

## Bis(2-aminopyridine- $\kappa N^1$ )bis(benzoato- $\kappa^2 O, O'$ )cadmium(II)

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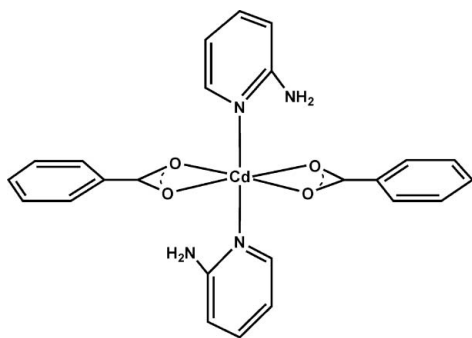
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(C-C) = 0.003$  Å;  $R$  factor = 0.022;  $wR$  factor = 0.057; data-to-parameter ratio = 18.2.

In the title compound,  $[Cd(C_7H_5O_2)_2(C_5H_6N_2)_2]$ , the Cd<sup>II</sup> atom is hexacoordinated by four O atoms from two crystallographically independent benzoate anions, and two pyridine N atoms from two crystallographically independent 2-aminopyridine molecules in a distorted octahedral geometry. In the crystal structure, the metal complexes are connected by N—H...O hydrogen bonding between the carboxylate O atoms of the benzoate anions and the amino H atoms of the 2-aminopyridine ligands. The benzoate and the aminopyridine rings are stacked in the direction of the crystallographic  $a$  axis, indicating  $\pi$ – $\pi$  stacking interactions are present [centroid-centroid distance = 3.6790 (15) Å].

### Related literature

For related literature, see: Kozlevčar *et al.* (2001); Shi *et al.* (2004); Tan *et al.* (2003); Wang *et al.* (2004); Zheng *et al.* (2004); Zhu, Shao *et al.* (2003); Zhu, Usman *et al.* (2003).



### Experimental

#### Crystal data

$[Cd(C_7H_5O_2)_2(C_5H_6N_2)_2]$   
 $M_r = 542.86$   
Monoclinic,  $P2_1/n$   
 $a = 9.1226$  (9) Å  
 $b = 11.4153$  (11) Å  
 $c = 22.520$  (2) Å  
 $\beta = 96.1090$  (10)°  
 $V = 2331.8$  (4) Å<sup>3</sup>  
 $Z = 4$   
Mo  $K\alpha$  radiation  
 $\mu = 0.97$  mm<sup>-1</sup>  
 $T = 296$  (2) K  
 $0.42 \times 0.36 \times 0.28$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{min} = 0.672$ ,  $T_{max} = 0.758$   
20104 measured reflections  
5418 independent reflections  
4817 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.020$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$   
 $wR(F^2) = 0.057$   
 $S = 1.04$   
5418 reflections  
298 parameters  
276 restraints  
H-atom parameters constrained  
 $\Delta\rho_{max} = 0.24$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.56$  e Å<sup>-3</sup>

**Table 1**

Selected bond lengths (Å).

Cd1—N3	2.2857 (15)	Cd1—O4	2.3251 (15)
Cd1—N1	2.2945 (15)	Cd1—O3	2.3936 (15)
Cd1—O2	2.3206 (15)	Cd1—O1	2.4287 (15)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2A...O3	0.86	2.15	2.999 (2)	170
N2—H2B...O1 <sup>i</sup>	0.86	2.08	2.897 (2)	157
N4—H4A...O2	0.86	2.03	2.880 (3)	169
N4—H4B...O4 <sup>ii</sup>	0.86	2.13	2.979 (2)	168

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2004); 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: NC2078).

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**supplementary materials**

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## Bis(2-aminopyridine- $\kappa N^1$ )bis(benzoato- $\kappa^2 O, O'$ )cadmium(II)

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### Comment

Over the past two decades, there has been considerable interest in the study of crystal structures and properties of cadmium complexes based on carboxyl ligand, owing to their photoluminescent behaviours. (Tan *et al.*, 2003; Zheng *et al.*, 2004; Wang *et al.*, 2004; Shi *et al.*, 2004). The structures of mixed ligand complexes containing benzoate anions and 2-aminopyridine ligands have also been reported (Kozlevčar *et al.*, 2001; Zhu, Usman *et al.*, 2003; Zhu, Shao *et al.*, 2004). As a part of our ongoing investigations in this field we report the synthesis and crystal structure of the title compound.

The structure of the title compound (I), is isostructural with the nickel (I) complex (Zhu, Shao *et al.*, 2003). The Cd<sup>II</sup> atom is hexa-coordinated by four O atoms of two crystallographically independent benzoate anions, and two pyridine N atoms from two crystallographically independent 2-aminopyridine molecules, within a distorted octahedron. The Cd—N bond lengths are 2.2857 (15) Å and 2.2945 (15) Å, and the Cd—O distances ranges from 2.3206 (15) to 2.4287 (15) Å. The molecules are connected *via* intermolecular O—H $\cdots$ N hydrogen bonding between the carboxyl oxygen atoms of the benzoate anions and the amino hydrogen atoms of the 2-aminopyridine ligands (Table 1 and Fig. 2). The benzoate and the aminopyridine rings are stacked in the direction of the crystallographic *a* axis indicating for  $\pi\cdots\pi$  stacking interaction (Fig. 2).

### Experimental

All reagents are commercially available and were used without further purification. CdCl<sub>2</sub>·2.5H<sub>2</sub>O (0.5 mmol), benzoate sodium (1 mmol) and 2-aminopyridine (1 mmol) were mixed in 8 ml of methanol and and 8 ml of water. After stirring for half an hour, the mixture was transferred in a 25 ml Teflon-lined reactor and heated at 130 °C for 7 days. The reaction mixture was filtered and the filtrate was allowed to stay at room temperature. Well shaped yellow crystals of the title compound suitable for X-rays diffraction were obtained after two weeks. Yield: 62% based on benzoate sodium.

### Refinement

All the H atoms were placed in geometrically idealized positions with N—H and C—H distances of 0.86 Å and 0.93 Å and were refined isotropic using a riding model with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C or N})$ .

Figures

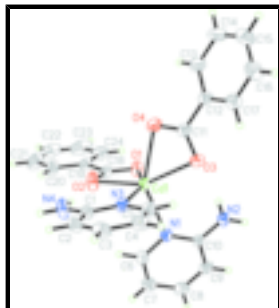


Fig. 1. The structure of (I), with labeling and displacement ellipsoids drawn at the 30% probability level.

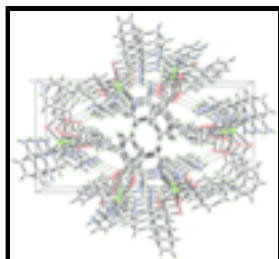


Fig. 2. Crystal structure of compound (I) with view along the crystallographic *a* axis (Hydrogen bonding is shown as dashed lines).

**Bis(2-aminopyridine- $\kappa N^1$ )bis(benzoato- $\kappa O^2$ )cadmium(II)**

*Crystal data*

[Cd(C <sub>7</sub> H <sub>5</sub> O <sub>2</sub> ) <sub>2</sub> (C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> ) <sub>2</sub> ]	<i>Z</i> = 4
<i>M<sub>r</sub></i> = 542.86	<i>F</i> <sub>000</sub> = 1096
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>	<i>D<sub>x</sub></i> = 1.546 Mg m <sup>-3</sup>
Hall symbol: - <i>P</i> 2yn	Mo <i>K</i> α radiation
<i>a</i> = 9.1226 (9) Å	λ = 0.71073 Å
<i>b</i> = 11.4153 (11) Å	θ = 2.3–27.7°
<i>c</i> = 22.520 (2) Å	μ = 0.97 mm <sup>-1</sup>
β = 96.1090 (10)°	<i>T</i> = 296 (2) K
<i>V</i> = 2331.8 (4) Å <sup>3</sup>	Block, yellow
	0.42 × 0.36 × 0.28 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer	5418 independent reflections
Radiation source: fine-focus sealed tube	4817 reflections with <i>I</i> > 2σ( <i>I</i> )
Monochromator: graphite	<i>R</i> <sub>int</sub> = 0.020
<i>T</i> = 296(2) K	θ <sub>max</sub> = 27.7°
φ and ω scans	θ <sub>min</sub> = 1.8°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>h</i> = -11→11
<i>T</i> <sub>min</sub> = 0.672, <i>T</i> <sub>max</sub> = 0.758	<i>k</i> = -14→14
20104 measured reflections	<i>l</i> = -29→28

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.022$	H-atom parameters constrained
$wR(F^2) = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2 + 0.8501P]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
5418 reflections	$(\Delta/\sigma)_{\max} = 0.022$
298 parameters	$\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$
276 restraints	$\Delta\rho_{\min} = -0.56 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Cd1	0.308844 (14)	0.551275 (12)	0.124286 (5)	0.03915 (5)
O1	0.56299 (16)	0.48583 (14)	0.14239 (6)	0.0541 (3)
O2	0.47033 (17)	0.59585 (17)	0.20791 (7)	0.0656 (4)
O3	0.15943 (18)	0.42390 (12)	0.05863 (6)	0.0517 (3)
O4	0.24832 (18)	0.35974 (13)	0.14697 (7)	0.0581 (4)
N1	0.38419 (17)	0.67576 (14)	0.05352 (6)	0.0406 (3)
N2	0.3290 (2)	0.55339 (14)	-0.02765 (7)	0.0490 (4)
H2A	0.2774	0.5107	-0.0063	0.059*
H2B	0.3365	0.5348	-0.0642	0.059*
N3	0.11118 (17)	0.65797 (14)	0.14799 (7)	0.0416 (3)
N4	0.2241 (2)	0.73593 (19)	0.23601 (8)	0.0658 (5)
H4A	0.3047	0.7018	0.2293	0.079*
H4B	0.2211	0.7777	0.2677	0.079*
C1	0.1026 (2)	0.72404 (16)	0.19711 (8)	0.0442 (4)
C2	-0.0298 (2)	0.78070 (18)	0.20682 (10)	0.0537 (5)
H2	-0.0352	0.8247	0.2413	0.064*
C3	-0.1490 (2)	0.77110 (19)	0.16603 (11)	0.0581 (5)

## supplementary materials

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H3	-0.2365	0.8088	0.1722	0.070*
C4	-0.1403 (2)	0.7043 (2)	0.11449 (11)	0.0573 (5)
H4	-0.2206	0.6976	0.0856	0.069*
C5	-0.0104 (2)	0.64945 (19)	0.10798 (9)	0.0499 (4)
H5	-0.0048	0.6035	0.0742	0.060*
C6	0.4484 (2)	0.77564 (18)	0.07639 (9)	0.0491 (4)
H6	0.4370	0.7946	0.1158	0.059*
C7	0.5282 (2)	0.84974 (19)	0.04511 (10)	0.0550 (5)
H7	0.5690	0.9180	0.0623	0.066*
C8	0.5467 (2)	0.81977 (19)	-0.01361 (10)	0.0547 (5)
H8	0.6027	0.8674	-0.0360	0.066*
C9	0.4830 (2)	0.72089 (18)	-0.03821 (9)	0.0492 (4)
H9	0.4952	0.7007	-0.0774	0.059*
C10	0.39819 (19)	0.64920 (16)	-0.00389 (7)	0.0387 (4)
C11	0.1700 (2)	0.34529 (17)	0.09790 (8)	0.0431 (4)
C12	0.0872 (2)	0.23300 (17)	0.08679 (8)	0.0437 (4)
C13	0.1306 (3)	0.13299 (19)	0.11883 (11)	0.0591 (5)
H13	0.2121	0.1355	0.1474	0.071*
C14	0.0532 (3)	0.0292 (2)	0.10853 (13)	0.0735 (7)
H14	0.0844	-0.0382	0.1293	0.088*
C15	-0.0691 (3)	0.0260 (2)	0.06784 (14)	0.0739 (7)
H15	-0.1222	-0.0433	0.0618	0.089*
C16	-0.1141 (3)	0.1243 (2)	0.03587 (13)	0.0716 (7)
H16	-0.1973	0.1214	0.0082	0.086*
C17	-0.0355 (2)	0.2279 (2)	0.04486 (11)	0.0568 (5)
H17	-0.0651	0.2941	0.0227	0.068*
C18	0.5755 (2)	0.53716 (16)	0.19175 (8)	0.0405 (4)
C19	0.7157 (2)	0.52812 (18)	0.23220 (9)	0.0455 (4)
C20	0.7305 (3)	0.5873 (2)	0.28624 (10)	0.0635 (6)
H20	0.6531	0.6320	0.2977	0.076*
C21	0.8625 (4)	0.5790 (3)	0.32314 (13)	0.0870 (9)
H21	0.8738	0.6185	0.3595	0.104*
C22	0.9756 (3)	0.5129 (3)	0.30603 (17)	0.0942 (10)
H22	1.0636	0.5083	0.3309	0.113*
C23	0.9618 (3)	0.4543 (3)	0.25367 (18)	0.0894 (10)
H23	1.0398	0.4094	0.2428	0.107*
C24	0.8304 (3)	0.4612 (2)	0.21574 (13)	0.0651 (6)
H24	0.8205	0.4209	0.1796	0.078*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cd1	0.04208 (8)	0.04492 (8)	0.03039 (7)	0.00135 (5)	0.00357 (5)	-0.00096 (5)
O1	0.0543 (8)	0.0687 (9)	0.0392 (7)	0.0014 (7)	0.0042 (6)	-0.0117 (7)
O2	0.0535 (9)	0.0896 (12)	0.0517 (9)	0.0229 (8)	-0.0033 (7)	-0.0207 (8)
O3	0.0677 (9)	0.0414 (7)	0.0463 (8)	-0.0019 (6)	0.0080 (7)	0.0074 (6)
O4	0.0652 (9)	0.0560 (9)	0.0506 (8)	-0.0115 (7)	-0.0052 (7)	0.0119 (7)
N1	0.0456 (8)	0.0433 (8)	0.0329 (7)	0.0031 (6)	0.0049 (6)	-0.0003 (6)

N2	0.0646 (11)	0.0494 (9)	0.0345 (8)	-0.0032 (8)	0.0122 (7)	-0.0055 (7)
N3	0.0445 (8)	0.0450 (8)	0.0362 (7)	0.0032 (7)	0.0085 (6)	-0.0001 (6)
N4	0.0578 (11)	0.0837 (14)	0.0553 (11)	0.0109 (10)	0.0032 (9)	-0.0319 (10)
C1	0.0500 (10)	0.0404 (9)	0.0439 (10)	-0.0004 (8)	0.0134 (8)	-0.0009 (7)
C2	0.0601 (12)	0.0433 (10)	0.0609 (12)	0.0059 (9)	0.0212 (10)	-0.0051 (9)
C3	0.0497 (11)	0.0471 (11)	0.0798 (15)	0.0106 (9)	0.0170 (10)	0.0042 (10)
C4	0.0486 (11)	0.0546 (12)	0.0674 (13)	0.0074 (9)	-0.0001 (10)	0.0067 (10)
C5	0.0511 (11)	0.0531 (11)	0.0449 (10)	0.0058 (9)	0.0023 (8)	0.0013 (9)
C6	0.0557 (11)	0.0501 (11)	0.0410 (10)	-0.0001 (9)	0.0020 (8)	-0.0039 (8)
C7	0.0549 (12)	0.0468 (11)	0.0618 (12)	-0.0051 (9)	-0.0005 (10)	-0.0010 (9)
C8	0.0524 (11)	0.0522 (12)	0.0611 (12)	-0.0005 (9)	0.0131 (9)	0.0126 (9)
C9	0.0558 (11)	0.0524 (11)	0.0414 (10)	0.0075 (9)	0.0148 (8)	0.0067 (8)
C10	0.0408 (9)	0.0411 (9)	0.0344 (8)	0.0096 (7)	0.0044 (7)	0.0030 (7)
C11	0.0434 (9)	0.0440 (10)	0.0435 (10)	0.0039 (8)	0.0116 (7)	0.0048 (8)
C12	0.0440 (9)	0.0433 (10)	0.0452 (10)	0.0014 (8)	0.0118 (8)	0.0041 (8)
C13	0.0653 (13)	0.0502 (12)	0.0609 (13)	-0.0029 (10)	0.0020 (10)	0.0121 (10)
C14	0.0891 (18)	0.0493 (13)	0.0830 (17)	-0.0043 (12)	0.0135 (14)	0.0159 (12)
C15	0.0734 (16)	0.0561 (14)	0.0943 (19)	-0.0182 (12)	0.0179 (14)	-0.0044 (13)
C16	0.0555 (13)	0.0692 (15)	0.0882 (17)	-0.0069 (11)	-0.0011 (12)	-0.0093 (13)
C17	0.0510 (11)	0.0526 (12)	0.0655 (13)	0.0035 (9)	0.0008 (10)	0.0034 (10)
C18	0.0430 (9)	0.0447 (10)	0.0340 (9)	-0.0028 (7)	0.0041 (7)	0.0024 (7)
C19	0.0419 (10)	0.0519 (11)	0.0424 (10)	-0.0073 (8)	0.0025 (8)	0.0129 (8)
C20	0.0657 (14)	0.0758 (15)	0.0463 (11)	-0.0165 (12)	-0.0059 (10)	0.0044 (10)
C21	0.089 (2)	0.104 (2)	0.0612 (15)	-0.0350 (17)	-0.0242 (14)	0.0168 (14)
C22	0.0589 (16)	0.119 (2)	0.097 (2)	-0.0305 (16)	-0.0255 (15)	0.0531 (19)
C23	0.0507 (14)	0.105 (2)	0.112 (2)	0.0073 (14)	0.0064 (15)	0.0476 (18)
C24	0.0494 (12)	0.0740 (15)	0.0723 (15)	0.0067 (11)	0.0083 (11)	0.0212 (12)

*Geometric parameters (Å, °)*

Cd1—N3	2.2857 (15)	C7—C8	1.393 (3)
Cd1—N1	2.2945 (15)	C7—H7	0.9300
Cd1—O2	2.3206 (15)	C8—C9	1.360 (3)
Cd1—O4	2.3251 (15)	C8—H8	0.9300
Cd1—O3	2.3936 (15)	C9—C10	1.412 (3)
Cd1—O1	2.4287 (15)	C9—H9	0.9300
O1—C18	1.251 (2)	C11—C12	1.495 (3)
O2—C18	1.255 (2)	C12—C13	1.386 (3)
O3—C11	1.256 (2)	C12—C17	1.386 (3)
O4—C11	1.261 (2)	C13—C14	1.386 (3)
N1—C10	1.347 (2)	C13—H13	0.9300
N1—C6	1.358 (2)	C14—C15	1.367 (4)
N2—C10	1.345 (2)	C14—H14	0.9300
N2—H2A	0.8600	C15—C16	1.372 (4)
N2—H2B	0.8600	C15—H15	0.9300
N3—C1	1.348 (2)	C16—C17	1.387 (3)
N3—C5	1.356 (2)	C16—H16	0.9300
N4—C1	1.344 (3)	C17—H17	0.9300
N4—H4A	0.8600	C18—C19	1.492 (3)



## supplementary materials

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N4—H4B	0.8600	C19—C24	1.378 (3)
C1—C2	1.407 (3)	C19—C20	1.386 (3)
C2—C3	1.351 (3)	C20—C21	1.392 (4)
C2—H2	0.9300	C20—H20	0.9300
C3—C4	1.398 (3)	C21—C22	1.366 (5)
C3—H3	0.9300	C21—H21	0.9300
C4—C5	1.361 (3)	C22—C23	1.350 (5)
C4—H4	0.9300	C22—H22	0.9300
C5—H5	0.9300	C23—C24	1.398 (4)
C6—C7	1.361 (3)	C23—H23	0.9300
C6—H6	0.9300	C24—H24	0.9300
N3—Cd1—N1	97.72 (5)	C9—C8—C7	120.03 (19)
N3—Cd1—O2	98.17 (5)	C9—C8—H8	120.0
N1—Cd1—O2	102.51 (6)	C7—C8—H8	120.0
N3—Cd1—O4	103.77 (6)	C8—C9—C10	119.57 (18)
N1—Cd1—O4	146.17 (5)	C8—C9—H9	120.2
O2—Cd1—O4	99.96 (6)	C10—C9—H9	120.2
N3—Cd1—O3	93.24 (5)	N2—C10—N1	118.46 (17)
N1—Cd1—O3	98.06 (5)	N2—C10—C9	120.98 (17)
O2—Cd1—O3	154.83 (6)	N1—C10—C9	120.56 (17)
O4—Cd1—O3	55.36 (5)	O3—C11—O4	121.14 (18)
N3—Cd1—O1	152.55 (5)	O3—C11—C12	119.67 (17)
N1—Cd1—O1	87.47 (5)	O4—C11—C12	119.19 (17)
O2—Cd1—O1	54.48 (5)	C13—C12—C17	119.0 (2)
O4—Cd1—O1	85.33 (6)	C13—C12—C11	120.52 (18)
O3—Cd1—O1	112.80 (5)	C17—C12—C11	120.46 (18)
C18—O1—Cd1	90.02 (12)	C14—C13—C12	120.3 (2)
C18—O2—Cd1	94.96 (12)	C14—C13—H13	119.9
C11—O3—Cd1	90.18 (12)	C12—C13—H13	119.9
C11—O4—Cd1	93.22 (11)	C15—C14—C13	120.1 (2)
C10—N1—C6	118.16 (17)	C15—C14—H14	120.0
C10—N1—Cd1	126.38 (12)	C13—C14—H14	120.0
C6—N1—Cd1	113.92 (12)	C14—C15—C16	120.5 (2)
C10—N2—H2A	120.0	C14—C15—H15	119.8
C10—N2—H2B	120.0	C16—C15—H15	119.8
H2A—N2—H2B	120.0	C15—C16—C17	119.9 (2)
C1—N3—C5	118.06 (17)	C15—C16—H16	120.0
C1—N3—Cd1	127.30 (13)	C17—C16—H16	120.0
C5—N3—Cd1	114.62 (12)	C16—C17—C12	120.2 (2)
C1—N4—H4A	120.0	C16—C17—H17	119.9
C1—N4—H4B	120.0	C12—C17—H17	119.9
H4A—N4—H4B	120.0	O1—C18—O2	120.48 (18)
N4—C1—N3	118.39 (17)	O1—C18—C19	120.08 (18)
N4—C1—C2	120.91 (19)	O2—C18—C19	119.43 (17)
N3—C1—C2	120.69 (19)	C24—C19—C20	120.0 (2)
C3—C2—C1	119.9 (2)	C24—C19—C18	120.0 (2)
C3—C2—H2	120.0	C20—C19—C18	120.0 (2)
C1—C2—H2	120.0	C19—C20—C21	119.2 (3)
C2—C3—C4	119.7 (2)	C19—C20—H20	120.4

C2—C3—H3	120.1	C21—C20—H20	120.4
C4—C3—H3	120.1	C22—C21—C20	120.0 (3)
C5—C4—C3	117.9 (2)	C22—C21—H21	120.0
C5—C4—H4	121.1	C20—C21—H21	120.0
C3—C4—H4	121.1	C23—C22—C21	121.1 (3)
N3—C5—C4	123.7 (2)	C23—C22—H22	119.4
N3—C5—H5	118.1	C21—C22—H22	119.4
C4—C5—H5	118.1	C22—C23—C24	120.0 (3)
N1—C6—C7	123.95 (19)	C22—C23—H23	120.0
N1—C6—H6	118.0	C24—C23—H23	120.0
C7—C6—H6	118.0	C19—C24—C23	119.6 (3)
C6—C7—C8	117.7 (2)	C19—C24—H24	120.2
C6—C7—H7	121.2	C23—C24—H24	120.2
C8—C7—H7	121.2		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N2—H2A $\cdots$ O3	0.86	2.15	2.999 (2)	170
N2—H2B $\cdots$ O1 <sup>i</sup>	0.86	2.08	2.897 (2)	157
N4—H4A $\cdots$ O2	0.86	2.03	2.880 (3)	169
N4—H4B $\cdots$ O4 <sup>ii</sup>	0.86	2.13	2.979 (2)	168

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

Fig. 1

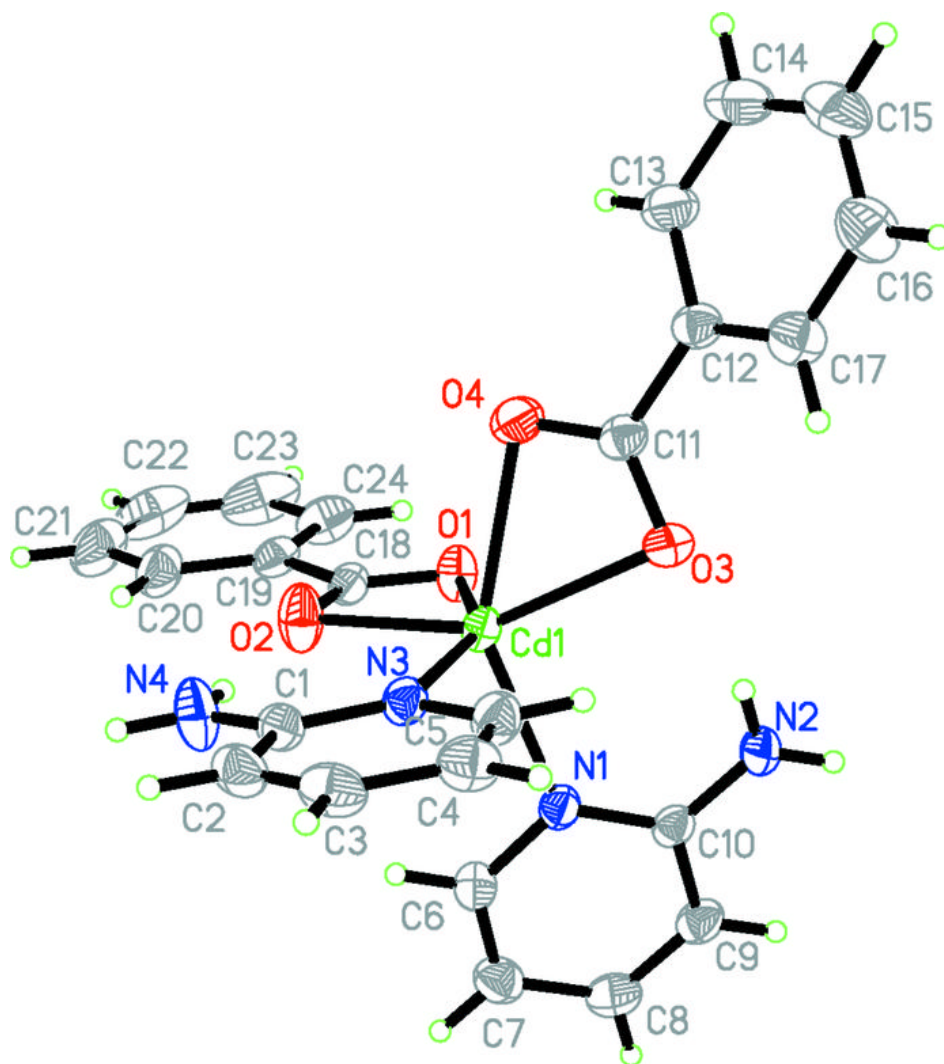


Fig. 2

