Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tris(phenyl 2-pyridyl ketone oxime-κ^2N,N')cadmium(II) dinitrate

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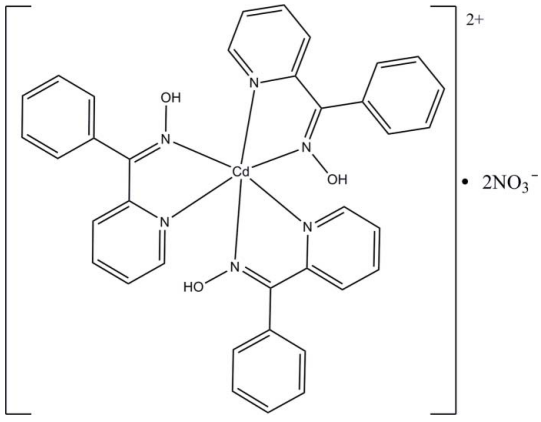
Received 5 May 2009; accepted 6 May 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.046; wR factor = 0.077; data-to-parameter ratio = 13.3.

The Cd atom in the title compound, $[Cd(C_{12}H_{10}N_2O)_3](NO_3)_2$, adopts a distorted octahedral geometry, being ligated by six N atoms from three different phenyl-2-pyridyl ketone oxime ligands. In the crystal structure, intermolecular O—H···O and C—H···O hydrogen bonds link the molecules into a chain structure propagating along [100]. The chains are further linked into a three-dimensional supramolecular structure *via* van der Waals forces.

Related literature

For related structures, see: Korpi *et al.* (2005); Pearse *et al.* (1989); Afrati *et al.* (2005); Stamatatos *et al.* (2006). For related literature on 2-pyridyl-substituted oximes, see: Papatriantafyllopoulou *et al.* (2007).



Experimental

Crystal data

$[Cd(C_{12}H_{10}N_2O)_3](NO_3)_2$
M_r = 831.08
Triclinic, $P\overline{1}$
a = 10.618 (3) Å
b = 11.687 (4) Å
c = 15.279 (5) Å
α = 101.263 (4)°
β = 100.166 (4)°
γ = 101.807 (4)°
V = 1773.3 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.68 mm^{-1}
T = 293 K
0.24 × 0.22 × 0.18 mm

Data collection

Bruker SMART Apex CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.853, T_{max} = 0.887
13329 measured reflections
6526 independent reflections
4387 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.077
S = 1.08
6526 reflections
490 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C32—H32···O8	0.93	2.48	3.355 (6)	157
C27—H27···O9^{i}	0.93	2.58	3.191 (6)	123
C14—H14···O5^{ii}	0.93	2.49	3.261 (6)	141
C4—H4···O3^{iii}	0.93	2.42	3.285 (5)	155
C3—H3*A*···O2^{iii}	0.93	2.56	3.461 (5)	164
O3—H3···O6	0.82	2.34	2.892 (4)	126
O3—H3···O4	0.82	2.00	2.820 (5)	176
O2—H2···O8	0.82	2.04	2.800 (5)	154
O2—H2···O7	0.82	2.21	2.939 (6)	149
O1—H1···O6	0.82	1.81	2.585 (4)	158

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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*.

This work was supported by the National Natural Science Foundation of China (No. 20731004), the Natural Science Foundation for Outstanding Scholars of Anhui Province, China (grant No. 044-J-04011) and the Natural Science Foundation of Education Commission of Anhui Province, China (No. KJ2008B004).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2779).

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supplementary materials

Acta Cryst. (2009). E**65**, m641 [**doi:10.1107/S1600536809017073**]

Tris(phenyl 2-pyridyl ketone oxime-κ^2N,N')cadmium(II) dinitrate

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Comment

Pyridine-2-carbaldehyde oxime ligands usually bind to metals in a bidentate fashion, either chelating one metal center or bridging two metals. Their complexes find application in diverse areas such as functional supramolecular design, magnetic materials and catalysis (Korpi *et al.*, 2005; Pearse *et al.*, 1989; Afrati *et al.*, 2005; Stamatatos *et al.*, 2006). The title compound is a new cadmium complex from the reaction of $Cd(NO_3)_2.4H_2O$ with phenyl-2-pyridyl ketone oxime (ppo). The compound consists of three N,N-chelating ligands and two nitrate anion. The three ppo ligands are coordinated to nickel to form three five-membered CdC_2N_2 rings.

The central cadmium atom adopts a distorted octahedral geometry (Fig. 1), which are ligated by six N atoms from three different phenyl-2-pyridyl ketone oxime ligands. The bond distances Cd—N, are in the expected ranges of 2.320 (3)–2.402 (3) Å, and the coordination angles around Ni atom are in the range 68.00 (11)–172.80 (12)°. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules into one-dimensional chain structure, which are further linker into three-dimensional supramolecular structure *via* van der Waals forces.

Experimental

A colourless solution of phenyl-2-pyridyl ketone oxime (0.394 g, 2.00 mmol) in MeOH (10 ml) was slowly added to a solution of $Cd(NO_3)_2.4H_2O$ (0.308 g, 1.00 mmol) in MeOH (10 ml) and the resulting colourless solution was stirred for 1 h at room temperature. A small quantity of undissolved material was removed by filtration. The filtrate was allowed to stand undisturbed in a closed flask for a period of 7–8 d. Colourless block crystals appeared which were collected by filtration, washed with cold MeOH (1 ml) and ice-cold Et_2O (2 ml), and dried in air [yield: 70%].

Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å and O—H = 0.82 Å, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for hydroxyl H and x = 1.2 for aromatic H atoms. The deepest hole is located 1.01Å from atom Cd1.

Figures

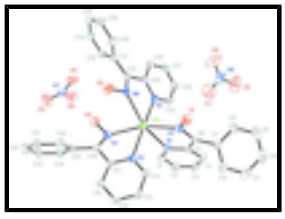


Fig. 1. The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

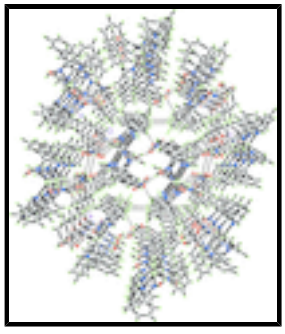


Fig. 2. A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

Tris(phenyl 2-pyridyl ketone oxime-k^2*N*,*N*')cadmium(II) dinitrate

Crystal data

$[Cd(C_{12}H_{10}N_2O)_3](NO_3)_2$	$Z = 2$
$M_r = 831.08$	$F_{000} = 844$
Triclinic, $P\overline{1}$	$D_x = 1.556$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 10.618$ (3) Å	Cell parameters from 3787 reflections
$b = 11.687$ (4) Å	$\theta = 2.4$–24.4°
$c = 15.279$ (5) Å	$\mu = 0.68$ mm^{-1}
$\alpha = 101.263$ (4)°	$T = 293$ K
$\beta = 100.166$ (4)°	Block, colourless
$\gamma = 101.807$ (4)°	0.24 × 0.22 × 0.18 mm
$V = 1773.3$ (10) Å^3	

Data collection

Bruker SMART Apex CCD area-detector diffractometer	6526 independent reflections
Radiation source: sealed tube	4387 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.041$
$T = 293$ K	$\theta_{max} = 25.5^\circ$
phi and ω scans	$\theta_{min} = 1.4^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -12 \rightarrow 12$
$T_{min} = 0.853$, $T_{max} = 0.887$	$k = -13 \rightarrow 14$
13329 measured reflections	$l = -18 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.077$	$w = 1/[\sigma^2(F_o^2) + (0.010P)^2 + 0.9209P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
6526 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
490 parameters	$\Delta\rho_{min} = -0.54$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.39932 (3)	0.31776 (3)	0.24172 (2)	0.04876 (12)
N1	0.6295 (3)	0.3685 (3)	0.2886 (2)	0.0444 (9)
N2	0.5000 (3)	0.2396 (3)	0.1219 (2)	0.0427 (8)
N3	0.4239 (3)	0.4973 (3)	0.1957 (2)	0.0421 (8)
N4	0.3093 (3)	0.4563 (3)	0.3321 (2)	0.0421 (8)
N5	0.3952 (3)	0.1499 (3)	0.3045 (2)	0.0426 (9)
N6	0.1810 (3)	0.1985 (3)	0.2194 (2)	0.0424 (8)
N7	0.1902 (3)	0.3451 (4)	0.0246 (3)	0.0670 (12)
N8	0.3849 (5)	0.2736 (4)	0.5251 (3)	0.0751 (13)
O1	0.4373 (3)	0.1901 (3)	0.02985 (19)	0.0568 (8)
H1	0.3608	0.1964	0.0215	0.085*
O2	0.2339 (3)	0.4255 (3)	0.39257 (19)	0.0524 (8)
H2	0.2688	0.3854	0.4232	0.079*
O3	0.0693 (3)	0.2320 (3)	0.1822 (2)	0.0615 (8)
H3	0.0886	0.2782	0.1498	0.092*
O4	0.1362 (3)	0.3998 (3)	0.0776 (2)	0.0938 (12)
O5	0.2140 (4)	0.3763 (4)	−0.0428 (3)	0.1087 (14)
O6	0.2210 (3)	0.2537 (4)	0.0439 (3)	0.0946 (12)
O7	0.4502 (5)	0.3435 (4)	0.4894 (3)	0.1285 (17)
O8	0.2671 (4)	0.2615 (4)	0.5008 (3)	0.1301 (18)
O9	0.4367 (5)	0.2216 (4)	0.5717 (3)	0.1331 (18)
C1	0.6938 (4)	0.4314 (4)	0.3723 (3)	0.0514 (11)
H1A	0.6469	0.4685	0.4103	0.062*
C2	0.8274 (4)	0.4444 (4)	0.4061 (3)	0.0586 (13)
H2A	0.8700	0.4908	0.4646	0.070*
C3	0.8948 (4)	0.3864 (4)	0.3503 (3)	0.0625 (14)

H3A	0.9836	0.3902	0.3715	0.075*
C4	0.8300 (4)	0.3226 (4)	0.2628 (3)	0.0484 (11)
H4	0.8751	0.2839	0.2242	0.058*
C5	0.6979 (4)	0.3163 (3)	0.2325 (3)	0.0376 (10)
C6	0.6255 (4)	0.2552 (3)	0.1382 (3)	0.0374 (10)
C7	0.7001 (4)	0.2251 (4)	0.0665 (3)	0.0426 (10)
C8	0.6898 (4)	0.1069 (4)	0.0231 (3)	0.0631 (13)
H8	0.6357	0.0441	0.0385	0.076*
C9	0.7599 (5)	0.0828 (5)	−0.0427 (4)	0.0842 (17)
H9	0.7527	0.0034	−0.0720	0.101*
C10	0.8401 (5)	0.1739 (6)	−0.0658 (4)	0.0833 (17)
H10	0.8877	0.1564	−0.1101	0.100*
C11	0.8501 (4)	0.2905 (5)	−0.0238 (3)	0.0689 (14)
H11	0.9036	0.3525	−0.0404	0.083*
C12	0.7816 (4)	0.3176 (4)	0.0431 (3)	0.0532 (12)
H12	0.7901	0.3974	0.0723	0.064*
C13	0.5020 (4)	0.5307 (4)	0.1411 (3)	0.0591 (13)
H13	0.5472	0.4764	0.1168	0.071*
C14	0.5201 (4)	0.6396 (4)	0.1186 (3)	0.0596 (13)
H14	0.5765	0.6591	0.0806	0.071*
C15	0.4529 (4)	0.7188 (4)	0.1534 (3)	0.0515 (12)
H15	0.4614	0.7931	0.1385	0.062*
C16	0.3725 (4)	0.6877 (3)	0.2106 (3)	0.0492 (11)
H16	0.3262	0.7408	0.2349	0.059*
C17	0.3608 (3)	0.5765 (3)	0.2320 (2)	0.0350 (9)
C18	0.2810 (3)	0.5415 (3)	0.2966 (2)	0.0352 (9)
C19	0.1797 (4)	0.6062 (3)	0.3191 (3)	0.0396 (10)
C20	0.0747 (4)	0.6039 (4)	0.2504 (3)	0.0551 (12)
H20	0.0691	0.5641	0.1903	0.066*
C21	−0.0220 (5)	0.6609 (5)	0.2712 (4)	0.0768 (16)
H21	−0.0921	0.6596	0.2246	0.092*
C22	−0.0163 (6)	0.7188 (5)	0.3584 (5)	0.086 (2)
H22	−0.0828	0.7553	0.3720	0.103*
C23	0.0890 (6)	0.7224 (4)	0.4261 (4)	0.0761 (16)
H23	0.0940	0.7627	0.4859	0.091*
C24	0.1879 (4)	0.6674 (3)	0.4070 (3)	0.0553 (12)
H24	0.2595	0.6719	0.4536	0.066*
C25	0.5031 (4)	0.1182 (4)	0.3414 (3)	0.0510 (12)
H25	0.5852	0.1662	0.3424	0.061*
C26	0.5001 (4)	0.0196 (4)	0.3777 (3)	0.0570 (12)
H26	0.5775	−0.0001	0.4014	0.068*
C27	0.3793 (4)	−0.0487 (4)	0.3776 (3)	0.0508 (11)
H27	0.3735	−0.1158	0.4024	0.061*
C28	0.2668 (4)	−0.0187 (3)	0.3412 (3)	0.0498 (11)
H28	0.1843	−0.0654	0.3405	0.060*
C29	0.2771 (4)	0.0812 (3)	0.3057 (2)	0.0342 (9)
C30	0.1588 (4)	0.1179 (3)	0.2634 (3)	0.0370 (9)
C31	0.0258 (4)	0.0574 (3)	0.2733 (3)	0.0404 (10)
C32	−0.0003 (4)	0.0635 (4)	0.3599 (3)	0.0518 (11)

H32	0.0635	0.1083	0.4118	0.062*
C33	−0.1227 (4)	0.0021 (4)	0.3680 (4)	0.0642 (14)
H33	−0.1416	0.0074	0.4256	0.077*
C34	−0.2156 (4)	−0.0661 (4)	0.2919 (4)	0.0690 (15)
H34	−0.2964	−0.1086	0.2982	0.083*
C35	−0.1901 (4)	−0.0721 (4)	0.2063 (4)	0.0726 (15)
H35	−0.2538	−0.1182	0.1547	0.087*
C36	−0.0694 (4)	−0.0095 (4)	0.1965 (3)	0.0597 (13)
H36	−0.0527	−0.0125	0.1385	0.072*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03717 (17)	0.04326 (19)	0.0802 (3)	0.01777 (14)	0.02862 (17)	0.02601 (17)
N1	0.041 (2)	0.036 (2)	0.057 (3)	0.0085 (16)	0.0198 (19)	0.0055 (19)
N2	0.040 (2)	0.043 (2)	0.041 (2)	0.0079 (17)	0.0013 (18)	0.0117 (18)
N3	0.0376 (19)	0.043 (2)	0.054 (2)	0.0149 (16)	0.0173 (17)	0.0192 (18)
N4	0.051 (2)	0.046 (2)	0.038 (2)	0.0164 (17)	0.0197 (17)	0.0167 (18)
N5	0.0320 (19)	0.045 (2)	0.059 (2)	0.0132 (16)	0.0172 (17)	0.0218 (18)
N6	0.0314 (18)	0.051 (2)	0.048 (2)	0.0167 (17)	0.0053 (17)	0.0173 (19)
N7	0.034 (2)	0.087 (4)	0.074 (3)	0.015 (2)	0.007 (2)	0.010 (3)
N8	0.086 (4)	0.054 (3)	0.077 (4)	0.034 (3)	−0.007 (3)	0.003 (3)
O1	0.0427 (18)	0.064 (2)	0.052 (2)	0.0047 (17)	−0.0019 (16)	0.0074 (17)
O2	0.070 (2)	0.060 (2)	0.0440 (19)	0.0276 (16)	0.0248 (17)	0.0282 (16)
O3	0.0425 (17)	0.078 (2)	0.080 (2)	0.0250 (16)	0.0141 (16)	0.0456 (19)
O4	0.062 (2)	0.109 (3)	0.093 (3)	0.022 (2)	0.018 (2)	−0.016 (2)
O5	0.132 (4)	0.123 (3)	0.101 (3)	0.045 (3)	0.053 (3)	0.058 (3)
O6	0.078 (3)	0.104 (3)	0.129 (4)	0.041 (2)	0.043 (2)	0.054 (3)
O7	0.152 (4)	0.094 (3)	0.141 (4)	0.023 (3)	0.040 (3)	0.032 (3)
O8	0.074 (3)	0.107 (3)	0.177 (5)	0.026 (3)	−0.015 (3)	−0.005 (3)
O9	0.183 (5)	0.126 (4)	0.120 (4)	0.095 (4)	0.011 (3)	0.059 (3)
C1	0.054 (3)	0.049 (3)	0.047 (3)	0.009 (2)	0.017 (2)	0.002 (2)
C2	0.052 (3)	0.070 (3)	0.040 (3)	−0.005 (3)	0.005 (2)	0.007 (3)
C3	0.031 (2)	0.100 (4)	0.055 (3)	0.008 (3)	0.007 (2)	0.026 (3)
C4	0.037 (2)	0.075 (3)	0.036 (3)	0.019 (2)	0.009 (2)	0.012 (2)
C5	0.034 (2)	0.036 (2)	0.044 (3)	0.0074 (19)	0.015 (2)	0.010 (2)
C6	0.031 (2)	0.032 (2)	0.048 (3)	0.0077 (18)	0.009 (2)	0.008 (2)
C7	0.037 (2)	0.050 (3)	0.042 (3)	0.015 (2)	0.009 (2)	0.010 (2)
C8	0.075 (3)	0.054 (3)	0.068 (3)	0.024 (3)	0.029 (3)	0.012 (3)
C9	0.100 (4)	0.075 (4)	0.079 (4)	0.033 (3)	0.038 (4)	−0.005 (3)
C10	0.076 (4)	0.115 (5)	0.071 (4)	0.041 (4)	0.040 (3)	0.014 (4)
C11	0.053 (3)	0.105 (4)	0.056 (3)	0.016 (3)	0.020 (3)	0.033 (3)
C12	0.048 (3)	0.065 (3)	0.044 (3)	0.014 (2)	0.008 (2)	0.010 (2)
C13	0.057 (3)	0.054 (3)	0.085 (4)	0.020 (2)	0.043 (3)	0.031 (3)
C14	0.055 (3)	0.061 (3)	0.076 (4)	0.012 (2)	0.034 (3)	0.034 (3)
C15	0.055 (3)	0.041 (3)	0.058 (3)	0.002 (2)	0.010 (2)	0.022 (2)
C16	0.059 (3)	0.035 (2)	0.056 (3)	0.011 (2)	0.018 (2)	0.014 (2)
C17	0.029 (2)	0.037 (2)	0.036 (2)	0.0046 (18)	0.0019 (19)	0.008 (2)

C18	0.037 (2)	0.036 (2)	0.030 (2)	0.0083 (19)	0.0039 (19)	0.007 (2)
C19	0.049 (3)	0.039 (2)	0.039 (3)	0.018 (2)	0.015 (2)	0.015 (2)
C20	0.061 (3)	0.071 (3)	0.045 (3)	0.031 (3)	0.014 (2)	0.024 (3)
C21	0.063 (3)	0.089 (4)	0.109 (5)	0.045 (3)	0.032 (3)	0.058 (4)
C22	0.104 (5)	0.071 (4)	0.134 (6)	0.056 (4)	0.082 (5)	0.056 (4)
C23	0.117 (5)	0.056 (3)	0.083 (4)	0.042 (3)	0.062 (4)	0.026 (3)
C24	0.074 (3)	0.042 (3)	0.060 (3)	0.018 (2)	0.032 (3)	0.017 (2)
C25	0.030 (2)	0.054 (3)	0.073 (3)	0.010 (2)	0.008 (2)	0.029 (3)
C26	0.051 (3)	0.055 (3)	0.073 (4)	0.020 (2)	0.018 (3)	0.024 (3)
C27	0.060 (3)	0.041 (3)	0.056 (3)	0.018 (2)	0.014 (3)	0.019 (2)
C28	0.049 (3)	0.039 (3)	0.068 (3)	0.011 (2)	0.022 (2)	0.019 (2)
C29	0.038 (2)	0.035 (2)	0.031 (2)	0.0114 (19)	0.0088 (19)	0.0081 (19)
C30	0.035 (2)	0.036 (2)	0.039 (3)	0.0088 (19)	0.010 (2)	0.005 (2)
C31	0.032 (2)	0.042 (3)	0.049 (3)	0.010 (2)	0.012 (2)	0.012 (2)
C32	0.046 (3)	0.051 (3)	0.055 (3)	0.005 (2)	0.016 (2)	0.009 (2)
C33	0.054 (3)	0.063 (3)	0.082 (4)	0.011 (3)	0.040 (3)	0.012 (3)
C34	0.040 (3)	0.061 (3)	0.100 (5)	0.002 (3)	0.023 (3)	0.009 (3)
C35	0.039 (3)	0.082 (4)	0.075 (4)	−0.008 (3)	0.003 (3)	−0.001 (3)
C36	0.043 (3)	0.066 (3)	0.064 (3)	0.005 (2)	0.016 (3)	0.007 (3)

Geometric parameters (Å, °)

Cd1—N3	2.320 (3)	C11—C12	1.380 (5)
Cd1—N1	2.337 (3)	C11—H11	0.9300
Cd1—N5	2.342 (3)	C12—H12	0.9300
Cd1—N6	2.376 (3)	C13—C14	1.368 (5)
Cd1—N4	2.380 (3)	C13—H13	0.9300
Cd1—N2	2.402 (3)	C14—C15	1.364 (5)
N1—C1	1.327 (5)	C14—H14	0.9300
N1—C5	1.353 (4)	C15—C16	1.374 (5)
N2—C6	1.279 (4)	C15—H15	0.9300
N2—O1	1.396 (4)	C16—C17	1.387 (5)
N3—C13	1.332 (4)	C16—H16	0.9300
N3—C17	1.341 (4)	C17—C18	1.474 (5)
N4—C18	1.285 (4)	C18—C19	1.486 (5)
N4—O2	1.378 (3)	C19—C24	1.372 (5)
N5—C25	1.340 (4)	C19—C20	1.382 (5)
N5—C29	1.349 (4)	C20—C21	1.382 (5)
N6—C30	1.269 (4)	C20—H20	0.9300
N6—O3	1.386 (3)	C21—C22	1.356 (7)
N7—O5	1.208 (5)	C21—H21	0.9300
N7—O4	1.227 (4)	C22—C23	1.370 (7)
N7—O6	1.252 (5)	C22—H22	0.9300
N8—O9	1.161 (5)	C23—C24	1.382 (6)
N8—O8	1.210 (5)	C23—H23	0.9300
N8—O7	1.234 (5)	C24—H24	0.9300
O1—H1	0.8200	C25—C26	1.371 (5)
O2—H2	0.8200	C25—H25	0.9300
O3—H3	0.8200	C26—C27	1.365 (5)

C1—C2	1.388 (5)	C26—H26	0.9300
C1—H1A	0.9300	C27—C28	1.369 (5)
C2—C3	1.373 (5)	C27—H27	0.9300
C2—H2A	0.9300	C28—C29	1.373 (5)
C3—C4	1.375 (5)	C28—H28	0.9300
C3—H3A	0.9300	C29—C30	1.490 (5)
C4—C5	1.380 (5)	C30—C31	1.491 (5)
C4—H4	0.9300	C31—C36	1.382 (5)
C5—C6	1.470 (5)	C31—C32	1.391 (5)
C6—C7	1.490 (5)	C32—C33	1.389 (5)
C7—C8	1.384 (5)	C32—H32	0.9300
C7—C12	1.387 (5)	C33—C34	1.368 (6)
C8—C9	1.373 (6)	C33—H33	0.9300
C8—H8	0.9300	C34—C35	1.374 (6)
C9—C10	1.366 (6)	C34—H34	0.9300
C9—H9	0.9300	C35—C36	1.387 (5)
C10—C11	1.362 (6)	C35—H35	0.9300
C10—H10	0.9300	C36—H36	0.9300
N3—Cd1—N1	86.23 (10)	C11—C12—C7	119.5 (4)
N3—Cd1—N5	172.80 (12)	C11—C12—H12	120.2
N1—Cd1—N5	88.33 (10)	C7—C12—H12	120.2
N3—Cd1—N6	117.48 (10)	N3—C13—C14	124.2 (4)
N1—Cd1—N6	156.28 (10)	N3—C13—H13	117.9
N5—Cd1—N6	68.00 (11)	C14—C13—H13	117.9
N3—Cd1—N4	69.06 (11)	C15—C14—C13	118.0 (4)
N1—Cd1—N4	110.42 (11)	C15—C14—H14	121.0
N5—Cd1—N4	108.62 (11)	C13—C14—H14	121.0
N6—Cd1—N4	80.07 (11)	C14—C15—C16	119.2 (4)
N3—Cd1—N2	89.14 (10)	C14—C15—H15	120.4
N1—Cd1—N2	68.22 (12)	C16—C15—H15	120.4
N5—Cd1—N2	93.23 (10)	C15—C16—C17	119.7 (4)
N6—Cd1—N2	110.04 (11)	C15—C16—H16	120.2
N4—Cd1—N2	158.13 (10)	C17—C16—H16	120.2
C1—N1—C5	118.6 (3)	N3—C17—C16	121.0 (3)
C1—N1—Cd1	122.8 (3)	N3—C17—C18	117.3 (3)
C5—N1—Cd1	117.9 (3)	C16—C17—C18	121.6 (3)
C6—N2—O1	113.9 (3)	N4—C18—C17	115.1 (3)
C6—N2—Cd1	119.3 (3)	N4—C18—C19	124.6 (3)
O1—N2—Cd1	126.3 (2)	C17—C18—C19	120.2 (3)
C13—N3—C17	117.8 (3)	C24—C19—C20	119.3 (4)
C13—N3—Cd1	125.2 (3)	C24—C19—C18	121.3 (4)
C17—N3—Cd1	116.9 (2)	C20—C19—C18	119.4 (4)
C18—N4—O2	114.0 (3)	C21—C20—C19	119.8 (4)
C18—N4—Cd1	115.8 (2)	C21—C20—H20	120.1
O2—N4—Cd1	123.5 (2)	C19—C20—H20	120.1
C25—N5—C29	117.2 (3)	C22—C21—C20	121.1 (5)
C25—N5—Cd1	124.3 (3)	C22—C21—H21	119.5
C29—N5—Cd1	118.5 (2)	C20—C21—H21	119.5
C30—N6—O3	114.2 (3)	C21—C22—C23	118.9 (5)

C30—N6—Cd1	119.8 (3)	C21—C22—H22	120.6
O3—N6—Cd1	123.4 (2)	C23—C22—H22	120.6
O5—N7—O4	122.9 (5)	C22—C23—C24	121.2 (5)
O5—N7—O6	120.6 (5)	C22—C23—H23	119.4
O4—N7—O6	116.5 (5)	C24—C23—H23	119.4
O9—N8—O8	126.6 (6)	C19—C24—C23	119.6 (5)
O9—N8—O7	120.3 (6)	C19—C24—H24	120.2
O8—N8—O7	112.9 (5)	C23—C24—H24	120.2
N2—O1—H1	109.5	N5—C25—C26	124.1 (4)
N4—O2—H2	109.5	N5—C25—H25	118.0
N6—O3—H3	109.5	C26—C25—H25	118.0
N1—C1—C2	123.3 (4)	C27—C26—C25	117.6 (4)
N1—C1—H1A	118.4	C27—C26—H26	121.2
C2—C1—H1A	118.4	C25—C26—H26	121.2
C3—C2—C1	117.8 (4)	C26—C27—C28	120.1 (4)
C3—C2—H2A	121.1	C26—C27—H27	120.0
C1—C2—H2A	121.1	C28—C27—H27	120.0
C2—C3—C4	119.5 (4)	C27—C28—C29	119.3 (4)
C2—C3—H3A	120.2	C27—C28—H28	120.4
C4—C3—H3A	120.2	C29—C28—H28	120.4
C3—C4—C5	119.7 (4)	N5—C29—C28	121.8 (3)
C3—C4—H4	120.1	N5—C29—C30	116.0 (3)
C5—C4—H4	120.1	C28—C29—C30	122.2 (3)
N1—C5—C4	121.0 (4)	N6—C30—C29	115.6 (3)
N1—C5—C6	116.9 (3)	N6—C30—C31	125.1 (3)
C4—C5—C6	122.0 (3)	C29—C30—C31	119.2 (3)
N2—C6—C5	116.2 (3)	C36—C31—C32	120.0 (4)
N2—C6—C7	123.9 (4)	C36—C31—C30	119.9 (4)
C5—C6—C7	119.6 (3)	C32—C31—C30	120.0 (4)
C8—C7—C12	119.5 (4)	C33—C32—C31	119.3 (4)
C8—C7—C6	121.3 (4)	C33—C32—H32	120.4
C12—C7—C6	119.2 (4)	C31—C32—H32	120.4
C9—C8—C7	119.6 (4)	C34—C33—C32	120.5 (4)
C9—C8—H8	120.2	C34—C33—H33	119.8
C7—C8—H8	120.2	C32—C33—H33	119.8
C10—C9—C8	120.9 (5)	C33—C34—C35	120.3 (4)
C10—C9—H9	119.5	C33—C34—H34	119.8
C8—C9—H9	119.5	C35—C34—H34	119.8
C11—C10—C9	119.8 (5)	C34—C35—C36	120.1 (5)
C11—C10—H10	120.1	C34—C35—H35	119.9
C9—C10—H10	120.1	C36—C35—H35	119.9
C10—C11—C12	120.6 (5)	C31—C36—C35	119.8 (4)
C10—C11—H11	119.7	C31—C36—H36	120.1
C12—C11—H11	119.7	C35—C36—H36	120.1
N3—Cd1—N1—C1	90.4 (3)	N2—C6—C7—C8	−69.3 (5)
N5—Cd1—N1—C1	−84.8 (3)	C5—C6—C7—C8	116.4 (4)
N6—Cd1—N1—C1	−88.5 (4)	N2—C6—C7—C12	110.8 (5)
N4—Cd1—N1—C1	24.4 (3)	C5—C6—C7—C12	−63.5 (5)
N2—Cd1—N1—C1	−179.0 (3)	C12—C7—C8—C9	−0.3 (7)

N3—Cd1—N1—C5	−99.7 (3)	C6—C7—C8—C9	179.8 (4)
N5—Cd1—N1—C5	85.0 (3)	C7—C8—C9—C10	0.2 (8)
N6—Cd1—N1—C5	81.4 (4)	C8—C9—C10—C11	−0.6 (9)
N4—Cd1—N1—C5	−165.7 (2)	C9—C10—C11—C12	1.1 (8)
N2—Cd1—N1—C5	−9.1 (2)	C10—C11—C12—C7	−1.1 (7)
N3—Cd1—N2—C6	89.4 (3)	C8—C7—C12—C11	0.7 (6)
N1—Cd1—N2—C6	3.1 (3)	C6—C7—C12—C11	−179.4 (4)
N5—Cd1—N2—C6	−83.8 (3)	C17—N3—C13—C14	−1.2 (7)
N6—Cd1—N2—C6	−151.5 (3)	Cd1—N3—C13—C14	−176.6 (3)
N4—Cd1—N2—C6	93.9 (4)	N3—C13—C14—C15	−0.7 (7)
N3—Cd1—N2—O1	−81.9 (3)	C13—C14—C15—C16	1.3 (7)
N1—Cd1—N2—O1	−168.2 (3)	C14—C15—C16—C17	−0.1 (6)
N5—Cd1—N2—O1	104.9 (3)	C13—N3—C17—C16	2.4 (6)
N6—Cd1—N2—O1	37.2 (3)	Cd1—N3—C17—C16	178.2 (3)
N4—Cd1—N2—O1	−77.4 (4)	C13—N3—C17—C18	−176.4 (4)
N1—Cd1—N3—C13	52.5 (3)	Cd1—N3—C17—C18	−0.6 (4)
N6—Cd1—N3—C13	−128.0 (3)	C15—C16—C17—N3	−1.8 (6)
N4—Cd1—N3—C13	166.1 (4)	C15—C16—C17—C18	177.0 (4)
N2—Cd1—N3—C13	−15.7 (3)	O2—N4—C18—C17	179.7 (3)
N1—Cd1—N3—C17	−122.9 (3)	Cd1—N4—C18—C17	−27.8 (4)
N6—Cd1—N3—C17	56.6 (3)	O2—N4—C18—C19	1.9 (5)
N4—Cd1—N3—C17	−9.3 (3)	Cd1—N4—C18—C19	154.4 (3)
N2—Cd1—N3—C17	168.9 (3)	N3—C17—C18—N4	19.4 (5)
N3—Cd1—N4—C18	20.4 (3)	C16—C17—C18—N4	−159.4 (4)
N1—Cd1—N4—C18	97.8 (3)	N3—C17—C18—C19	−162.7 (3)
N5—Cd1—N4—C18	−166.9 (3)	C16—C17—C18—C19	18.5 (6)
N6—Cd1—N4—C18	−104.3 (3)	N4—C18—C19—C24	58.9 (6)
N2—Cd1—N4—C18	15.6 (5)	C17—C18—C19—C24	−118.8 (4)
N3—Cd1—N4—O2	170.0 (3)	N4—C18—C19—C20	−120.5 (4)
N1—Cd1—N4—O2	−112.6 (3)	C17—C18—C19—C20	61.8 (5)
N5—Cd1—N4—O2	−17.3 (3)	C24—C19—C20—C21	−1.3 (6)
N6—Cd1—N4—O2	45.3 (3)	C18—C19—C20—C21	178.1 (4)
N2—Cd1—N4—O2	165.2 (3)	C19—C20—C21—C22	−0.5 (7)
N1—Cd1—N5—C25	−4.0 (3)	C20—C21—C22—C23	1.5 (8)
N6—Cd1—N5—C25	174.4 (3)	C21—C22—C23—C24	−0.7 (8)
N4—Cd1—N5—C25	−115.1 (3)	C20—C19—C24—C23	2.1 (6)
N2—Cd1—N5—C25	64.0 (3)	C18—C19—C24—C23	−177.3 (4)
N1—Cd1—N5—C29	174.6 (3)	C22—C23—C24—C19	−1.1 (7)
N6—Cd1—N5—C29	−7.0 (3)	C29—N5—C25—C26	1.7 (6)
N4—Cd1—N5—C29	63.5 (3)	Cd1—N5—C25—C26	−179.7 (3)
N2—Cd1—N5—C29	−117.4 (3)	N5—C25—C26—C27	−1.4 (7)
N3—Cd1—N6—C30	−161.7 (3)	C25—C26—C27—C28	0.8 (6)
N1—Cd1—N6—C30	17.1 (5)	C26—C27—C28—C29	−0.6 (6)
N5—Cd1—N6—C30	13.1 (3)	C25—N5—C29—C28	−1.4 (5)
N4—Cd1—N6—C30	−101.7 (3)	Cd1—N5—C29—C28	179.9 (3)
N2—Cd1—N6—C30	98.4 (3)	C25—N5—C29—C30	−179.4 (3)
N3—Cd1—N6—O3	−1.1 (3)	Cd1—N5—C29—C30	1.9 (4)
N1—Cd1—N6—O3	177.7 (3)	C27—C28—C29—N5	1.0 (6)
N5—Cd1—N6—O3	173.7 (3)	C27—C28—C29—C30	178.8 (4)

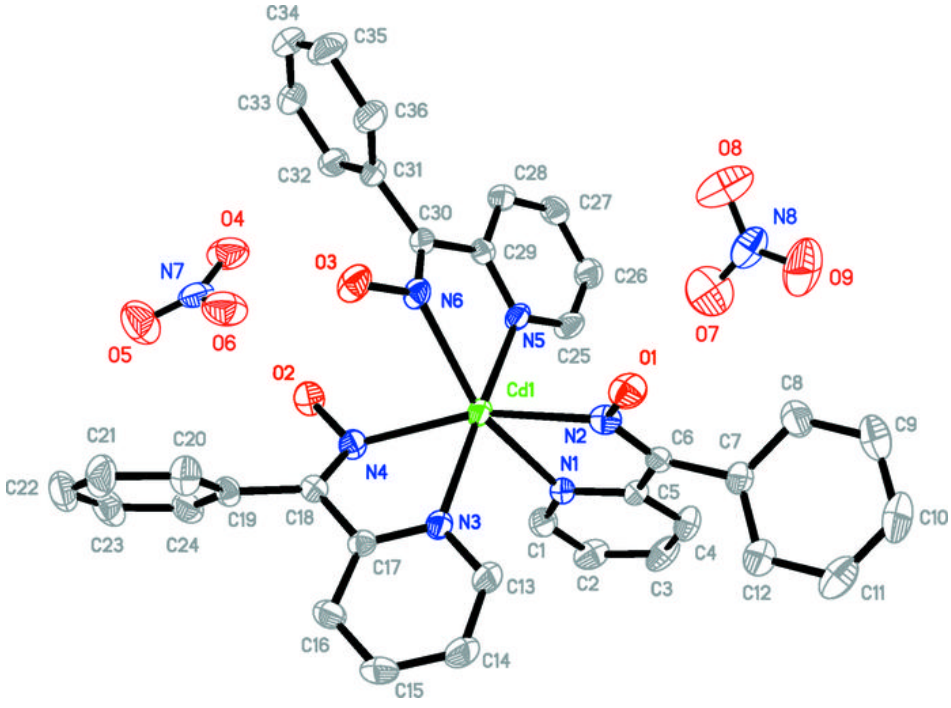
N4—Cd1—N6—O3	58.9 (3)	O3—N6—C30—C29	−179.0 (3)
N2—Cd1—N6—O3	−101.0 (3)	Cd1—N6—C30—C29	−16.7 (4)
C5—N1—C1—C2	−1.3 (6)	O3—N6—C30—C31	2.5 (5)
Cd1—N1—C1—C2	168.5 (3)	Cd1—N6—C30—C31	164.8 (3)
N1—C1—C2—C3	−1.7 (6)	N5—C29—C30—N6	9.7 (5)
C1—C2—C3—C4	2.7 (6)	C28—C29—C30—N6	−168.2 (4)
C2—C3—C4—C5	−0.8 (6)	N5—C29—C30—C31	−171.7 (3)
C1—N1—C5—C4	3.4 (5)	C28—C29—C30—C31	10.4 (5)
Cd1—N1—C5—C4	−167.0 (3)	N6—C30—C31—C36	61.6 (5)
C1—N1—C5—C6	−175.6 (3)	C29—C30—C31—C36	−116.9 (4)
Cd1—N1—C5—C6	14.1 (4)	N6—C30—C31—C32	−121.4 (4)
C3—C4—C5—N1	−2.3 (6)	C29—C30—C31—C32	60.1 (5)
C3—C4—C5—C6	176.5 (4)	C36—C31—C32—C33	−0.1 (6)
O1—N2—C6—C5	175.1 (3)	C30—C31—C32—C33	−177.1 (4)
Cd1—N2—C6—C5	2.7 (4)	C31—C32—C33—C34	1.6 (7)
O1—N2—C6—C7	0.6 (5)	C32—C33—C34—C35	−1.7 (7)
Cd1—N2—C6—C7	−171.7 (3)	C33—C34—C35—C36	0.4 (8)
N1—C5—C6—N2	−11.1 (5)	C32—C31—C36—C35	−1.2 (6)
C4—C5—C6—N2	170.0 (4)	C30—C31—C36—C35	175.8 (4)
N1—C5—C6—C7	163.6 (3)	C34—C35—C36—C31	1.0 (7)
C4—C5—C6—C7	−15.3 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C32—H32···O8	0.93	2.48	3.355 (6)	157
C27—H27···O9^{i}	0.93	2.58	3.191 (6)	123
C14—H14···O5^{ii}	0.93	2.49	3.261 (6)	141
C4—H4···O3^{iii}	0.93	2.42	3.285 (5)	155
C3—H3A···O2^{iii}	0.93	2.56	3.461 (5)	164
O3—H3···O6	0.82	2.34	2.892 (4)	126
O3—H3···O4	0.82	2.00	2.820 (5)	176
O2—H2···O8	0.82	2.04	2.800 (5)	154
O2—H2···O7	0.82	2.21	2.939 (6)	149
O1—H1···O6	0.82	1.81	2.585 (4)	158

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

Fig. 1


C34
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C20
N2
C6
C7
C22
N4
N1
C5
C10
C19
C18
N3
C1
C4
C23
C24
C17
C13
C2
C3
C12
C11
C16
C14
C15

Fig. 2