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Dichloridobis{2-[(triphenylmethyl)amino]pyridine-κN}cadmium(II)

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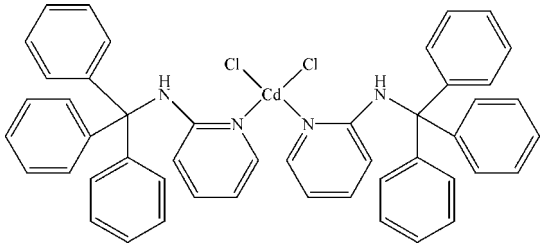
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.040; wR factor = 0.091; data-to-parameter ratio = 18.4.

In the molecule of the title compound, $[CdCl_2(C_{24}H_{20}N_2)_2]$, the Cd^{II} centre has a distorted tetrahedral coordination geometry defined by two chloride ions and two pyridine N atoms of the monodentate 2-[(triphenylmethyl)amino]-pyridine ligands. Weak intramolecular N—H···Cl hydrogen bonds help to establish the three-dimensional architecture.

Related literature

For related literature, see: Fang *et al.* (2006); Zhang *et al.* (2007).



Experimental

Crystal data

$[CdCl_2(C_{24}H_{20}N_2)_2]$
M_r = 856.15
Monoclinic, $P2_1/n$
a = 10.0531 (11) Å
b = 22.903 (2) Å
c = 17.5659 (18) Å
β = 98.693 (2)°
V = 3998.0 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 295 (2) K
0.09 × 0.06 × 0.05 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.937, T_{max} = 0.968
25067 measured reflections
9118 independent reflections
5827 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.091
S = 0.97
9118 reflections
496 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.284 (2)	Cd1—Cl2	2.3850 (9)
Cd1—N3	2.286 (2)	Cd1—Cl1	2.3878 (8)
N1—Cd1—N3	95.24 (8)	N1—Cd1—Cl1	110.82 (6)
N1—Cd1—Cl2	109.63 (6)	N3—Cd1—Cl1	108.47 (6)
N3—Cd1—Cl2	108.33 (6)	Cl2—Cd1—Cl1	121.18 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Cl2	0.86	2.79	3.630 (2)	165
N4—H4A···Cl1	0.86	2.87	3.693 (2)	160

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2417).

References

Bruker (2005). *APEX2* and *SAINT*. Bruker AXS inc., Madison, Wisconsin, USA.
Fang, Y., Huang, C.-Y., Zhu, Z.-M., Yu, X.-L. & You, W.-S. (2006). *Acta Cryst.* E**62**, m3347–m3348.
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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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supplementary materials

Acta Cryst. (2008). E**64**, m357 [**doi:10.1107/S1600536808000986**]

Dichloridobis{2-[(triphenylmethyl)amino]pyridine-*κN*}cadmium(II)

G.-N. Zhang

Comment

As part of our ongoing studies on different metal complexes with 2-[N-(tri- phenylmethyl)imino] pyridine ligand, we synthesized the title compound, (I), and report herein its crystal structure. It is isomorphic with $[CoCl_2(C_{24}H_{20}N_2)_2]$ (Fang *et al.*, 2006) and $[ZnCl_2(C_{24}H_{20}N_2)_2]$ (Zhang *et al.*, 2007) and exhibits approximate C2 local point symmetry.

In the molecule of the title compound, (I), (Fig. 1) C d atom adopts a distorted tetrahedral coordination geometry with two chloride ions and two N atoms of the pyridine rings of the monodentate 2-[*N*-(triphenylmethyl)imino]pyridine ligands (Table 1). Because of the large volume of the 2-[*N*-(triphenylmethyl)imino]- pyridine ligand, the formation of a four-coordinate complex is more possible rather than six-coordinate one. Weak intramolecular N—H···Cl hydrogen bonds (Table 2) help to establish the three-dimensional architecture.

As shown in Fig. 2, the complex molecules stack in the A—B—A—B sequence along the *b* axis.

Experimental

For the preparation of the title compound, (I), 2-[*N*-(triphenylmethyl)imino]- pyridine ligand (30 mg, 0.09 mmol) and $CdCl_2$ (25 mg, 0.14 mmol) were dissolved in 5 ml and 10 ml of ethanol, respectively, and then mixed. The mixed solution was stirred about 30 min and covered with hexane (10 ml). After two months, colorless crystals of (I) were obtained.

Refinement

H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Figures

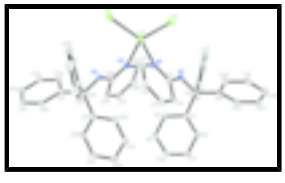

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 15% probability level. Hydrogen atoms have been omitted for clarity.

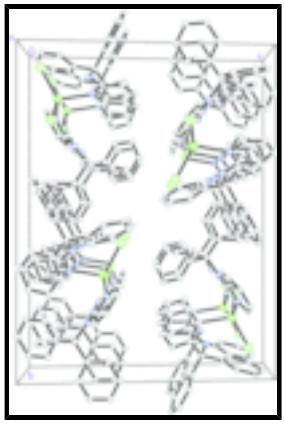

Fig. 2. A packing diagram of (I). Hydrogen atoms have been omitted for clarity.

Dichloridobis{2-[(triphenylmethyl)amino]pyridine-κ*N*}cadmium(II)

Crystal data

$[CdCl_2(C_{24}H_{20}N_2)_2]$	F_{000} = 1752
M_r = 856.15	D_x = 1.422 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 4517 reflections
a = 10.0531 (11) Å	θ = 2.2–24.1º
b = 22.903 (2) Å	μ = 0.72 mm^{-1}
c = 17.5659 (18) Å	T = 295 (2) K
β = 98.693 (2)º	Plate, colorless
V = 3998.0 (7) Å^3	0.09 × 0.06 × 0.05 mm
Z = 4	

Data collection

Bruker SMART APEXII CCD diffractometer	9118 independent reflections
Radiation source: fine-focus sealed tube	5827 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.044
T = 295(2) K	θ_{max} = 27.5º
CCD scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −13→12
T_{min} = 0.937, T_{max} = 0.968	k = −29→28
25067 measured reflections	l = −17→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H-atom parameters constrained

$wR(F^2) = 0.091$	$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{max} = 0.001$
9118 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
496 parameters	$\Delta\rho_{min} = -0.34$ 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^ > σ(*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	0.22022 (2)	0.180326 (9)	0.164854 (12)	0.04388 (8)
Cl1	0.18946 (8)	0.08877 (3)	0.09955 (5)	0.0580 (2)
Cl2	0.40291 (10)	0.24316 (4)	0.14838 (6)	0.0852 (3)
N1	0.0244 (2)	0.23247 (10)	0.14942 (13)	0.0404 (5)
N2	0.1196 (2)	0.31010 (9)	0.22081 (12)	0.0375 (5)
H2A	0.1946	0.2951	0.2127	0.045*
N3	0.2253 (2)	0.16432 (9)	0.29372 (13)	0.0374 (5)
N4	0.0345 (2)	0.10679 (10)	0.27581 (12)	0.0404 (6)
H4A	0.0486	0.1046	0.2288	0.048*
C1	−0.0853 (3)	0.20510 (13)	0.11086 (17)	0.0513 (8)
H1A	−0.0718	0.1713	0.0837	0.062*
C2	−0.2141 (3)	0.22420 (14)	0.10963 (18)	0.0555 (8)
H2B	−0.2865	0.2039	0.0828	0.067*
C3	−0.2336 (3)	0.27467 (14)	0.14947 (17)	0.0487 (8)
H3A	−0.3203	0.2886	0.1503	0.058*
C4	−0.1251 (3)	0.30426 (12)	0.18791 (16)	0.0418 (7)
H4B	−0.1379	0.3384	0.2145	0.050*
C5	0.0060 (3)	0.28270 (12)	0.18684 (15)	0.0374 (6)
C6	0.1295 (3)	0.36288 (11)	0.27025 (15)	0.0346 (6)
C7	0.0422 (3)	0.35458 (12)	0.33435 (15)	0.0362 (6)
C8	0.0536 (3)	0.30209 (12)	0.37457 (16)	0.0437 (7)
H8A	0.1032	0.2718	0.3576	0.052*
C9	−0.0070 (3)	0.29417 (14)	0.43891 (17)	0.0515 (8)
H9A	0.0016	0.2586	0.4648	0.062*
C10	−0.0801 (3)	0.33843 (14)	0.46514 (18)	0.0534 (8)

H10A	−0.1191	0.3335	0.5095	0.064*
C11	−0.0951 (3)	0.39013 (14)	0.42521 (18)	0.0508 (8)
H11A	−0.1456	0.4201	0.4422	0.061*
C12	−0.0354 (3)	0.39804 (13)	0.35958 (17)	0.0436 (7)
H12A	−0.0479	0.4330	0.3324	0.052*
C13	0.2786 (3)	0.36728 (11)	0.30850 (16)	0.0375 (6)
C14	0.3146 (3)	0.37696 (15)	0.38628 (18)	0.0620 (9)
H14A	0.2482	0.3798	0.4177	0.074*
C15	0.4485 (4)	0.38248 (18)	0.4181 (2)	0.0788 (12)
H15A	0.4716	0.3902	0.4704	0.095*
C16	0.5476 (4)	0.37651 (17)	0.3726 (3)	0.0777 (12)
H16A	0.6377	0.3780	0.3945	0.093*
C17	0.5135 (3)	0.36846 (15)	0.2952 (2)	0.0710 (10)
H17A	0.5801	0.3660	0.2639	0.085*
C18	0.3793 (3)	0.36399 (12)	0.26346 (18)	0.0502 (8)
H18A	0.3566	0.3587	0.2106	0.060*
C19	0.0974 (3)	0.41857 (11)	0.22183 (16)	0.0372 (6)
C20	0.0453 (3)	0.41674 (14)	0.14404 (17)	0.0494 (8)
H20A	0.0274	0.3810	0.1196	0.059*
C21	0.0197 (3)	0.46849 (16)	0.1023 (2)	0.0632 (9)
H21A	−0.0160	0.4669	0.0504	0.076*
C22	0.0467 (3)	0.52172 (15)	0.1373 (2)	0.0648 (10)
H22A	0.0285	0.5560	0.1094	0.078*
C23	0.1006 (3)	0.52379 (14)	0.2135 (2)	0.0586 (9)
H23A	0.1203	0.5597	0.2373	0.070*
C24	0.1262 (3)	0.47306 (12)	0.25542 (18)	0.0483 (7)
H24A	0.1633	0.4753	0.3071	0.058*
C25	0.3258 (3)	0.19135 (13)	0.34048 (17)	0.0471 (7)
H25A	0.3926	0.2099	0.3182	0.057*
C26	0.3341 (3)	0.19281 (14)	0.41855 (18)	0.0561 (9)
H26A	0.4031	0.2129	0.4489	0.067*
C27	0.2372 (3)	0.16361 (13)	0.45119 (17)	0.0510 (8)
H27A	0.2411	0.1633	0.5044	0.061*
C28	0.1352 (3)	0.13498 (12)	0.40572 (15)	0.0438 (7)
H28A	0.0693	0.1155	0.4277	0.053*
C29	0.1310 (3)	0.13526 (11)	0.32565 (15)	0.0366 (6)
C30	−0.0912 (3)	0.07931 (11)	0.29282 (15)	0.0373 (6)
C31	−0.1649 (3)	0.12273 (12)	0.33877 (16)	0.0401 (7)
C32	−0.1876 (3)	0.17884 (13)	0.31017 (18)	0.0509 (8)
H32A	−0.1555	0.1894	0.2651	0.061*
C33	−0.2564 (3)	0.21912 (15)	0.3470 (2)	0.0601 (9)
H33A	−0.2728	0.2561	0.3257	0.072*
C34	−0.3012 (3)	0.20559 (16)	0.4144 (2)	0.0626 (9)
H34A	−0.3475	0.2330	0.4393	0.075*
C35	−0.2765 (3)	0.15041 (16)	0.4449 (2)	0.0638 (9)
H35A	−0.3051	0.1409	0.4913	0.077*
C36	−0.2098 (3)	0.10921 (14)	0.40748 (17)	0.0509 (8)
H36A	−0.1948	0.0721	0.4285	0.061*
C37	−0.0639 (3)	0.02013 (12)	0.33347 (15)	0.0394 (7)

C38	0.0644 (3)	−0.00021 (13)	0.36006 (16)	0.0464 (7)
H38A	0.1386	0.0221	0.3525	0.056*
C39	0.0838 (3)	−0.05327 (14)	0.39767 (18)	0.0544 (8)
H39A	0.1707	−0.0660	0.4158	0.065*
C40	−0.0238 (3)	−0.08734 (14)	0.40857 (18)	0.0567 (8)
H40A	−0.0103	−0.1229	0.4342	0.068*
C41	−0.1525 (3)	−0.06832 (13)	0.38105 (18)	0.0553 (8)
H41A	−0.2261	−0.0913	0.3878	0.066*
C42	−0.1721 (3)	−0.01555 (13)	0.34372 (17)	0.0499 (8)
H42A	−0.2592	−0.0034	0.3250	0.060*
C43	−0.3090 (3)	0.08348 (14)	0.19416 (18)	0.0548 (8)
H43A	−0.3518	0.1024	0.2306	0.066*
C44	−0.3791 (4)	0.07201 (15)	0.1217 (2)	0.0672 (10)
H44A	−0.4689	0.0831	0.1101	0.081*
C45	−0.3187 (4)	0.04481 (16)	0.0669 (2)	0.0684 (10)
H45A	−0.3656	0.0385	0.0178	0.082*
C46	−0.1881 (4)	0.02697 (15)	0.08543 (19)	0.0633 (9)
H46A	−0.1465	0.0079	0.0487	0.076*
C47	−0.1165 (3)	0.03688 (13)	0.15848 (17)	0.0503 (8)
H47A	−0.0288	0.0232	0.1708	0.060*
C48	−0.1759 (3)	0.06707 (12)	0.21270 (16)	0.0406 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.04738 (13)	0.04593 (14)	0.04041 (13)	−0.00364 (11)	0.01342 (9)	−0.00233 (11)
Cl1	0.0686 (5)	0.0518 (5)	0.0532 (5)	−0.0031 (4)	0.0082 (4)	−0.0104 (4)
Cl2	0.0828 (6)	0.0833 (7)	0.1021 (8)	−0.0386 (5)	0.0545 (6)	−0.0328 (6)
N1	0.0427 (13)	0.0382 (13)	0.0391 (14)	−0.0040 (11)	0.0021 (11)	−0.0003 (11)
N2	0.0322 (12)	0.0398 (14)	0.0402 (13)	−0.0004 (10)	0.0042 (10)	−0.0039 (10)
N3	0.0342 (12)	0.0421 (14)	0.0364 (13)	−0.0047 (10)	0.0074 (10)	−0.0018 (10)
N4	0.0428 (13)	0.0482 (14)	0.0310 (12)	−0.0120 (11)	0.0083 (10)	0.0013 (11)
C1	0.066 (2)	0.0422 (18)	0.0412 (18)	−0.0066 (16)	−0.0055 (16)	−0.0015 (14)
C2	0.052 (2)	0.054 (2)	0.053 (2)	−0.0128 (16)	−0.0146 (16)	0.0082 (17)
C3	0.0381 (16)	0.0521 (19)	0.053 (2)	−0.0042 (14)	−0.0030 (14)	0.0146 (16)
C4	0.0410 (16)	0.0400 (17)	0.0432 (17)	−0.0009 (13)	0.0029 (13)	0.0067 (13)
C5	0.0421 (16)	0.0394 (16)	0.0294 (15)	−0.0034 (13)	0.0017 (12)	0.0077 (12)
C6	0.0366 (15)	0.0316 (15)	0.0353 (15)	−0.0005 (12)	0.0042 (12)	−0.0012 (12)
C7	0.0311 (14)	0.0409 (16)	0.0360 (15)	−0.0023 (12)	0.0024 (12)	0.0010 (13)
C8	0.0453 (17)	0.0425 (17)	0.0435 (17)	0.0022 (13)	0.0076 (14)	0.0045 (14)
C9	0.0534 (19)	0.0553 (19)	0.0466 (19)	−0.0037 (16)	0.0107 (15)	0.0143 (16)
C10	0.0490 (18)	0.070 (2)	0.0438 (18)	−0.0096 (16)	0.0156 (15)	−0.0051 (16)
C11	0.0405 (17)	0.056 (2)	0.057 (2)	−0.0034 (15)	0.0136 (15)	−0.0109 (16)
C12	0.0410 (16)	0.0413 (17)	0.0487 (18)	−0.0003 (13)	0.0072 (14)	0.0010 (14)
C13	0.0383 (15)	0.0322 (15)	0.0406 (16)	−0.0031 (12)	0.0010 (13)	0.0024 (12)
C14	0.053 (2)	0.086 (3)	0.0459 (19)	−0.0131 (18)	0.0017 (16)	−0.0019 (18)
C15	0.064 (2)	0.110 (3)	0.055 (2)	−0.021 (2)	−0.015 (2)	0.007 (2)
C16	0.042 (2)	0.087 (3)	0.096 (3)	−0.0079 (19)	−0.016 (2)	0.003 (2)

C17	0.0358 (18)	0.080 (3)	0.097 (3)	−0.0067 (17)	0.0103 (19)	−0.012 (2)
C18	0.0435 (18)	0.0524 (19)	0.0548 (19)	−0.0044 (15)	0.0076 (15)	−0.0047 (16)
C19	0.0323 (14)	0.0380 (16)	0.0419 (17)	0.0010 (12)	0.0079 (12)	0.0048 (13)
C20	0.0518 (18)	0.0496 (19)	0.0471 (19)	−0.0056 (15)	0.0078 (15)	0.0102 (15)
C21	0.062 (2)	0.070 (2)	0.056 (2)	−0.0057 (18)	0.0035 (17)	0.0261 (19)
C22	0.058 (2)	0.052 (2)	0.086 (3)	0.0032 (17)	0.014 (2)	0.033 (2)
C23	0.057 (2)	0.0400 (19)	0.081 (3)	−0.0011 (16)	0.0193 (19)	0.0103 (18)
C24	0.0506 (18)	0.0416 (18)	0.0534 (19)	−0.0031 (14)	0.0105 (15)	0.0026 (15)
C25	0.0405 (16)	0.0527 (19)	0.0488 (19)	−0.0079 (14)	0.0089 (14)	−0.0052 (15)
C26	0.0429 (18)	0.071 (2)	0.053 (2)	−0.0138 (16)	0.0001 (15)	−0.0120 (17)
C27	0.0560 (19)	0.064 (2)	0.0327 (16)	−0.0026 (16)	0.0037 (14)	−0.0055 (15)
C28	0.0444 (17)	0.0520 (19)	0.0360 (16)	−0.0060 (14)	0.0097 (13)	0.0025 (14)
C29	0.0370 (15)	0.0368 (16)	0.0359 (15)	−0.0006 (12)	0.0051 (12)	−0.0001 (12)
C30	0.0362 (15)	0.0381 (16)	0.0366 (15)	−0.0066 (12)	0.0029 (12)	0.0065 (12)
C31	0.0340 (14)	0.0447 (17)	0.0403 (16)	−0.0022 (13)	0.0011 (12)	0.0033 (14)
C32	0.0570 (19)	0.0457 (18)	0.0514 (19)	0.0002 (16)	0.0131 (15)	0.0049 (16)
C33	0.061 (2)	0.046 (2)	0.075 (3)	0.0007 (16)	0.0131 (19)	0.0080 (18)
C34	0.0482 (19)	0.063 (2)	0.079 (3)	0.0064 (17)	0.0169 (18)	−0.011 (2)
C35	0.060 (2)	0.074 (2)	0.061 (2)	0.0042 (19)	0.0224 (18)	0.004 (2)
C36	0.0540 (19)	0.0533 (19)	0.0464 (19)	−0.0001 (15)	0.0105 (15)	0.0100 (15)
C37	0.0392 (16)	0.0435 (17)	0.0358 (16)	−0.0040 (13)	0.0066 (13)	0.0057 (13)
C38	0.0460 (17)	0.0473 (18)	0.0464 (18)	−0.0023 (14)	0.0093 (14)	0.0058 (15)
C39	0.0493 (19)	0.058 (2)	0.056 (2)	0.0101 (16)	0.0072 (16)	0.0093 (17)
C40	0.071 (2)	0.050 (2)	0.0499 (19)	0.0051 (17)	0.0105 (17)	0.0150 (16)
C41	0.057 (2)	0.0486 (19)	0.062 (2)	−0.0084 (16)	0.0130 (17)	0.0115 (16)
C42	0.0440 (17)	0.0479 (19)	0.058 (2)	−0.0013 (14)	0.0073 (15)	0.0114 (15)
C43	0.0496 (19)	0.061 (2)	0.051 (2)	−0.0043 (16)	−0.0013 (16)	0.0037 (17)
C44	0.057 (2)	0.070 (2)	0.067 (2)	−0.0059 (18)	−0.016 (2)	0.010 (2)
C45	0.081 (3)	0.068 (2)	0.049 (2)	−0.017 (2)	−0.015 (2)	0.0100 (19)
C46	0.078 (3)	0.060 (2)	0.051 (2)	−0.0174 (19)	0.0069 (19)	−0.0066 (17)
C47	0.0505 (18)	0.0513 (19)	0.0468 (19)	−0.0102 (15)	−0.0005 (15)	−0.0016 (15)
C48	0.0429 (17)	0.0388 (16)	0.0381 (16)	−0.0099 (13)	−0.0001 (13)	0.0081 (13)

Geometric parameters (Å, °)

Cd1—N1	2.284 (2)	C21—C22	1.374 (5)
Cd1—N3	2.286 (2)	C21—H21A	0.9300
Cd1—Cl2	2.3850 (9)	C22—C23	1.366 (5)
Cd1—Cl1	2.3878 (8)	C22—H22A	0.9300
N1—C5	1.351 (3)	C23—C24	1.379 (4)
N1—C1	1.357 (3)	C23—H23A	0.9300
N2—C5	1.360 (3)	C24—H24A	0.9300
N2—C6	1.483 (3)	C25—C26	1.362 (4)
N2—H2A	0.8600	C25—H25A	0.9300
N3—C29	1.348 (3)	C26—C27	1.376 (4)
N3—C25	1.352 (3)	C26—H26A	0.9300
N4—C29	1.370 (3)	C27—C28	1.368 (4)
N4—C30	1.482 (3)	C27—H27A	0.9300
N4—H4A	0.8600	C28—C29	1.401 (4)

C1—C2	1.364 (4)	C28—H28A	0.9300
C1—H1A	0.9300	C30—C37	1.537 (4)
C2—C3	1.381 (4)	C30—C31	1.539 (4)
C2—H2B	0.9300	C30—C48	1.556 (4)
C3—C4	1.372 (4)	C31—C36	1.386 (4)
C3—H3A	0.9300	C31—C32	1.386 (4)
C4—C5	1.410 (4)	C32—C33	1.372 (4)
C4—H4B	0.9300	C32—H32A	0.9300
C6—C19	1.540 (3)	C33—C34	1.365 (4)
C6—C7	1.540 (3)	C33—H33A	0.9300
C6—C13	1.551 (4)	C34—C35	1.381 (5)
C7—C12	1.379 (4)	C34—H34A	0.9300
C7—C8	1.390 (4)	C35—C36	1.381 (4)
C8—C9	1.375 (4)	C35—H35A	0.9300
C8—H8A	0.9300	C36—H36A	0.9300
C9—C10	1.372 (4)	C37—C38	1.385 (4)
C9—H9A	0.9300	C37—C42	1.394 (4)
C10—C11	1.373 (4)	C38—C39	1.383 (4)
C10—H10A	0.9300	C38—H38A	0.9300
C11—C12	1.390 (4)	C39—C40	1.370 (4)
C11—H11A	0.9300	C39—H39A	0.9300
C12—H12A	0.9300	C40—C41	1.381 (4)
C13—C14	1.377 (4)	C40—H40A	0.9300
C13—C18	1.378 (4)	C41—C42	1.375 (4)
C14—C15	1.384 (4)	C41—H41A	0.9300
C14—H14A	0.9300	C42—H42A	0.9300
C15—C16	1.375 (5)	C43—C48	1.380 (4)
C15—H15A	0.9300	C43—C44	1.384 (4)
C16—C17	1.363 (5)	C43—H43A	0.9300
C16—H16A	0.9300	C44—C45	1.363 (5)
C17—C18	1.383 (4)	C44—H44A	0.9300
C17—H17A	0.9300	C45—C46	1.366 (5)
C18—H18A	0.9300	C45—H45A	0.9300
C19—C20	1.388 (4)	C46—C47	1.392 (4)
C19—C24	1.392 (4)	C46—H46A	0.9300
C20—C21	1.397 (4)	C47—C48	1.383 (4)
C20—H20A	0.9300	C47—H47A	0.9300
N1—Cd1—N3	95.24 (8)	C23—C22—C21	119.4 (3)
N1—Cd1—Cl2	109.63 (6)	C23—C22—H22A	120.3
N3—Cd1—Cl2	108.33 (6)	C21—C22—H22A	120.3
N1—Cd1—Cl1	110.82 (6)	C22—C23—C24	120.5 (3)
N3—Cd1—Cl1	108.47 (6)	C22—C23—H23A	119.7
Cl2—Cd1—Cl1	121.18 (3)	C24—C23—H23A	119.7
C5—N1—C1	118.4 (2)	C23—C24—C19	121.3 (3)
C5—N1—Cd1	124.49 (17)	C23—C24—H24A	119.4
C1—N1—Cd1	116.00 (19)	C19—C24—H24A	119.4
C5—N2—C6	127.6 (2)	N3—C25—C26	123.4 (3)
C5—N2—H2A	116.2	N3—C25—H25A	118.3
C6—N2—H2A	116.2	C26—C25—H25A	118.3

C29—N3—C25	118.8 (2)	C25—C26—C27	117.9 (3)
C29—N3—Cd1	125.40 (17)	C25—C26—H26A	121.0
C25—N3—Cd1	115.54 (18)	C27—C26—H26A	121.0
C29—N4—C30	128.1 (2)	C28—C27—C26	120.3 (3)
C29—N4—H4A	116.0	C28—C27—H27A	119.8
C30—N4—H4A	116.0	C26—C27—H27A	119.8
N1—C1—C2	123.9 (3)	C27—C28—C29	119.3 (3)
N1—C1—H1A	118.1	C27—C28—H28A	120.3
C2—C1—H1A	118.1	C29—C28—H28A	120.3
C1—C2—C3	117.9 (3)	N3—C29—N4	116.4 (2)
C1—C2—H2B	121.1	N3—C29—C28	120.3 (2)
C3—C2—H2B	121.1	N4—C29—C28	123.4 (2)
C4—C3—C2	120.0 (3)	N4—C30—C37	111.7 (2)
C4—C3—H3A	120.0	N4—C30—C31	108.9 (2)
C2—C3—H3A	120.0	C37—C30—C31	113.1 (2)
C3—C4—C5	119.7 (3)	N4—C30—C48	105.1 (2)
C3—C4—H4B	120.1	C37—C30—C48	107.2 (2)
C5—C4—H4B	120.1	C31—C30—C48	110.5 (2)
N1—C5—N2	116.0 (2)	C36—C31—C32	117.7 (3)
N1—C5—C4	120.1 (2)	C36—C31—C30	123.9 (3)
N2—C5—C4	123.9 (3)	C32—C31—C30	118.3 (3)
N2—C6—C19	111.2 (2)	C33—C32—C31	121.3 (3)
N2—C6—C7	109.4 (2)	C33—C32—H32A	119.4
C19—C6—C7	114.3 (2)	C31—C32—H32A	119.4
N2—C6—C13	106.3 (2)	C34—C33—C32	120.8 (3)
C19—C6—C13	107.0 (2)	C34—C33—H33A	119.6
C7—C6—C13	108.2 (2)	C32—C33—H33A	119.6
C12—C7—C8	117.9 (3)	C33—C34—C35	118.8 (3)
C12—C7—C6	123.9 (2)	C33—C34—H34A	120.6
C8—C7—C6	117.8 (2)	C35—C34—H34A	120.6
C9—C8—C7	121.3 (3)	C34—C35—C36	120.8 (3)
C9—C8—H8A	119.4	C34—C35—H35A	119.6
C7—C8—H8A	119.4	C36—C35—H35A	119.6
C10—C9—C8	120.3 (3)	C35—C36—C31	120.5 (3)
C10—C9—H9A	119.8	C35—C36—H36A	119.7
C8—C9—H9A	119.8	C31—C36—H36A	119.7
C9—C10—C11	119.3 (3)	C38—C37—C42	117.7 (3)
C9—C10—H10A	120.4	C38—C37—C30	123.0 (2)
C11—C10—H10A	120.4	C42—C37—C30	119.3 (2)
C10—C11—C12	120.6 (3)	C39—C38—C37	120.9 (3)
C10—C11—H11A	119.7	C39—C38—H38A	119.6
C12—C11—H11A	119.7	C37—C38—H38A	119.6
C7—C12—C11	120.6 (3)	C40—C39—C38	120.7 (3)
C7—C12—H12A	119.7	C40—C39—H39A	119.7
C11—C12—H12A	119.7	C38—C39—H39A	119.7
C14—C13—C18	118.2 (3)	C39—C40—C41	119.2 (3)
C14—C13—C6	122.1 (3)	C39—C40—H40A	120.4
C18—C13—C6	119.6 (2)	C41—C40—H40A	120.4
C13—C14—C15	120.6 (3)	C42—C41—C40	120.2 (3)

C13—C14—H14A	119.7	C42—C41—H41A	119.9
C15—C14—H14A	119.7	C40—C41—H41A	119.9
C16—C15—C14	120.1 (3)	C41—C42—C37	121.2 (3)
C16—C15—H15A	120.0	C41—C42—H42A	119.4
C14—C15—H15A	120.0	C37—C42—H42A	119.4
C17—C16—C15	119.9 (3)	C48—C43—C44	120.4 (3)
C17—C16—H16A	120.0	C48—C43—H43A	119.8
C15—C16—H16A	120.0	C44—C43—H43A	119.8
C16—C17—C18	119.7 (3)	C45—C44—C43	121.1 (3)
C16—C17—H17A	120.2	C45—C44—H44A	119.4
C18—C17—H17A	120.2	C43—C44—H44A	119.4
C13—C18—C17	121.4 (3)	C44—C45—C46	118.9 (3)
C13—C18—H18A	119.3	C44—C45—H45A	120.6
C17—C18—H18A	119.3	C46—C45—H45A	120.6
C20—C19—C24	117.9 (3)	C45—C46—C47	121.0 (3)
C20—C19—C6	122.3 (2)	C45—C46—H46A	119.5
C24—C19—C6	119.7 (2)	C47—C46—H46A	119.5
C19—C20—C21	120.2 (3)	C48—C47—C46	120.0 (3)
C19—C20—H20A	119.9	C48—C47—H47A	120.0
C21—C20—H20A	119.9	C46—C47—H47A	120.0
C22—C21—C20	120.7 (3)	C43—C48—C47	118.5 (3)
C22—C21—H21A	119.7	C43—C48—C30	122.9 (3)
C20—C21—H21A	119.7	C47—C48—C30	118.6 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···Cl2	0.86	2.79	3.630 (2)	165
N4—H4A···Cl1	0.86	2.87	3.693 (2)	160

Fig. 1

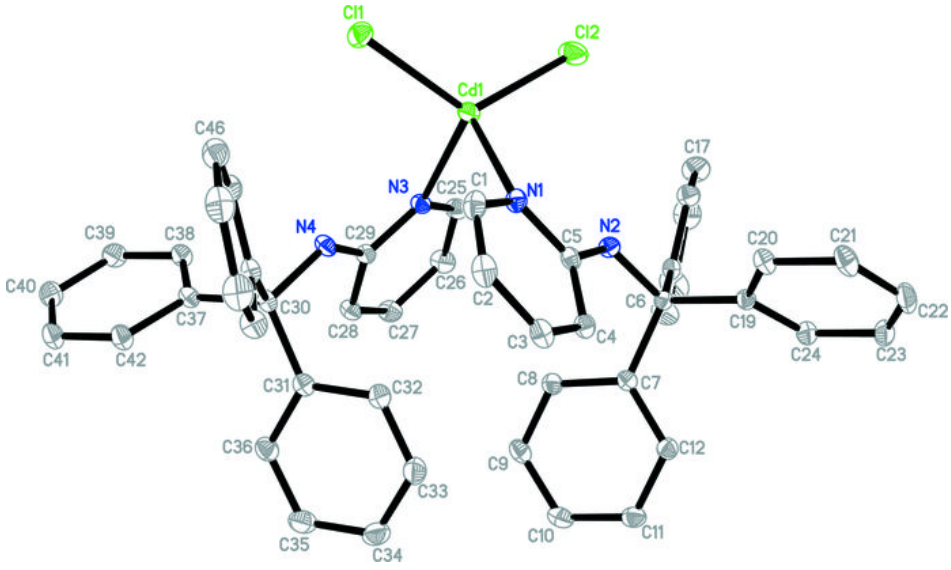
Cl1
Cl2
Cd1
C46
N3
C25
C1
N1
C17
N4
C29
C5
N2
C39
C38
C20
C21
C40
C26
C2
C6
C22
C37
C30
C28
C27
C3
C4
C19
C24
C23
C41
C42
C31
C32
C8
C7
C36
C12
C9
C33
C10
C11
C35
C34

Fig. 2