Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(7-amino-2,4-dimethyl-1,8-naphthyridine)dinitratocadmium(II)

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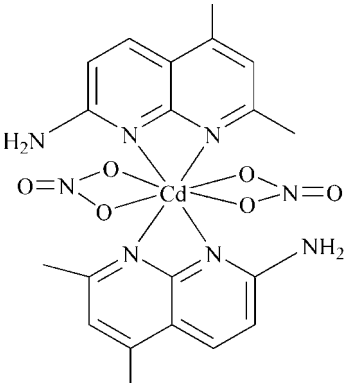
Received 15 November 2007; accepted 23 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.035; wR factor = 0.081; data-to-parameter ratio = 12.8.

In the title compound, $[Cd(NO_3)_2(C_{10}H_{11}N_3)_2]$, two naphthyridine ring systems are coordinated to the Cd ion through the two N atoms in a bidentate chelating mode, whereas the remaining coordination sites are occupied by two O atoms from two different nitrate groups to complete the octahedral geometry. Intermoleular N—H···O hydrogen bonds link the molecules to form a one-dimensionnal sheet parallel to the *ac* plane. Weak slipped π–π stacking involving the naphthyridine ring systems stabilizes the structure.

Related literature

For related literature, see: Bayer (1979); Che *et al.* (2001); Gavrilova & Bosnich (2004); Jin *et al.* (2007); Kukrek *et al.* (2006); Mintert & Sheldrick (1995*a*,*b*); Oskui & Sheldrick (1999); Oskui, Mintert & Sheldrick (1999).



Experimental

Crystal data

$[Cd(NO_3)_2(C_{10}H_{11}N_3)_2]$
M_r = 582.86
Triclinic, $P\overline{1}$
a = 9.308 (2) Å
b = 9.584 (2) Å
c = 15.067 (4) Å
α = 95.497 (3)°
β = 95.224 (3)°
γ = 116.865 (3)°
V = 1179.8 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.98 mm^{-1}
T = 298 (2) K
0.45 × 0.37 × 0.31 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.667, T_{max} = 0.751
6136 measured reflections
4101 independent reflections
3346 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.081
S = 1.09
4101 reflections
320 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O2	0.86	2.23	3.033 (4)	155
N3—H3B···O5^{i}	0.86	2.38	3.161 (4)	151
N6—H6A···O5	0.86	2.11	2.902 (4)	153
N6—H6B···O3^{ii}	0.86	2.18	2.979 (4)	154

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

Table 2
Main π–π interactions (Å, °).

α is the dihedral angle between the planes. DCC is the length of the CC vector (centroid to centroid). τ is the angle(s) subtended by the plane(s) normal to CC (offset angle). *Cg*1 is the centroid of ring N1/C1/C5–C8; *Cg*2 is the centroid of ring N2/C1/C5–C2.

Centroid 1	Centroid 2	α	DCC	τ
*Cg*1	*Cg*2^{iii}	1.32	3.862 (2)	26
*Cg*2	*Cg*2^{iii}	0.0	3.823 (2)	25

Symmetry code: (iii) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors thank the Zhejiang Forestry University Science Foundation for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2283).

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supporting information

Acta Cryst. (2008). E**64**, m54–m55 [https://doi.org/10.1107/S160053680706271X]

Bis(7-amino-2,4-dimethyl-1,8-naphthyridine)dinitratocadmium(II)

Shou-Wen Jin, Qi-Jun Zhao, Xian-Gang Qian, Ru-Xiang Chen and Yan-Fen Shi

S1. Comment

Molecular structures and chemical properties of transition metal complexes of 1,8-naphthyridine (napy) and its derivatives have received much attention(Kukrek *et al.*, 2006; Che *et al.*, 2001), because the ligands can link to metals with several coordination modes such as monodentate, chelating bidentate, and dinuclear bridging binding fashion (Gavrilova & Bosnich, 2004). 5,7-dimethyl-1,8-naphthyridin-2-amine (*L*) is a potentially tridentate ligand and is capable of linking two to four metal atoms together to form metal aggregates (Oskui *et al.*, 1999; Mintert & Sheldrick, 1995*a*; Oskui & Sheldrick, 1999; Mintert & Sheldrick, 1995*b*). The coordination chemistry of 5,7-dimethyl-1,8-naphthyridine-2-amine has not been well studied before although a series of transiton metal complex ($M_{(L)}2_{Cl}2$) were once described in a US patent (Bayer, 1979). As an extension of our study on naphthyridine coordination chemistry(Jin *et al.*, 2007), herein the title complex $[Cd(L)_2(NO_3)_{2]}$ is reported.

In the title compound, two naphthyridine are coordinated to the Cd ion through two nitrogen atoms in bidentate chelating mode whereas the remaining coordination sites are occupied by two oxygen atoms from two different nitrates (Fig. 1). The two nitrate ligands display a dissymetric chelating mode with Cd—O distances of 2.357 (4) and 2.718 (4). The remaining distances are within the usual range. The two naphthyridine rings were almost perpendicular to each other making dihedral angle of 80.22 (7)°. The two chelating Cd—O—N—O group make dihedral angle of 81.21 (12)°.

Intermoleular N—H···O hydrogen bonds link the molecules to form a one dimensionnal sheet parallel to the *a* axis (Table 1, Fig. 2). Weak slippest π-π stackings involving the naphthyridine rings stabilize the structure (Table 2).

S2. Experimental

All reagents and solvents were used as obtained without further purification. The CHN elemental analyses were performed on a Perkin-Elmer model 2400 elemental analyzer. A solution of cadmium nitrate tetrahydrate (31.4 mg, 0.1 mmol) in methanol (3 ml) was added to *L* (52.2 mg, 0.3 mmol) in methanol (10 ml) to give a colorless solution. The methanol solution was filtered. The solution was left standing at room temperature for several days, colorless block crystals were isolated. Yield: 41 mg, 70.3%. Anal. Calcd. for $C_{20}H_{22}Cd_N8_O6$: C, 41.18; H, 3.77; N, 19.22. Found: C, 41.14; H, 3.72; N, 19.18.

S3. Refinement

All H atoms attached to C atoms and N atom were fixed geometrically and treated as riding with C—H = 0.93 Å (aromatic) or 0.96 Å (methyl) and N—H = 0.86 Å with U_{iso}(H) = 1.2U_{eq}(Caromatic or N) or U_{iso}(H) = 1.5U_{eq}(Cmethyl).

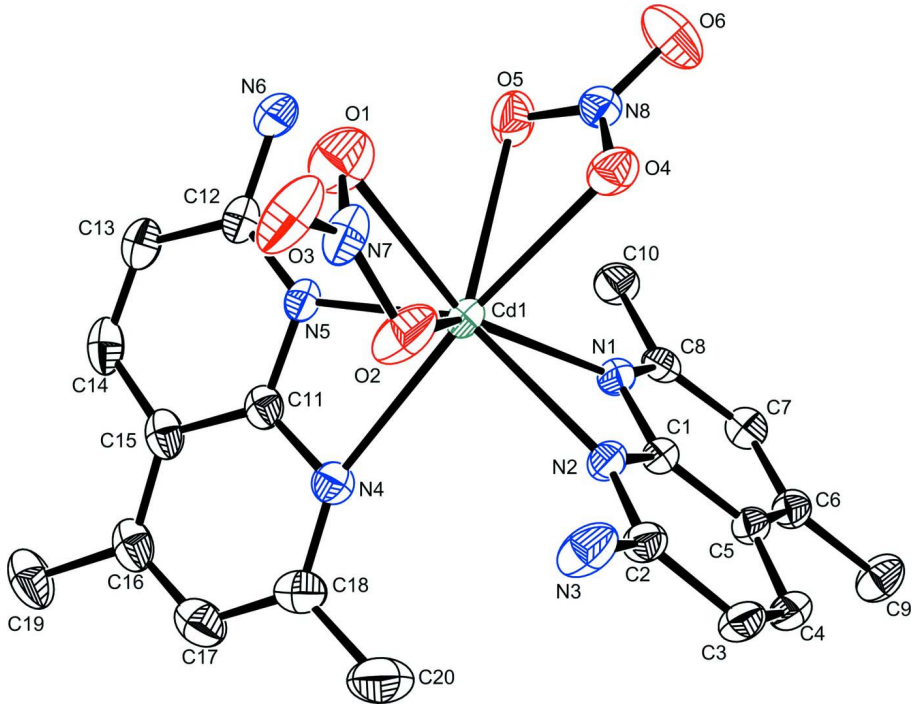

Figure 1

Molecular view of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

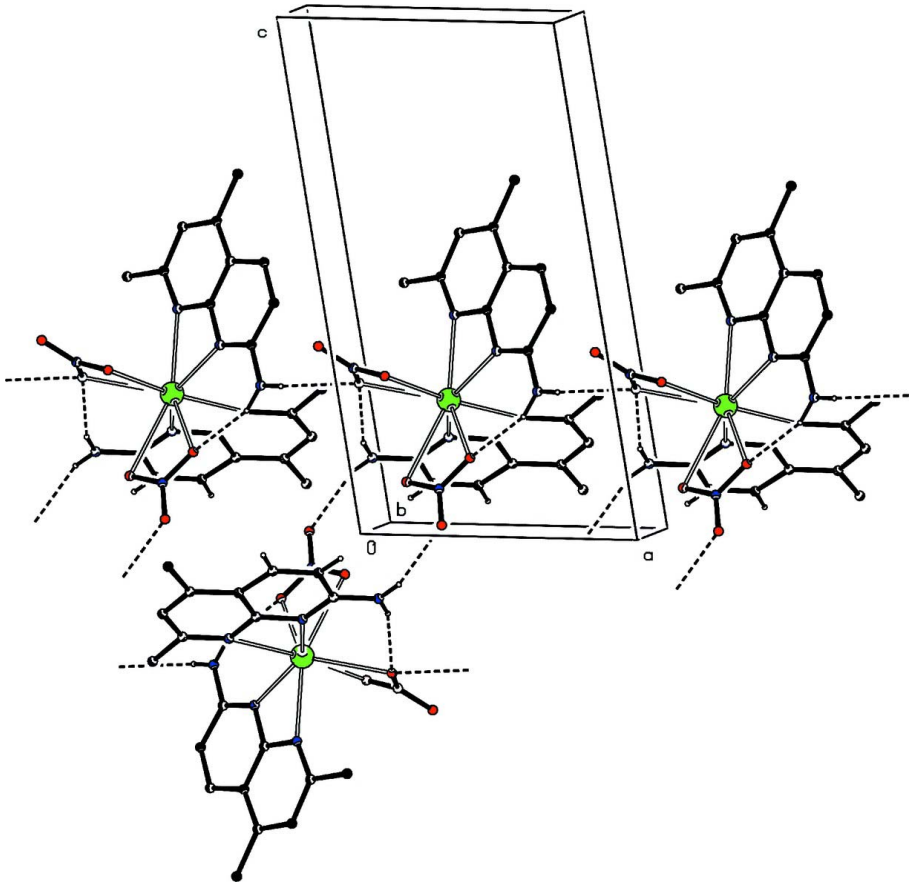

Figure 2

Partial packing view showing the N—H···O hydrogen bonds. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bondings have been omitted for clarity.

Dinitratobis(7-amino-2,4-dimethyl-1,8-naphthyridine)cadmium(II)

Crystal data

$[Cd(NO_3)_2(C_{10}H_{11}N_3)_2]$
$M_r = 582.86$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.308\ (2)$ Å
$b = 9.584\ (2)$ Å
$c = 15.067\ (4)$ Å
$\alpha = 95.497\ (3)°$
$\beta = 95.224\ (3)°$
$\gamma = 116.865\ (3)°$
$V = 1179.8\ (5)$ Å^3
$Z = 2$
$F(000) = 588$
$D_x = 1.641$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2793 reflections
$\theta = 2.4–26.1°$
$\mu = 0.98$ mm^{-1}
$T = 298$ K
Block, colorless
0.45 × 0.37 × 0.31 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.667$, $T_{max} = 0.751$
6136 measured reflections
4101 independent reflections

3346 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -11 \rightarrow 6$
$k = -11 \rightarrow 11$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.081$
$S = 1.09$
4101 reflections
320 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
$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.1524P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.32533 (3)	0.63678 (3)	0.248895 (17)	0.04168 (11)
N1	0.3847 (3)	0.7270 (3)	0.41178 (18)	0.0381 (7)
N2	0.5294 (3)	0.6210 (3)	0.34613 (18)	0.0385 (7)
N3	0.6662 (4)	0.5103 (4)	0.2720 (2)	0.0624 (10)
H3A	0.6026	0.4943	0.2228	0.075*
H3B	0.7418	0.4820	0.2719	0.075*
N4	0.5509 (4)	0.8962 (4)	0.2110 (2)	0.0448 (7)
N5	0.2822 (4)	0.8123 (3)	0.17237 (18)	0.0407 (7)
N6	0.0057 (4)	0.7107 (4)	0.1316 (2)	0.0616 (9)
H6A	−0.0097	0.6348	0.1619	0.074*
H6B	−0.0763	0.7152	0.1034	0.074*
N7	0.2627 (5)	0.4197 (4)	0.0808 (2)	0.0568 (9)
N8	0.0220 (4)	0.4282 (4)	0.3115 (2)	0.0459 (8)
O1	0.1458 (4)	0.4451 (4)	0.0924 (2)	0.0826 (10)
O2	0.3852 (4)	0.4845 (4)	0.1406 (2)	0.0784 (10)
O3	0.2607 (4)	0.3373 (4)	0.0126 (2)	0.0803 (10)
O4	0.1344 (3)	0.3951 (3)	0.29808 (18)	0.0550 (7)
O5	0.0207 (4)	0.5429 (4)	0.27969 (18)	0.0622 (8)
O6	−0.0832 (5)	0.3513 (4)	0.3543 (2)	0.0927 (11)
C1	0.5092 (4)	0.6900 (4)	0.4236 (2)	0.0342 (8)
C2	0.6476 (4)	0.5792 (4)	0.3489 (2)	0.0395 (8)
C3	0.7515 (4)	0.6041 (4)	0.4305 (2)	0.0447 (9)

H3	0.8323	0.5722	0.4311	0.054*
C4	0.7316 (4)	0.6744 (4)	0.5071 (2)	0.0427 (9)
H4	0.8013	0.6939	0.5603	0.051*
C5	0.6056 (4)	0.7189 (4)	0.5074 (2)	0.0361 (8)
C6	0.5702 (4)	0.7900 (4)	0.5826 (2)	0.0403 (8)
C7	0.4400 (5)	0.8216 (4)	0.5692 (2)	0.0449 (9)
H7	0.4116	0.8652	0.6181	0.054*
C8	0.3495 (4)	0.7898 (4)	0.4836 (2)	0.0386 (8)
C9	0.6701 (5)	0.8290 (5)	0.6740 (2)	0.0586 (11)
H9A	0.6225	0.8677	0.7177	0.088*
H9B	0.7791	0.9088	0.6724	0.088*
H9C	0.6725	0.7356	0.6902	0.088*
C10	0.2099 (5)	0.8259 (5)	0.4700 (3)	0.0533 (10)
H10A	0.1851	0.8294	0.4073	0.080*
H10B	0.2383	0.9266	0.5047	0.080*
H10C	0.1165	0.7451	0.4893	0.080*
C11	0.4365 (5)	0.9236 (4)	0.1670 (2)	0.0406 (8)
C12	0.1564 (5)	0.8210 (5)	0.1283 (2)	0.0470 (9)
C13	0.1818 (6)	0.9478 (5)	0.0788 (3)	0.0560 (11)
H13	0.0928	0.9539	0.0496	0.067*
C14	0.3334 (6)	1.0585 (5)	0.0741 (3)	0.0571 (11)
H14	0.3489	1.1410	0.0419	0.069*
C15	0.4704 (5)	1.0502 (4)	0.1182 (2)	0.0466 (9)
C16	0.6348 (6)	1.1545 (5)	0.1155 (3)	0.0545 (11)
C17	0.7501 (6)	1.1242 (5)	0.1602 (3)	0.0623 (12)
H17	0.8598	1.1908	0.1592	0.075*
C18	0.7068 (5)	0.9956 (5)	0.2072 (3)	0.0554 (10)
C19	0.6828 (6)	1.2936 (5)	0.0644 (3)	0.0732 (14)
H19A	0.7992	1.3479	0.0680	0.110*
H19B	0.6461	1.3648	0.0904	0.110*
H19C	0.6336	1.2561	0.0023	0.110*
C20	0.8329 (5)	0.9635 (6)	0.2569 (4)	0.0837 (15)
H20A	0.8194	0.9630	0.3193	0.126*
H20B	0.9396	1.0446	0.2521	0.126*
H20C	0.8206	0.8624	0.2313	0.126*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03665 (17)	0.05040 (19)	0.03889 (17)	0.02133 (13)	−0.00124 (11)	0.01172 (12)
N1	0.0334 (16)	0.0441 (18)	0.0397 (17)	0.0198 (15)	0.0055 (13)	0.0101 (14)
N2	0.0343 (16)	0.0515 (19)	0.0318 (16)	0.0219 (15)	0.0033 (13)	0.0070 (13)
N3	0.056 (2)	0.103 (3)	0.0426 (19)	0.053 (2)	0.0011 (16)	−0.0061 (19)
N4	0.0439 (19)	0.0461 (19)	0.0428 (18)	0.0198 (17)	0.0060 (15)	0.0060 (14)
N5	0.0465 (19)	0.0442 (18)	0.0313 (16)	0.0218 (16)	0.0004 (14)	0.0064 (13)
N6	0.047 (2)	0.072 (3)	0.064 (2)	0.026 (2)	−0.0057 (17)	0.0254 (19)
N7	0.076 (3)	0.057 (2)	0.041 (2)	0.037 (2)	−0.0073 (19)	0.0058 (17)
N8	0.0391 (18)	0.054 (2)	0.0418 (18)	0.0183 (17)	0.0073 (15)	0.0091 (16)

O1	0.083 (2)	0.101 (3)	0.081 (2)	0.061 (2)	0.0066 (19)	0.0053 (19)
O2	0.073 (2)	0.100 (3)	0.0541 (19)	0.044 (2)	−0.0205 (16)	−0.0151 (17)
O3	0.111 (3)	0.096 (3)	0.0524 (19)	0.077 (2)	−0.0252 (18)	−0.0190 (17)
O4	0.0460 (16)	0.0676 (19)	0.0608 (18)	0.0351 (15)	0.0044 (13)	0.0099 (14)
O5	0.072 (2)	0.071 (2)	0.0607 (18)	0.0446 (18)	0.0102 (15)	0.0249 (16)
O6	0.089 (3)	0.092 (3)	0.100 (3)	0.032 (2)	0.060 (2)	0.037 (2)
C1	0.0311 (18)	0.0372 (19)	0.0331 (19)	0.0152 (16)	0.0029 (15)	0.0069 (15)
C2	0.033 (2)	0.048 (2)	0.039 (2)	0.0206 (18)	0.0045 (16)	0.0052 (17)
C3	0.034 (2)	0.055 (2)	0.049 (2)	0.0253 (19)	−0.0001 (17)	0.0072 (19)
C4	0.035 (2)	0.050 (2)	0.039 (2)	0.0176 (18)	−0.0038 (16)	0.0045 (17)
C5	0.0343 (19)	0.0355 (19)	0.0347 (19)	0.0139 (17)	0.0013 (15)	0.0042 (15)
C6	0.041 (2)	0.039 (2)	0.037 (2)	0.0156 (18)	0.0013 (16)	0.0029 (16)
C7	0.048 (2)	0.042 (2)	0.043 (2)	0.0206 (19)	0.0096 (18)	0.0027 (17)
C8	0.0327 (19)	0.034 (2)	0.048 (2)	0.0130 (16)	0.0113 (17)	0.0103 (17)
C9	0.062 (3)	0.076 (3)	0.037 (2)	0.036 (2)	−0.0058 (19)	−0.006 (2)
C10	0.046 (2)	0.059 (3)	0.067 (3)	0.032 (2)	0.014 (2)	0.014 (2)
C11	0.050 (2)	0.037 (2)	0.0300 (19)	0.0172 (19)	0.0063 (17)	−0.0007 (15)
C12	0.057 (3)	0.052 (2)	0.035 (2)	0.029 (2)	0.0013 (18)	0.0076 (18)
C13	0.069 (3)	0.062 (3)	0.046 (2)	0.038 (3)	0.003 (2)	0.015 (2)
C14	0.090 (4)	0.051 (3)	0.041 (2)	0.040 (3)	0.013 (2)	0.0157 (19)
C15	0.067 (3)	0.038 (2)	0.034 (2)	0.023 (2)	0.0129 (19)	0.0019 (17)
C16	0.075 (3)	0.040 (2)	0.036 (2)	0.016 (2)	0.014 (2)	−0.0011 (18)
C17	0.059 (3)	0.053 (3)	0.060 (3)	0.013 (2)	0.018 (2)	0.002 (2)
C18	0.044 (2)	0.056 (3)	0.059 (3)	0.019 (2)	0.007 (2)	0.000 (2)
C19	0.097 (4)	0.043 (3)	0.057 (3)	0.011 (3)	0.028 (3)	0.009 (2)
C20	0.047 (3)	0.082 (4)	0.118 (4)	0.027 (3)	0.008 (3)	0.020 (3)

Geometric parameters (Å, º)

Cd1—N5	2.284 (3)	C4—H4	0.9300
Cd1—O2	2.355 (3)	C5—C6	1.408 (5)
Cd1—N2	2.361 (3)	C6—C7	1.379 (5)
Cd1—O4	2.433 (3)	C6—C9	1.501 (5)
Cd1—N1	2.448 (3)	C7—C8	1.400 (5)
Cd1—N4	2.586 (3)	C7—H7	0.9300
N1—C8	1.326 (4)	C8—C10	1.490 (5)
N1—C1	1.359 (4)	C9—H9A	0.9600
N2—C2	1.328 (4)	C9—H9B	0.9600
N2—C1	1.356 (4)	C9—H9C	0.9600
N3—C2	1.343 (4)	C10—H10A	0.9600
N3—H3A	0.8600	C10—H10B	0.9600
N3—H3B	0.8600	C10—H10C	0.9600
N4—C18	1.339 (5)	C11—C15	1.406 (5)
N4—C11	1.342 (5)	C12—C13	1.427 (5)
N5—C12	1.333 (4)	C13—C14	1.342 (6)
N5—C11	1.364 (5)	C13—H13	0.9300
N6—C12	1.330 (5)	C14—C15	1.422 (6)
N6—H6A	0.8600	C14—H14	0.9300

N6—H6B	0.8600	C15—C16	1.406 (6)
N7—O3	1.229 (4)	C16—C17	1.370 (6)
N7—O1	1.241 (4)	C16—C19	1.514 (5)
N7—O2	1.250 (4)	C17—C18	1.398 (6)
N8—O6	1.213 (4)	C17—H17	0.9300
N8—O5	1.246 (4)	C18—C20	1.498 (6)
N8—O4	1.250 (4)	C19—H19A	0.9600
C1—C5	1.405 (4)	C19—H19B	0.9600
C2—C3	1.423 (5)	C19—H19C	0.9600
C3—C4	1.351 (5)	C20—H20A	0.9600
C3—H3	0.9300	C20—H20B	0.9600
C4—C5	1.418 (5)	C20—H20C	0.9600

N5—Cd1—O2	104.91 (11)	C7—C6—C9	121.4 (3)
N5—Cd1—N2	140.76 (11)	C5—C6—C9	121.2 (3)
O2—Cd1—N2	84.14 (10)	C6—C7—C8	121.6 (3)
N5—Cd1—O4	130.94 (10)	C6—C7—H7	119.2
O2—Cd1—O4	89.68 (11)	C8—C7—H7	119.2
N2—Cd1—O4	86.30 (9)	N1—C8—C7	121.4 (3)
N5—Cd1—N1	111.10 (9)	N1—C8—C10	117.6 (3)
O2—Cd1—N1	139.39 (10)	C7—C8—C10	121.0 (3)
N2—Cd1—N1	56.05 (9)	C6—C9—H9A	109.5
O4—Cd1—N1	80.82 (9)	C6—C9—H9B	109.5
N5—Cd1—N4	54.63 (10)	H9A—C9—H9B	109.5
O2—Cd1—N4	91.13 (11)	C6—C9—H9C	109.5
N2—Cd1—N4	87.67 (10)	H9A—C9—H9C	109.5
O4—Cd1—N4	173.80 (9)	H9B—C9—H9C	109.5
N1—Cd1—N4	94.61 (9)	C8—C10—H10A	109.5
C8—N1—C1	118.2 (3)	C8—C10—H10B	109.5
C8—N1—Cd1	148.2 (2)	H10A—C10—H10B	109.5
C1—N1—Cd1	93.59 (19)	C8—C10—H10C	109.5
C2—N2—C1	118.5 (3)	H10A—C10—H10C	109.5
C2—N2—Cd1	143.8 (2)	H10B—C10—H10C	109.5
C1—N2—Cd1	97.6 (2)	N4—C11—N5	112.6 (3)
C2—N3—H3A	120.0	N4—C11—C15	124.2 (4)
C2—N3—H3B	120.0	N5—C11—C15	123.2 (3)
H3A—N3—H3B	120.0	N6—C12—N5	119.3 (3)
C18—N4—C11	117.4 (3)	N6—C12—C13	120.0 (4)
C18—N4—Cd1	152.3 (3)	N5—C12—C13	120.7 (4)
C11—N4—Cd1	89.8 (2)	C14—C13—C12	120.4 (4)
C12—N5—C11	119.0 (3)	C14—C13—H13	119.8
C12—N5—Cd1	137.6 (3)	C12—C13—H13	119.8
C11—N5—Cd1	102.9 (2)	C13—C14—C15	120.3 (4)
C12—N6—H6A	120.0	C13—C14—H14	119.8
C12—N6—H6B	120.0	C15—C14—H14	119.8
H6A—N6—H6B	120.0	C11—C15—C16	117.8 (4)
O3—N7—O1	121.8 (4)	C11—C15—C14	116.3 (4)
O3—N7—O2	120.9 (4)	C16—C15—C14	125.9 (4)

O1—N7—O2	117.3 (3)	C17—C16—C15	117.4 (4)
O6—N8—O5	120.6 (3)	C17—C16—C19	121.2 (4)
O6—N8—O4	121.3 (4)	C15—C16—C19	121.5 (4)
O5—N8—O4	118.1 (3)	C16—C17—C18	121.5 (4)
N7—O2—Cd1	105.8 (3)	C16—C17—H17	119.2
N8—O4—Cd1	100.6 (2)	C18—C17—H17	119.2
N2—C1—N1	112.7 (3)	N4—C18—C17	121.8 (4)
N2—C1—C5	123.7 (3)	N4—C18—C20	116.7 (4)
N1—C1—C5	123.5 (3)	C17—C18—C20	121.6 (4)
N2—C2—N3	118.1 (3)	C16—C19—H19A	109.5
N2—C2—C3	121.8 (3)	C16—C19—H19B	109.5
N3—C2—C3	120.1 (3)	H19A—C19—H19B	109.5
C4—C3—C2	119.3 (3)	C16—C19—H19C	109.5
C4—C3—H3	120.4	H19A—C19—H19C	109.5
C2—C3—H3	120.4	H19B—C19—H19C	109.5
C3—C4—C5	120.7 (3)	C18—C20—H20A	109.5
C3—C4—H4	119.7	C18—C20—H20B	109.5
C5—C4—H4	119.7	H20A—C20—H20B	109.5
C1—C5—C6	117.8 (3)	C18—C20—H20C	109.5
C1—C5—C4	116.0 (3)	H20A—C20—H20C	109.5
C6—C5—C4	126.2 (3)	H20B—C20—H20C	109.5
C7—C6—C5	117.4 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O2	0.86	2.23	3.033 (4)	155
N3—H3*B*···O5^{i}	0.86	2.38	3.161 (4)	151
N6—H6*A*···O5	0.86	2.11	2.902 (4)	153
N6—H6*B*···O3^{ii}	0.86	2.18	2.979 (4)	154

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*, −*y*+1, −*z*.