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Dichlorido{2,6-bis[1-(2,4,6-trimethylphenylimino)ethyl]pyridine-κ^3N,N',N''}cadmium(II) acetonitrile solvate

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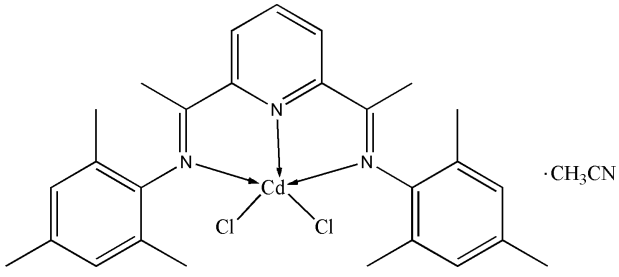
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.042; wR factor = 0.091; data-to-parameter ratio = 17.8.

In the title compound, $[Cd(C_{27}H_{31}N_3)Cl_2]\cdot CH_3CN$, the coordination geometry around the five-coordinated Cd^{II} atom can be described as distorted trigonal–bipyramidal, formed by two Cl atoms, one pyridine N and two imine N atoms from the bis(iminoalkyl)pyridine ligand. The dihedral angles between the substituted phenyl rings and the plane formed by the three coordinated N atoms are 90.6 (1) and 86.0 (1)°. C—H···Cl hydrogen bonds link the molecules into a three-dimensional supramolecular network.

Related literature

For related literature, see: Fan *et al.* (2004); Tang & Vanslyke (1987); Wang (2001).



Experimental

Crystal data

$[Cd(C_{27}H_{31}N_3)Cl_2]\cdot C_2H_3N$
M_r = 621.90
Monoclinic, $P2_1/n$
a = 14.545 (3) Å
b = 15.074 (3) Å
c = 14.758 (3) Å
β = 111.516 (2)°
V = 3010.3 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.93 mm^{-1}
T = 295 (2) K
0.42 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.697, T_{max} = 0.851
16698 measured reflections
5948 independent reflections
4046 reflections with $I > 2\sigma(I)$
R_{int} = 0.086

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.091
S = 0.88
5948 reflections
334 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N2	2.306 (3)	Cd1—N3	2.416 (3)
Cd1—N1	2.410 (3)	Cd1—Cl1	2.4369 (11)
Cd1—Cl2	2.4097 (10)		
N2—Cd1—N1	69.50 (10)	Cl2—Cd1—N3	99.21 (7)
N2—Cd1—Cl2	126.50 (7)	N2—Cd1—Cl1	118.86 (7)
N1—Cd1—Cl2	102.89 (7)	N1—Cd1—Cl1	97.85 (7)
N2—Cd1—N3	68.88 (10)	Cl2—Cd1—Cl1	114.64 (4)
N1—Cd1—N3	138.28 (10)	N3—Cd1—Cl1	104.43 (7)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8C···Cl1^{i}	0.96	2.66	3.614 (4)	172
C16—H16A···Cl2^{ii}	0.96	2.84	3.681 (4)	146
C16—H16C···Cl2	0.96	2.80	3.680 (4)	153
C29—H29B···Cl2^{iii}	0.96	2.81	3.721 (6)	159
C5—H5···Cl1^{iii}	0.93	2.74	3.622 (4)	158

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+2, -y, -z+1$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); 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: HY2081).

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supplementary materials

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Dichlorido{2,6-bis[1-(2,4,6-trimethylphenylimino)ethyl]pyridine-κ^3N,N',N''}cadmium(II) acetonitrile solvate

R.-Q. Fan, P. Wang, Y.-L. Yang and Z.-W. Lv

Comment

Luminescent coordination compounds based on pyridine-type ligands have attracted intensive attention due to their potential applications in the areas of sensor technologies and electro-luminescent devices (Tang & Vanslyke, 1987; Wang, 2001). In order to explore potential luminescent complexes of this type, we have reported a series of cadmium complexes derived from bis(iminoalkyl)pyridine ligands (Fan *et al.*, 2004). We report here the crystal structure of the title compound, a new cadmium complex with 2,6-bis[1-(2,4,6-trimethylphenylimino)ethyl]pyridine ligand.

As shown in Fig. 1, the asymmetric unit of the title compound contains one independent complex molecule and a solvated acetonitrile molecule. The central Cd^{II} atom is five-coordinated in a distorted trigonal-bipyramidal geometry, defined by two Cl atoms, one pyridine N and two imine N atoms from the bis(iminoalkyl)pyridine ligand. The Cd—N bond lengths [2.306 (3)–2.416 (3) Å] (Table 1) fall into the range of observed values in the similar cadmium complexes (Fan *et al.*, 2004). The dihedral angles between the substituted phenyl rings and the plane formed by three coordinated N atoms are 90.6 (1)° and 86.0 (1)°, respectively.

In the crystal structure, weak intermolecular C—H···Cl hydrogen bonds (Table 2) play an important role to link the molecules into a three-dimensional supramolecular network (Fig.2).

Experimental

The title complex was synthesized according to the literature procedure (Fan *et al.*, 2004). To a solution of 2,6-diacetylpyridine (2.4 g, 14.7 mmol) in absolute methanol (50 ml) was added 2,4,6-trimethylaniline (6.2 ml, 44.1 mmol). After the addition of several drops of formic acid, the reaction mixture was refluxed for 24 h and then allowed to cool down to room temperature. The crude product precipitated as yellow powder. Pure 2,6-bis[1-(2,4,6-trimethylphenylimino)ethyl]pyridine was obtained in 83% yield (4.8 g). A mixture of this ligand (0.30 g, 0.75 mmol) and $CdCl_2{\cdot}2.5H_2O$ (0.17 g, 0.75 mmol) in acetonitrile was stirred at room temperature for 12 h. Evaporation of the solvent gave the crude product as a yellowish powder. Yellowish needle crystals suitable for X-ray diffraction were obtained upon recrystallization from acetonitrile/dichloromethane (2:1 *v*/*v*) (yield 84%, 0.39 g).

Refinement

H atoms were positioned geometrically and refined as riding, with C—H = 0.93Å (CH) and U_{iso}(H) = 1.2U_{eq}(C), and with C—H = 0.96Å (CH_3) and U_{iso}(H) = 1.5U_{eq}(C).

Figures

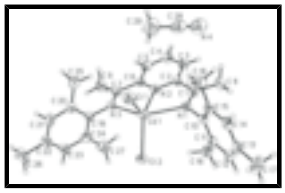


Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

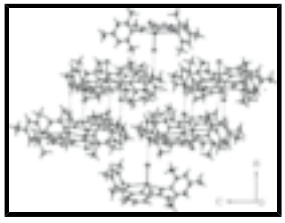


Fig. 2. Packing diagram of the title compound along the *b* axis. Hydrogen bonds are indicated by dashed lines.

Dichlorido{2,6-bis[1-(2,4,6-trimethylphenylimino)ethyl] pyridine-κ3 *N*,*N*',*N*''}cadmium(II) acetonitrile solvate

Crystal data

$[Cd(C_{27}H_{31}N_3)Cl_2]\cdot C_2H_3N$	F_{000} = 1272
M_r = 621.90	D_x = 1.372 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 6108 reflections
a = 14.545 (3) Å	θ = 1.7–26.1º
b = 15.074 (3) Å	μ = 0.93 mm^{-1}
c = 14.758 (3) Å	T = 295 (2) K
β = 111.516 (2)º	Needle, yellow
V = 3010.3 (11) Å^3	0.42 × 0.20 × 0.18 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	5948 independent reflections
Radiation source: fine-focus sealed tube	4046 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.086
T = 295(2) K	θ_{max} = 26.1º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −17→17
T_{min} = 0.697, T_{max} = 0.851	k = −16→18
16698 measured reflections	l = −18→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.091$

$S = 0.88$

5948 reflections

334 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.009$

$\Delta\rho_{max} = 0.69$ e Å^{-3}

$\Delta\rho_{min} = -0.39$ e Å^{-3}

Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.749428 (18)	0.180077 (17)	0.306446 (18)	0.04833 (11)
Cl1	0.57035 (7)	0.16398 (7)	0.23566 (9)	0.0755 (3)
Cl2	0.84039 (7)	0.04834 (7)	0.29937 (8)	0.0713 (3)
N1	0.76671 (19)	0.18576 (18)	0.4751 (2)	0.0456 (7)
N2	0.81540 (19)	0.31434 (18)	0.3745 (2)	0.0466 (7)
N3	0.7892 (2)	0.2711 (2)	0.1911 (2)	0.0529 (7)
N4	0.6107 (4)	0.4175 (3)	0.5283 (5)	0.1161 (18)
C1	0.7983 (2)	0.2586 (2)	0.5210 (2)	0.0468 (9)
C2	0.8220 (2)	0.3328 (2)	0.4650 (3)	0.0475 (9)
C3	0.8523 (3)	0.4155 (3)	0.5056 (3)	0.0644 (11)
H3	0.8580	0.4278	0.5692	0.077*
C4	0.8738 (3)	0.4796 (3)	0.4492 (3)	0.0695 (12)
H4	0.8911	0.5366	0.4736	0.083*
C5	0.8697 (3)	0.4589 (2)	0.3582 (3)	0.0645 (11)
H5	0.8878	0.5006	0.3214	0.077*
C6	0.8381 (2)	0.3750 (2)	0.3204 (3)	0.0508 (9)
C7	0.8266 (3)	0.3479 (3)	0.2199 (3)	0.0547 (10)
C8	0.8127 (3)	0.2753 (3)	0.6248 (3)	0.0652 (11)
H8A	0.7982	0.2221	0.6529	0.098*
H8B	0.7692	0.3219	0.6284	0.098*
H8C	0.8800	0.2924	0.6601	0.098*
C9	0.8587 (3)	0.4115 (3)	0.1586 (3)	0.0799 (13)
H9A	0.8544	0.3829	0.0991	0.120*
H9B	0.9258	0.4294	0.1937	0.120*
H9C	0.8166	0.4627	0.1440	0.120*
C10	0.7476 (2)	0.1111 (2)	0.5263 (2)	0.0453 (8)
C11	0.8242 (3)	0.0495 (3)	0.5670 (3)	0.0547 (10)
C12	0.8031 (3)	−0.0242 (3)	0.6125 (3)	0.0657 (11)
H12	0.8530	−0.0655	0.6407	0.079*
C13	0.7121 (3)	−0.0390 (3)	0.6178 (3)	0.0653 (11)
C14	0.6400 (3)	0.0233 (3)	0.5782 (3)	0.0611 (10)
H14	0.5783	0.0146	0.5824	0.073*
C15	0.6555 (3)	0.0993 (2)	0.5317 (3)	0.0525 (9)
C16	0.9252 (3)	0.0656 (3)	0.5663 (3)	0.0762 (13)

H16A	0.9659	0.0146	0.5920	0.114*
H16B	0.9537	0.1165	0.6057	0.114*
H16C	0.9208	0.0761	0.5007	0.114*
C17	0.6943 (4)	−0.1210 (3)	0.6687 (4)	0.1025 (17)
H17A	0.6443	−0.1087	0.6949	0.154*
H17B	0.7545	−0.1374	0.7206	0.154*
H17C	0.6730	−0.1689	0.6228	0.154*
C18	0.5753 (3)	0.1681 (3)	0.4925 (3)	0.0726 (12)
H18A	0.5961	0.2225	0.5278	0.109*
H18B	0.5160	0.1474	0.4998	0.109*
H18C	0.5628	0.1781	0.4247	0.109*
C19	0.7759 (3)	0.2367 (2)	0.0965 (3)	0.0545 (9)
C20	0.6847 (3)	0.2440 (3)	0.0224 (3)	0.0680 (11)
C21	0.6716 (4)	0.2024 (3)	−0.0655 (3)	0.0825 (14)
H21	0.6104	0.2065	−0.1160	0.099*
C22	0.7456 (5)	0.1553 (3)	−0.0807 (4)	0.0856 (15)
C23	0.8366 (4)	0.1519 (3)	−0.0054 (4)	0.0835 (14)
H23	0.8880	0.1216	−0.0150	0.100*
C24	0.8540 (3)	0.1918 (3)	0.0835 (3)	0.0681 (11)
C25	0.6026 (3)	0.2975 (3)	0.0350 (3)	0.0898 (15)
H25A	0.5823	0.2700	0.0833	0.135*
H25B	0.5475	0.3000	−0.0258	0.135*
H25C	0.6256	0.3565	0.0555	0.135*
C26	0.7284 (5)	0.1099 (4)	−0.1777 (4)	0.132 (2)
H26A	0.6675	0.0772	−0.1976	0.198*
H26B	0.7820	0.0701	−0.1707	0.198*
H26C	0.7247	0.1539	−0.2260	0.198*
C27	0.9545 (3)	0.1863 (3)	0.1635 (4)	0.0876 (15)
H27A	0.9981	0.1525	0.1412	0.131*
H27B	0.9488	0.1578	0.2194	0.131*
H27C	0.9807	0.2449	0.1808	0.131*
C28	0.5801 (5)	0.4177 (4)	0.4466 (6)	0.098 (2)
C29	0.5408 (5)	0.4164 (5)	0.3409 (5)	0.156 (3)
H29A	0.5294	0.3561	0.3185	0.234*
H29B	0.5874	0.4434	0.3172	0.234*
H29C	0.4797	0.4487	0.3171	0.234*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.05459 (18)	0.04431 (16)	0.04645 (17)	0.00312 (13)	0.01896 (13)	−0.00318 (12)
Cl1	0.0547 (6)	0.0804 (8)	0.0827 (8)	0.0069 (5)	0.0148 (5)	−0.0143 (6)
Cl2	0.0732 (7)	0.0640 (7)	0.0751 (8)	0.0229 (5)	0.0252 (6)	−0.0017 (5)
N1	0.0445 (16)	0.0469 (17)	0.0471 (18)	0.0001 (14)	0.0189 (14)	−0.0005 (14)
N2	0.0485 (17)	0.0431 (16)	0.0477 (19)	−0.0003 (14)	0.0169 (14)	−0.0012 (14)
N3	0.0654 (19)	0.053 (2)	0.0445 (19)	0.0105 (16)	0.0254 (15)	0.0009 (14)
N4	0.109 (4)	0.097 (4)	0.147 (5)	−0.001 (3)	0.052 (4)	0.015 (4)
C1	0.043 (2)	0.059 (2)	0.038 (2)	0.0008 (17)	0.0146 (16)	−0.0017 (17)

C2	0.046 (2)	0.050 (2)	0.044 (2)	−0.0054 (16)	0.0139 (17)	−0.0056 (17)
C3	0.078 (3)	0.061 (3)	0.054 (3)	−0.013 (2)	0.025 (2)	−0.014 (2)
C4	0.087 (3)	0.050 (2)	0.067 (3)	−0.016 (2)	0.023 (2)	−0.011 (2)
C5	0.079 (3)	0.046 (2)	0.070 (3)	−0.007 (2)	0.028 (2)	0.006 (2)
C6	0.055 (2)	0.048 (2)	0.052 (2)	0.0065 (18)	0.0226 (19)	0.0077 (18)
C7	0.059 (2)	0.052 (2)	0.057 (3)	0.0104 (19)	0.026 (2)	0.0110 (18)
C8	0.071 (3)	0.078 (3)	0.048 (2)	−0.013 (2)	0.023 (2)	−0.008 (2)
C9	0.120 (4)	0.062 (3)	0.073 (3)	−0.008 (3)	0.053 (3)	0.010 (2)
C10	0.050 (2)	0.049 (2)	0.038 (2)	−0.0051 (17)	0.0179 (17)	−0.0026 (15)
C11	0.061 (2)	0.063 (3)	0.041 (2)	0.005 (2)	0.0196 (19)	0.0036 (18)
C12	0.085 (3)	0.062 (3)	0.046 (3)	0.014 (2)	0.019 (2)	0.0099 (19)
C13	0.086 (3)	0.065 (3)	0.048 (3)	−0.011 (2)	0.028 (2)	0.002 (2)
C14	0.072 (3)	0.067 (3)	0.054 (3)	−0.017 (2)	0.034 (2)	−0.008 (2)
C15	0.056 (2)	0.052 (2)	0.054 (2)	−0.0070 (19)	0.0249 (19)	−0.0075 (18)
C16	0.063 (3)	0.098 (4)	0.067 (3)	0.018 (2)	0.024 (2)	0.019 (2)
C17	0.134 (4)	0.084 (4)	0.095 (4)	−0.012 (3)	0.049 (3)	0.033 (3)
C18	0.060 (3)	0.073 (3)	0.094 (4)	0.001 (2)	0.040 (2)	−0.003 (2)
C19	0.072 (3)	0.056 (2)	0.043 (2)	0.011 (2)	0.031 (2)	0.0057 (18)
C20	0.087 (3)	0.064 (3)	0.054 (3)	0.013 (2)	0.027 (2)	0.006 (2)
C21	0.109 (4)	0.082 (3)	0.046 (3)	0.004 (3)	0.016 (3)	0.008 (2)
C22	0.139 (5)	0.069 (3)	0.061 (3)	0.011 (3)	0.051 (3)	−0.003 (2)
C23	0.123 (4)	0.072 (3)	0.079 (4)	0.026 (3)	0.065 (3)	0.008 (3)
C24	0.094 (3)	0.061 (3)	0.062 (3)	0.016 (2)	0.044 (3)	0.011 (2)
C25	0.094 (3)	0.106 (4)	0.065 (3)	0.036 (3)	0.024 (3)	0.011 (3)
C26	0.222 (7)	0.123 (5)	0.065 (4)	0.012 (4)	0.069 (4)	−0.024 (3)
C27	0.077 (3)	0.102 (4)	0.096 (4)	0.025 (3)	0.047 (3)	0.019 (3)
C28	0.093 (4)	0.072 (3)	0.144 (6)	0.005 (3)	0.060 (5)	0.023 (4)
C29	0.188 (7)	0.158 (7)	0.131 (7)	−0.002 (5)	0.069 (5)	0.037 (5)

Geometric parameters (Å, °)

Cd1—N2	2.306 (3)	C14—C15	1.396 (5)
Cd1—N1	2.410 (3)	C14—H14	0.9300
Cd1—Cl2	2.4097 (10)	C15—C18	1.507 (5)
Cd1—N3	2.416 (3)	C16—H16A	0.9600
Cd1—Cl1	2.4369 (11)	C16—H16B	0.9600
N1—C1	1.284 (4)	C16—H16C	0.9600
N1—C10	1.438 (4)	C17—H17A	0.9600
N2—C6	1.332 (4)	C17—H17B	0.9600
N2—C2	1.332 (4)	C17—H17C	0.9600
N3—C7	1.284 (4)	C18—H18A	0.9600
N3—C19	1.434 (4)	C18—H18B	0.9600
N4—C28	1.123 (7)	C18—H18C	0.9600
C1—C8	1.490 (5)	C19—C20	1.380 (5)
C1—C2	1.504 (5)	C19—C24	1.395 (5)
C2—C3	1.385 (5)	C20—C21	1.390 (6)
C3—C4	1.383 (5)	C20—C25	1.507 (5)
C3—H3	0.9300	C21—C22	1.374 (6)
C4—C5	1.358 (5)	C21—H21	0.9300

C4—H4	0.9300	C22—C23	1.383 (6)
C5—C6	1.391 (5)	C22—C26	1.523 (6)
C5—H5	0.9300	C23—C24	1.380 (6)
C6—C7	1.488 (5)	C23—H23	0.9300
C7—C9	1.505 (5)	C24—C27	1.507 (6)
C8—H8A	0.9600	C25—H25A	0.9600
C8—H8B	0.9600	C25—H25B	0.9600
C8—H8C	0.9600	C25—H25C	0.9600
C9—H9A	0.9600	C26—H26A	0.9600
C9—H9B	0.9600	C26—H26B	0.9600
C9—H9C	0.9600	C26—H26C	0.9600
C10—C15	1.382 (4)	C27—H27A	0.9600
C10—C11	1.405 (5)	C27—H27B	0.9600
C11—C12	1.389 (5)	C27—H27C	0.9600
C11—C16	1.493 (5)	C28—C29	1.451 (8)
C12—C13	1.373 (5)	C29—H29A	0.9600
C12—H12	0.9300	C29—H29B	0.9600
C13—C14	1.369 (5)	C29—H29C	0.9600
C13—C17	1.517 (5)		
N2—Cd1—N1	69.50 (10)	C15—C14—H14	118.8
N2—Cd1—Cl2	126.50 (7)	C10—C15—C14	117.9 (4)
N1—Cd1—Cl2	102.89 (7)	C10—C15—C18	121.2 (3)
N2—Cd1—N3	68.88 (10)	C14—C15—C18	120.8 (3)
N1—Cd1—N3	138.28 (10)	C11—C16—H16A	109.5
Cl2—Cd1—N3	99.21 (7)	C11—C16—H16B	109.5
N2—Cd1—Cl1	118.86 (7)	H16A—C16—H16B	109.5
N1—Cd1—Cl1	97.85 (7)	C11—C16—H16C	109.5
Cl2—Cd1—Cl1	114.64 (4)	H16A—C16—H16C	109.5
N3—Cd1—Cl1	104.43 (7)	H16B—C16—H16C	109.5
C1—N1—C10	119.5 (3)	C13—C17—H17A	109.5
C1—N1—Cd1	117.2 (2)	C13—C17—H17B	109.5
C10—N1—Cd1	123.2 (2)	H17A—C17—H17B	109.5
C6—N2—C2	121.0 (3)	C13—C17—H17C	109.5
C6—N2—Cd1	119.8 (2)	H17A—C17—H17C	109.5
C2—N2—Cd1	119.0 (2)	H17B—C17—H17C	109.5
C7—N3—C19	122.6 (3)	C15—C18—H18A	109.5
C7—N3—Cd1	117.4 (2)	C15—C18—H18B	109.5
C19—N3—Cd1	120.0 (2)	H18A—C18—H18B	109.5
N1—C1—C8	125.1 (3)	C15—C18—H18C	109.5
N1—C1—C2	117.1 (3)	H18A—C18—H18C	109.5
C8—C1—C2	117.8 (3)	H18B—C18—H18C	109.5
N2—C2—C3	121.1 (3)	C20—C19—C24	121.7 (4)
N2—C2—C1	116.7 (3)	C20—C19—N3	119.3 (3)
C3—C2—C1	122.1 (3)	C24—C19—N3	118.9 (3)
C4—C3—C2	118.3 (4)	C19—C20—C21	117.8 (4)
C4—C3—H3	120.8	C19—C20—C25	121.3 (4)
C2—C3—H3	120.8	C21—C20—C25	120.9 (4)
C5—C4—C3	119.8 (4)	C22—C21—C20	122.5 (4)
C5—C4—H4	120.1	C22—C21—H21	118.7

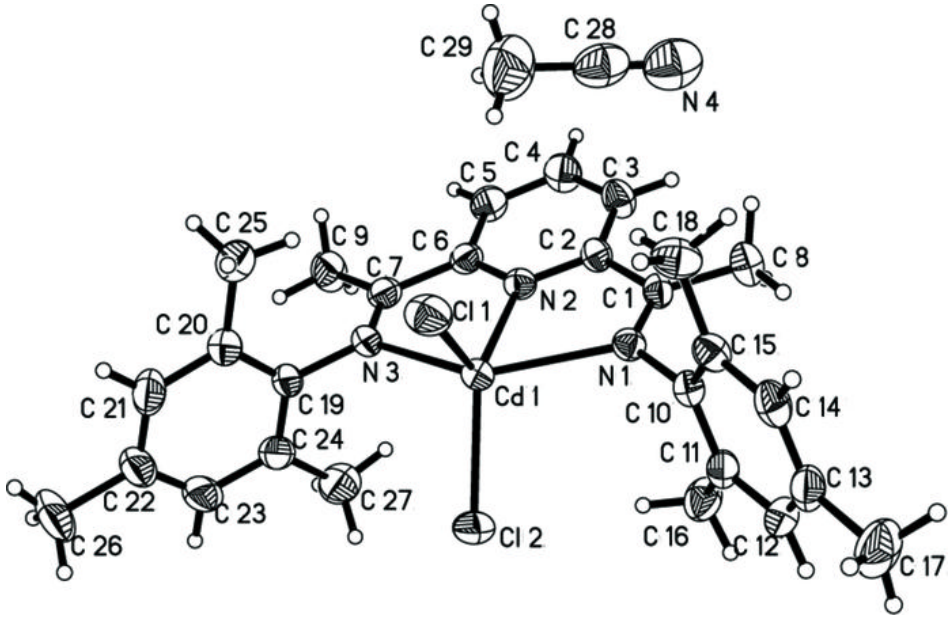
C3—C4—H4	120.1	C20—C21—H21	118.7
C4—C5—C6	119.5 (4)	C21—C22—C23	117.7 (4)
C4—C5—H5	120.2	C21—C22—C26	121.1 (5)
C6—C5—H5	120.2	C23—C22—C26	121.2 (5)
N2—C6—C5	120.1 (4)	C24—C23—C22	122.3 (4)
N2—C6—C7	116.6 (3)	C24—C23—H23	118.8
C5—C6—C7	123.3 (3)	C22—C23—H23	118.8
N3—C7—C6	117.2 (3)	C23—C24—C19	117.9 (4)
N3—C7—C9	124.2 (4)	C23—C24—C27	120.5 (4)
C6—C7—C9	118.6 (4)	C19—C24—C27	121.6 (4)
C1—C8—H8A	109.5	C20—C25—H25A	109.5
C1—C8—H8B	109.5	C20—C25—H25B	109.5
H8A—C8—H8B	109.5	H25A—C25—H25B	109.5
C1—C8—H8C	109.5	C20—C25—H25C	109.5
H8A—C8—H8C	109.5	H25A—C25—H25C	109.5
H8B—C8—H8C	109.5	H25B—C25—H25C	109.5
C7—C9—H9A	109.5	C22—C26—H26A	109.5
C7—C9—H9B	109.5	C22—C26—H26B	109.5
H9A—C9—H9B	109.5	H26A—C26—H26B	109.5
C7—C9—H9C	109.5	C22—C26—H26C	109.5
H9A—C9—H9C	109.5	H26A—C26—H26C	109.5
H9B—C9—H9C	109.5	H26B—C26—H26C	109.5
C15—C10—C11	121.6 (3)	C24—C27—H27A	109.5
C15—C10—N1	120.6 (3)	C24—C27—H27B	109.5
C11—C10—N1	117.8 (3)	H27A—C27—H27B	109.5
C12—C11—C10	117.1 (3)	C24—C27—H27C	109.5
C12—C11—C16	121.7 (4)	H27A—C27—H27C	109.5
C10—C11—C16	121.2 (3)	H27B—C27—H27C	109.5
C13—C12—C11	123.0 (4)	N4—C28—C29	179.0 (7)
C13—C12—H12	118.5	C28—C29—H29A	109.5
C11—C12—H12	118.5	C28—C29—H29B	109.5
C14—C13—C12	117.9 (4)	H29A—C29—H29B	109.5
C14—C13—C17	121.9 (4)	C28—C29—H29C	109.5
C12—C13—C17	120.2 (4)	H29A—C29—H29C	109.5
C13—C14—C15	122.5 (4)	H29B—C29—H29C	109.5
C13—C14—H14	118.8		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8C···Cl1^{i}	0.96	2.66	3.614 (4)	172
C16—H16A···Cl2^{ii}	0.96	2.84	3.681 (4)	146
C16—H16C···Cl2	0.96	2.80	3.680 (4)	153
C29—H29B···Cl2^{iii}	0.96	2.81	3.721 (6)	159
C5—H5···Cl1^{iii}	0.93	2.74	3.622 (4)	158

Symmetry codes: (i) $x+1/2, -y+1/2, z+1/2$; (ii) $-x+2, -y, -z+1$; (iii) $-x+3/2, y+1/2, -z+1/2$.

Fig. 1


C 29
C 28
N 4
C 4
C 5
C 3
C 25
C 9
C 6
C 2
C 18
C 8
C 7
Cl 1
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C 1
C 20
N 3
Cd 1
N 1
C 15
C 21
C 19
C 10
C 14
C 24
C 11
C 22
C 23
C 27
C 13
C 26
Cl 2
C 16
C 12
C 17

Fig. 2