121.8 (4)
N2—N1—Cd1	118.2 (2)	C6—C5—H5	119.1
N2—N1—C1	110.0 (3)	H7B—C7—H7A	107.9
N2—N3—C2	111.1 (3)	C8—N4—C7	124.7 (3)
N2—N3—C7	119.4 (3)	C8—C9—N5	109.1 (4)
N3—C2—C1	104.2 (3)	C8—C9—H9	125.4
N3—C2—C3	133.2 (3)	C9—N5—Cd1 <sup>ii</sup>	123.7 (3)
N3—C7—H7B	109.2	C9—C8—N4	106.6 (4)
N3—C7—H7A	109.2	C9—C8—H8	126.7
N4—C7—N3	112.0 (3)	C10—N4—C7	127.5 (3)
N4—C7—H7B	109.2	C10—N4—C8	107.9 (3)
N4—C7—H7A	109.2	C10—N5—Cd1 <sup>ii</sup>	129.2 (3)
N4—C8—H8	126.7	C10—N5—C9	106.8 (3)
N4—C10—C11	124.9 (4)	C10—C11—H11B	108.5
N5 <sup>ii</sup> —Cd1—C11	106.55 (8)	C10—C11—H11A	108.5
N5 <sup>ii</sup> —Cd1—C12 <sup>i</sup>	88.42 (8)	C10—C11—C12	115.0 (3)
N5 <sup>ii</sup> —Cd1—C12	131.58 (8)	C11—C12—H12A	109.5
N5 <sup>ii</sup> —Cd1—N1	90.57 (11)	C11—C12—H12B	109.5
N5—C9—H9	125.4	C11—C12—H12C	109.5
N5—C10—N4	109.5 (3)	H11B—C11—H11A	107.5
N5—C10—C11	125.5 (4)	C12—C11—H11B	108.5
C1—N1—Cd1	131.7 (2)	C12—C11—H11A	108.5
C1—C2—C3	122.5 (3)	H12A—C12—H12B	109.5
C1—C6—H6	121.7	H12A—C12—H12C	109.5
C2—N3—C7	129.5 (3)	H12B—C12—H12C	109.5
C2—C3—H3	122.5		
Cd1—N1—N2—N3	-177.7 (2)	N4—C10—C11—C12	81.6 (5)
Cd1—N1—C1—C2	176.9 (2)	N5 <sup>ii</sup> —Cd1—C12—Cd1 <sup>i</sup>	-79.87 (11)
Cd1—N1—C1—C6	-0.9 (6)	N5 <sup>ii</sup> —Cd1—N1—N2	-47.0 (3)
Cd1 <sup>ii</sup> —N5—C9—C8	-174.2 (2)	N5 <sup>ii</sup> —Cd1—N1—C1	136.3 (3)
Cd1 <sup>ii</sup> —N5—C10—N4	173.7 (2)	N5—C10—C11—C12	-100.9 (4)
Cd1 <sup>ii</sup> —N5—C10—C11	-4.0 (5)	C1—N1—N2—N3	-0.3 (4)
C11—Cd1—C12—Cd1 <sup>i</sup>	99.25 (4)	C1—C2—C3—C4	-1.8 (5)
C11—Cd1—N1—N2	-153.7 (2)	C2—N3—C7—N4	-87.5 (4)
C11—Cd1—N1—C1	29.6 (3)	C2—C1—C6—C5	-1.4 (5)
C12 <sup>i</sup> —Cd1—C12—Cd1 <sup>i</sup>	0.000 (2)	C2—C3—C4—C5	-0.1 (6)
C12 <sup>i</sup> —Cd1—N1—N2	39.8 (4)	C3—C4—C5—C6	1.3 (6)

## supplementary materials

---

C12—Cd1—N1—N2	84.7 (2)	C4—C5—C6—C1	-0.5 (6)
C12—Cd1—N1—C1	-92.0 (3)	C6—C1—C2—N3	178.3 (3)
C12 <sup>i</sup> —Cd1—N1—C1	-136.9 (3)	C6—C1—C2—C3	2.7 (6)
N1—Cd1—C12—Cd1 <sup>i</sup>	-166.64 (8)	C7—N3—C2—C1	175.8 (3)
N1—N2—N3—C2	0.5 (4)	C7—N3—C2—C3	-9.3 (6)
N1—N2—N3—C7	-176.2 (3)	C7—N4—C8—C9	-179.5 (3)
N1—C1—C2—N3	0.3 (4)	C7—N4—C10—N5	179.6 (3)
N1—C1—C2—C3	-175.3 (3)	C7—N4—C10—C11	-2.6 (6)
N1—C1—C6—C5	176.1 (4)	C8—N4—C7—N3	70.3 (4)
N2—N1—C1—C2	0.0 (4)	C8—N4—C10—N5	0.1 (4)
N2—N1—C1—C6	-177.7 (4)	C8—N4—C10—C11	177.9 (3)
N2—N3—C2—C1	-0.5 (4)	C9—N5—C10—N4	-0.2 (4)
N2—N3—C2—C3	174.4 (4)	C9—N5—C10—C11	-178.0 (3)
N2—N3—C7—N4	88.6 (4)	C10—N4—C7—N3	-109.1 (4)
N3—C2—C3—C4	-176.0 (4)	C10—N4—C8—C9	0.0 (4)
N4—C8—C9—N5	-0.1 (4)	C10—N5—C9—C8	0.2 (4)

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



Fig. 1

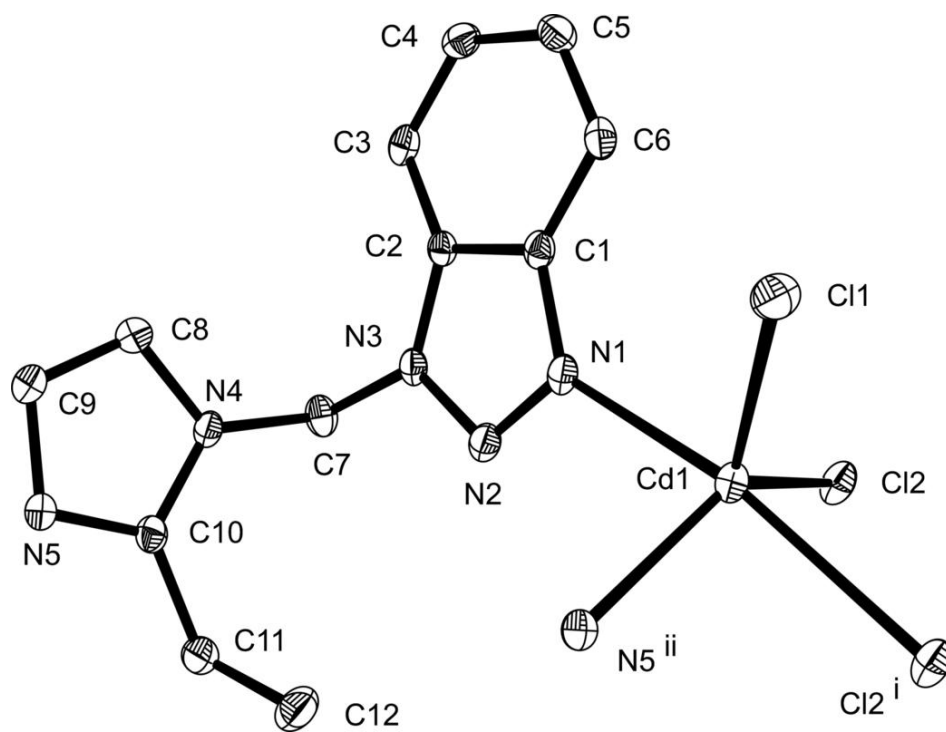


Fig. 2

