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Bis(1*H*-imidazole- κ N³)bis(1-naphthaleneacetato- κ^2 O, O')cadmium(II)

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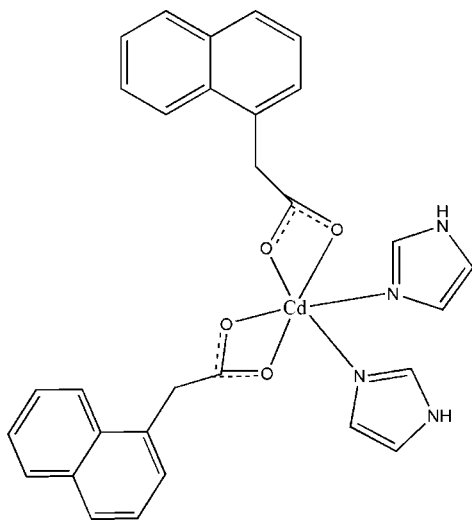
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 Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.010$ Å; R factor = 0.052; wR factor = 0.143; data-to-parameter ratio = 15.9.

In the mononuclear title compound, $[\text{Cd}(\text{C}_{12}\text{H}_9\text{O}_2)_2(\text{C}_3\text{H}_4\text{N}_2)_2]$, the Cd^{II} centre has a distorted octahedral coordination geometry defined by four O atoms from two naphthaleneacetate ligands and two N atoms from two imidazole ligands. The molecules are linked by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a layer network.

Related literature

 For related literature, see: Duan *et al.* (2007); Liu *et al.* (2006).


Experimental

Crystal data

 $[\text{Cd}(\text{C}_{12}\text{H}_9\text{O}_2)_2(\text{C}_3\text{H}_4\text{N}_2)_2]$
 $M_r = 618.95$

 Monoclinic, $P2_1/n$
 $a = 8.5275$ (3) Å

 $b = 17.1596$ (7) Å

 $c = 19.1198$ (6) Å

 $\beta = 100.735$ (2)°

 $V = 2748.81$ (17) Å³
 $Z = 4$

 Mo $K\alpha$ radiation

 $\mu = 0.84$ mm⁻¹
 $T = 296$ (2) K

 $0.26 \times 0.23 \times 0.21$ mm

Data collection

Bruker APEXII area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{\text{min}} = 0.812$, $T_{\text{max}} = 0.844$

26061 measured reflections

5399 independent reflections

 3336 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.089$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.142$
 $S = 0.99$

5399 reflections

340 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.57$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.16$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2}\cdots\text{O4}^{\text{i}}$	0.86	1.92	2.735 (6)	159
$\text{N4}-\text{H4A}\cdots\text{O2}^{\text{ii}}$	0.86	1.95	2.772 (6)	159

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: XP in SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

The authors acknowledge Guang Dong Ocean University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2436).

References

- Bruker (2004). APEX2 and SAINT. Bruker AXS Inc, Madison, Wisconsin, USA.
 Duan, J.-G., Liu, J.-W. & Wu, S. (2007). *Acta Cryst.* E63, m692–m694.
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 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* A64, 112–122.

supplementary materials

Acta Cryst. (2008). E64, m653 [doi:10.1107/S1600536808009409]

Bis(1*H*-imidazole- κN^3)bis(1-naphthaleneacetato- $\kappa^2 O, O'$)cadmium(II)

W.-D. Song, L.-L. Ji and H.-M. Wu

Comment

naphthaleneacetate is nice ligand which has versatile bonding modes to metal ions and easily forms simple complexes (Liu *et al.*, 2006; Duan *et al.*, 2007). Recently, we obtained the mononuclear cadmium complex, (I), its crystal structure is reported here. Recently, we obtained the title novel mononuclear complex (I), by the reaction of cadmium chloride, 1-naphthylacetic acid and imidazole in an aqueous solution, and its crystal structure is reported here.

As depicted in Fig. 1, the Cd^{II} centre in (I) presents a distorted octahedral coordination geometry, defined by four O atoms from two 1-naphthaleneacetate ligands, and two N atoms from two imidazole ligands. The structural packing is governed by N—H \cdots O hydrogen bonding interaction (Table 1) to form a layered network (Fig. 2).

Experimental

The title complex was prepared by the addition of a stoichiometric amount of cadmium chloride (1 mmol) and imidazole (1 mmol) to a hot aqueous solution(10 ml) of 1-naphthylacetic acid (1 mmol). the pH was then adjusted to 7.0 to 8.0 with NaOH (1 mmol). The resulting solution was filtered, and colorless single crystals were obtained at room temperature over several days.

Refinement

All H-atoms were placed in calculated positions with C—H = 0.93–0.97 Å, N—H = 0.86 Å; refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5 U_{\text{eq}}(\text{C}, \text{N})$.

Figures

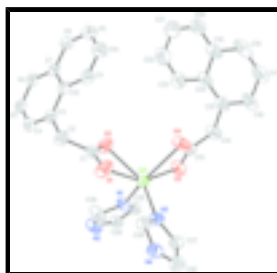


Fig. 1. The structure of (I), showing the atomic numbering scheme. Non-H atoms are shown as 30% probability displacement ellipsoids.

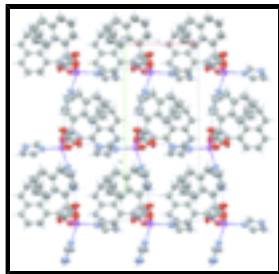


Fig. 2. The packing of structure (I).

Bis(1H-imidazole- κ N³)bis(1-naphthaleneacetato- κ^2 O,O')cadmium(II)

Crystal data

[Cd(C₁₂H₉O₂)₂(C₃H₄N₂)₂]

$M_r = 618.95$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 8.5275$ (3) Å

$b = 17.1596$ (7) Å

$c = 19.1198$ (6) Å

$\beta = 100.735$ (2)°

$V = 2748.81$ (17) Å³

$Z = 4$

$F_{000} = 1256$

$D_x = 1.496$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 5300 reflections

$\theta = 1.3$ – 28.0°

$\mu = 0.84$ mm⁻¹

$T = 296$ (2) K

Block, colorless

$0.26 \times 0.23 \times 0.21$ mm

Data collection

Bruker APEXII area-detector
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 296$ (2) K

φ and ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.812$, $T_{\max} = 0.844$

26061 measured reflections

5399 independent reflections

3336 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.089$

$\theta_{\max} = 26.0^\circ$

$\theta_{\min} = 2.2^\circ$

$h = -9 \rightarrow 10$

$k = -16 \rightarrow 21$

$l = -23 \rightarrow 23$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.143$

$S = 0.99$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0533P)^2 + 1.0058P]$

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

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

5399 reflections $\Delta\rho_{\max} = 0.57 \text{ e } \text{\AA}^{-3}$
 340 parameters $\Delta\rho_{\min} = -1.16 \text{ e } \text{\AA}^{-3}$
 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.3023 (7)	0.6405 (3)	0.3585 (3)	0.0583 (14)
C2	0.3810 (7)	0.6218 (4)	0.4342 (3)	0.0694 (16)
H2A	0.3450	0.6594	0.4656	0.083*
H2B	0.3449	0.5708	0.4463	0.083*
C3	0.5602 (7)	0.6219 (3)	0.4484 (2)	0.0581 (14)
C4	0.6434 (8)	0.6822 (3)	0.4844 (3)	0.0656 (16)
H4	0.5878	0.7224	0.5016	0.079*
C5	0.8115 (8)	0.6849 (3)	0.4962 (3)	0.0639 (15)
H5	0.8652	0.7265	0.5212	0.077*
C6	0.8959 (7)	0.6271 (3)	0.4713 (2)	0.0595 (14)
H6	1.0067	0.6297	0.4790	0.071*
C7	0.8159 (7)	0.5633 (3)	0.4339 (2)	0.0540 (13)
C8	0.9015 (7)	0.5033 (4)	0.4069 (3)	0.0649 (15)
H8	1.0124	0.5052	0.4145	0.078*
C9	0.8232 (9)	0.4431 (4)	0.3701 (3)	0.0785 (18)
H9	0.8802	0.4038	0.3525	0.094*
C10	0.6560 (9)	0.4402 (4)	0.3585 (4)	0.088 (2)
H10	0.6025	0.3991	0.3326	0.105*
C11	0.5716 (7)	0.4966 (4)	0.3845 (3)	0.0716 (16)
H11	0.4609	0.4927	0.3771	0.086*
C12	0.6464 (6)	0.5606 (3)	0.4223 (2)	0.0543 (13)
C13	0.2197 (7)	0.6142 (3)	0.1108 (2)	0.0593 (14)
C14	0.2727 (9)	0.5800 (4)	0.0458 (3)	0.0794 (19)
H14A	0.1911	0.5918	0.0046	0.095*
H14B	0.3691	0.6070	0.0394	0.095*
C15	0.3051 (9)	0.4945 (4)	0.0457 (3)	0.0718 (17)
C16	0.2010 (9)	0.4454 (4)	0.0041 (3)	0.092 (2)
H16	0.1081	0.4658	-0.0230	0.111*

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C17	0.2301 (11)	0.3654 (5)	0.0011 (4)	0.101 (3)
H17	0.1559	0.3335	-0.0272	0.121*
C18	0.3651 (12)	0.3339 (5)	0.0390 (5)	0.102 (3)
H18	0.3832	0.2806	0.0361	0.122*
C19	0.4786 (9)	0.3811 (4)	0.0827 (3)	0.0738 (18)
C20	0.6198 (11)	0.3493 (5)	0.1221 (4)	0.091 (2)
H20	0.6394	0.2962	0.1192	0.109*
C21	0.7265 (12)	0.3946 (6)	0.1637 (4)	0.113 (3)
H21	0.8192	0.3730	0.1898	0.135*
C22	0.6983 (11)	0.4739 (6)	0.1678 (4)	0.108 (3)
H22	0.7731	0.5048	0.1968	0.129*
C23	0.5650 (10)	0.5074 (4)	0.1308 (3)	0.085 (2)
H23	0.5502	0.5608	0.1348	0.102*
C24	0.4467 (9)	0.4625 (3)	0.0858 (3)	0.0684 (18)
C25	-0.1907 (7)	0.6672 (3)	0.2707 (3)	0.0589 (14)
H25	-0.1394	0.6407	0.3110	0.071*
C26	-0.2362 (7)	0.7286 (3)	0.1729 (3)	0.0626 (15)
H26	-0.2210	0.7536	0.1315	0.075*
C27	-0.3772 (8)	0.7215 (4)	0.1936 (3)	0.0734 (16)
H27	-0.4758	0.7394	0.1699	0.088*
C28	0.2489 (10)	0.8574 (4)	0.2921 (3)	0.099 (3)
H28	0.2326	0.8398	0.3362	0.118*
C29	0.2722 (7)	0.8611 (3)	0.1845 (3)	0.0635 (15)
H29	0.2723	0.8466	0.1376	0.076*
C30	0.3157 (7)	0.9321 (4)	0.2124 (3)	0.0698 (16)
H30	0.3521	0.9743	0.1894	0.084*
Cd1	0.14721 (4)	0.68863 (2)	0.227269 (18)	0.05146 (17)
N1	0.2286 (6)	0.8142 (2)	0.2344 (2)	0.0604 (12)
N2	0.2951 (7)	0.9287 (3)	0.2801 (3)	0.0800 (15)
H2	0.3095	0.9664	0.3103	0.096*
N3	-0.1180 (5)	0.6943 (2)	0.2210 (2)	0.0542 (11)
N4	-0.3455 (6)	0.6822 (3)	0.2569 (3)	0.0648 (13)
H4A	-0.4137	0.6697	0.2829	0.078*
O1	0.1546 (5)	0.6372 (3)	0.3436 (2)	0.0823 (9)
O2	0.3806 (5)	0.6581 (3)	0.3125 (2)	0.0823 (9)
O3	0.2221 (6)	0.6855 (2)	0.1175 (2)	0.0803 (9)
O4	0.1694 (6)	0.5712 (2)	0.1548 (2)	0.0803 (9)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.051 (4)	0.061 (4)	0.066 (3)	0.015 (3)	0.019 (3)	0.004 (3)
C2	0.059 (4)	0.093 (5)	0.059 (3)	0.003 (3)	0.016 (3)	0.003 (3)
C3	0.056 (4)	0.074 (4)	0.044 (3)	0.010 (3)	0.009 (3)	0.005 (3)
C4	0.073 (5)	0.074 (4)	0.048 (3)	0.014 (3)	0.006 (3)	-0.005 (3)
C5	0.076 (5)	0.064 (4)	0.048 (3)	-0.007 (3)	0.001 (3)	0.000 (3)
C6	0.054 (4)	0.064 (4)	0.057 (3)	-0.002 (3)	0.001 (3)	0.007 (3)
C7	0.056 (4)	0.062 (3)	0.043 (2)	0.004 (3)	0.005 (2)	0.012 (2)

C8	0.054 (4)	0.070 (4)	0.068 (3)	0.011 (3)	0.004 (3)	0.002 (3)
C9	0.076 (5)	0.069 (4)	0.089 (4)	0.020 (4)	0.012 (4)	-0.002 (3)
C10	0.088 (6)	0.067 (4)	0.101 (5)	0.003 (4)	0.002 (4)	-0.019 (4)
C11	0.054 (4)	0.075 (4)	0.081 (4)	-0.005 (3)	-0.001 (3)	-0.004 (3)
C12	0.050 (3)	0.061 (3)	0.051 (3)	0.002 (3)	0.006 (3)	0.005 (2)
C13	0.070 (4)	0.060 (4)	0.050 (3)	0.011 (3)	0.017 (3)	0.009 (2)
C14	0.109 (6)	0.077 (4)	0.061 (3)	0.011 (4)	0.036 (4)	0.007 (3)
C15	0.092 (5)	0.078 (4)	0.053 (3)	0.004 (4)	0.034 (3)	-0.011 (3)
C16	0.095 (6)	0.103 (6)	0.084 (4)	0.011 (5)	0.030 (4)	-0.037 (4)
C17	0.092 (6)	0.097 (6)	0.121 (6)	-0.013 (5)	0.038 (5)	-0.055 (5)
C18	0.118 (7)	0.078 (5)	0.130 (6)	-0.013 (5)	0.076 (6)	-0.036 (5)
C19	0.098 (6)	0.061 (4)	0.072 (4)	0.002 (4)	0.041 (4)	-0.009 (3)
C20	0.127 (7)	0.072 (5)	0.081 (4)	0.014 (5)	0.040 (5)	0.002 (4)
C21	0.145 (9)	0.113 (7)	0.080 (5)	0.028 (6)	0.019 (5)	0.005 (5)
C22	0.122 (8)	0.106 (7)	0.091 (5)	-0.014 (6)	0.007 (5)	-0.020 (5)
C23	0.120 (7)	0.065 (4)	0.074 (4)	-0.007 (5)	0.027 (4)	-0.002 (4)
C24	0.104 (5)	0.057 (4)	0.055 (3)	-0.010 (4)	0.043 (4)	-0.007 (3)
C25	0.046 (3)	0.070 (4)	0.063 (3)	0.003 (3)	0.014 (3)	0.011 (3)
C26	0.072 (4)	0.058 (3)	0.057 (3)	0.005 (3)	0.011 (3)	0.008 (3)
C27	0.056 (4)	0.079 (4)	0.080 (4)	-0.002 (3)	0.002 (3)	0.004 (4)
C28	0.166 (8)	0.062 (4)	0.088 (4)	-0.022 (4)	0.077 (5)	-0.009 (3)
C29	0.082 (4)	0.052 (4)	0.058 (3)	0.002 (3)	0.019 (3)	0.004 (3)
C30	0.079 (5)	0.059 (4)	0.076 (4)	0.003 (3)	0.028 (3)	0.010 (3)
Cd1	0.0507 (3)	0.0500 (3)	0.0565 (2)	-0.00004 (18)	0.01726 (19)	0.00188 (17)
N1	0.067 (3)	0.054 (3)	0.066 (3)	-0.004 (2)	0.029 (2)	-0.008 (2)
N2	0.106 (4)	0.050 (3)	0.094 (3)	-0.017 (3)	0.045 (3)	-0.014 (3)
N3	0.048 (3)	0.058 (3)	0.059 (2)	0.004 (2)	0.017 (2)	0.009 (2)
N4	0.053 (3)	0.071 (3)	0.074 (3)	-0.003 (2)	0.023 (2)	0.005 (2)
O1	0.0491 (18)	0.123 (3)	0.0752 (18)	0.0087 (18)	0.0131 (15)	0.0229 (18)
O2	0.0491 (18)	0.123 (3)	0.0752 (18)	0.0087 (18)	0.0131 (15)	0.0229 (18)
O3	0.125 (3)	0.0522 (18)	0.0756 (17)	0.0066 (17)	0.0499 (18)	0.0068 (14)
O4	0.125 (3)	0.0522 (18)	0.0756 (17)	0.0066 (17)	0.0499 (18)	0.0068 (14)

Geometric parameters (Å, °)

C1—O2	1.236 (6)	C18—C19	1.412 (10)
C1—O1	1.240 (6)	C18—H18	0.9300
C1—C2	1.513 (7)	C19—C20	1.407 (9)
C2—C3	1.501 (8)	C19—C24	1.426 (8)
C2—H2A	0.9700	C20—C21	1.340 (11)
C2—H2B	0.9700	C20—H20	0.9300
C3—C4	1.366 (8)	C21—C22	1.386 (11)
C3—C12	1.425 (7)	C21—H21	0.9300
C4—C5	1.410 (9)	C22—C23	1.350 (10)
C4—H4	0.9300	C22—H22	0.9300
C5—C6	1.362 (7)	C23—C24	1.423 (9)
C5—H5	0.9300	C23—H23	0.9300
C6—C7	1.413 (7)	C25—N3	1.313 (6)
C6—H6	0.9300	C25—N4	1.323 (7)

supplementary materials

C7—C8	1.414 (7)	C25—H25	0.9300
C7—C12	1.422 (7)	C26—C27	1.340 (8)
C8—C9	1.354 (8)	C26—N3	1.365 (7)
C8—H8	0.9300	C26—H26	0.9300
C9—C10	1.402 (9)	C27—N4	1.367 (8)
C9—H9	0.9300	C27—H27	0.9300
C10—C11	1.356 (8)	C28—N1	1.315 (7)
C10—H10	0.9300	C28—N2	1.319 (7)
C11—C12	1.402 (7)	C28—H28	0.9300
C11—H11	0.9300	C29—N1	1.352 (6)
C13—O3	1.230 (6)	C29—C30	1.355 (7)
C13—O4	1.252 (6)	C29—H29	0.9300
C13—C14	1.517 (7)	C30—N2	1.339 (7)
C14—C15	1.494 (8)	C30—H30	0.9300
C14—H14A	0.9700	Cd1—N3	2.244 (4)
C14—H14B	0.9700	Cd1—N1	2.259 (4)
C15—C16	1.367 (9)	Cd1—O3	2.306 (3)
C15—C24	1.415 (9)	Cd1—O1	2.384 (4)
C16—C17	1.398 (10)	Cd1—O2	2.384 (4)
C16—H16	0.9300	Cd1—O4	2.473 (4)
C17—C18	1.353 (11)	N2—H2	0.8600
C17—H17	0.9300	N4—H4A	0.8600
O2—C1—O1	120.6 (5)	C21—C20—H20	119.6
O2—C1—C2	122.0 (5)	C19—C20—H20	119.6
O1—C1—C2	117.4 (4)	C20—C21—C22	119.8 (9)
C3—C2—C1	115.3 (4)	C20—C21—H21	120.1
C3—C2—H2A	108.4	C22—C21—H21	120.1
C1—C2—H2A	108.4	C23—C22—C21	121.7 (8)
C3—C2—H2B	108.4	C23—C22—H22	119.1
C1—C2—H2B	108.4	C21—C22—H22	119.1
H2A—C2—H2B	107.5	C22—C23—C24	121.3 (7)
C4—C3—C12	118.8 (5)	C22—C23—H23	119.4
C4—C3—C2	120.5 (5)	C24—C23—H23	119.4
C12—C3—C2	120.6 (5)	C15—C24—C23	123.8 (6)
C3—C4—C5	121.5 (5)	C15—C24—C19	120.4 (6)
C3—C4—H4	119.3	C23—C24—C19	115.8 (7)
C5—C4—H4	119.3	N3—C25—N4	112.0 (5)
C6—C5—C4	120.5 (5)	N3—C25—H25	124.0
C6—C5—H5	119.7	N4—C25—H25	124.0
C4—C5—H5	119.7	C27—C26—N3	110.7 (5)
C5—C6—C7	120.3 (5)	C27—C26—H26	124.7
C5—C6—H6	119.8	N3—C26—H26	124.7
C7—C6—H6	119.8	C26—C27—N4	105.4 (6)
C6—C7—C8	121.1 (5)	C26—C27—H27	127.3
C6—C7—C12	119.0 (5)	N4—C27—H27	127.3
C8—C7—C12	119.9 (5)	N1—C28—N2	112.0 (5)
C9—C8—C7	120.5 (6)	N1—C28—H28	124.0
C9—C8—H8	119.8	N2—C28—H28	124.0
C7—C8—H8	119.8	N1—C29—C30	110.4 (5)

C8—C9—C10	119.9 (6)	N1—C29—H29	124.8
C8—C9—H9	120.1	C30—C29—H29	124.8
C10—C9—H9	120.1	N2—C30—C29	105.4 (5)
C11—C10—C9	120.7 (6)	N2—C30—H30	127.3
C11—C10—H10	119.7	C29—C30—H30	127.3
C9—C10—H10	119.7	N3—Cd1—N1	104.92 (16)
C10—C11—C12	121.8 (6)	N3—Cd1—O3	113.55 (17)
C10—C11—H11	119.1	N1—Cd1—O3	86.72 (14)
C12—C11—H11	119.1	N3—Cd1—O1	85.25 (14)
C11—C12—C7	117.2 (5)	N1—Cd1—O1	110.02 (16)
C11—C12—C3	123.0 (5)	O3—Cd1—O1	151.34 (16)
C7—C12—C3	119.8 (5)	N3—Cd1—O2	138.65 (14)
O3—C13—O4	121.1 (5)	N1—Cd1—O2	87.71 (17)
O3—C13—C14	117.9 (5)	O3—Cd1—O2	106.24 (15)
O4—C13—C14	121.0 (5)	O1—Cd1—O2	53.62 (13)
C15—C14—C13	117.6 (4)	N3—Cd1—O4	100.77 (15)
C15—C14—H14A	107.9	N1—Cd1—O4	139.07 (13)
C13—C14—H14A	107.9	O3—Cd1—O4	53.65 (12)
C15—C14—H14B	107.9	O1—Cd1—O4	103.32 (14)
C13—C14—H14B	107.9	O2—Cd1—O4	93.62 (16)
H14A—C14—H14B	107.2	C28—N1—C29	104.2 (5)
C16—C15—C24	118.3 (6)	C28—N1—Cd1	125.4 (4)
C16—C15—C14	120.4 (7)	C29—N1—Cd1	130.3 (3)
C24—C15—C14	121.3 (6)	C28—N2—C30	107.8 (5)
C15—C16—C17	121.9 (8)	C28—N2—H2	126.1
C15—C16—H16	119.1	C30—N2—H2	126.1
C17—C16—H16	119.1	C25—N3—C26	104.5 (5)
C18—C17—C16	120.7 (8)	C25—N3—Cd1	123.6 (4)
C18—C17—H17	119.6	C26—N3—Cd1	131.7 (3)
C16—C17—H17	119.6	C25—N4—C27	107.4 (5)
C17—C18—C19	120.5 (8)	C25—N4—H4A	126.3
C17—C18—H18	119.7	C27—N4—H4A	126.3
C19—C18—H18	119.7	C1—O1—Cd1	92.6 (3)
C20—C19—C18	121.2 (7)	C1—O2—Cd1	92.7 (3)
C20—C19—C24	120.6 (7)	C13—O3—Cd1	96.7 (3)
C18—C19—C24	118.2 (8)	C13—O4—Cd1	88.2 (3)
C21—C20—C19	120.8 (8)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2 \cdots O4 ⁱ	0.86	1.92	2.735 (6)	159
N4—H4A \cdots O2 ⁱⁱ	0.86	1.95	2.772 (6)	159

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

Fig. 1

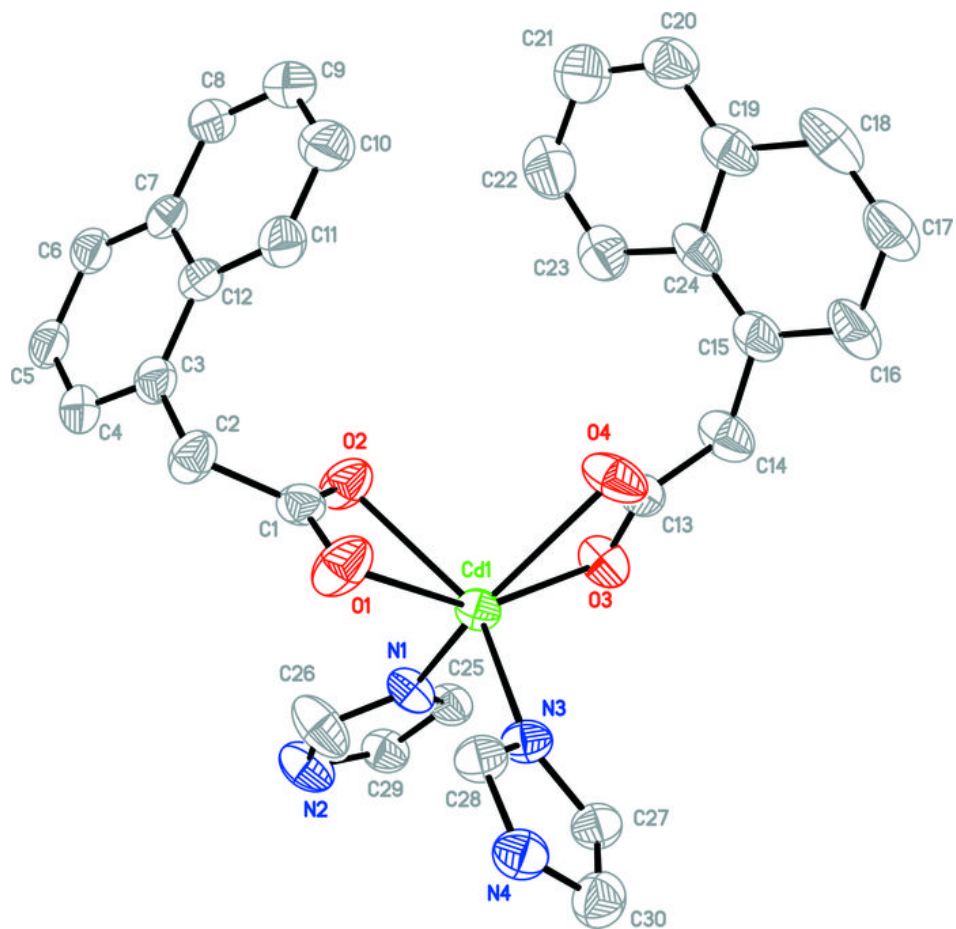


Fig. 2

