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Poly[bis[μ-1,4-bis(imidazol-1-ylmethyl)-benzene]dichloridocadmium(II)]

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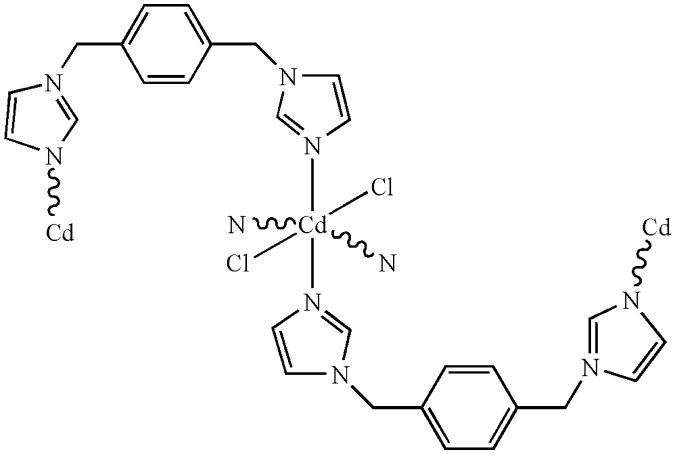
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.024; wR factor = 0.058; data-to-parameter ratio = 15.3.

The title compound, $[CdCl_2(C_{14}H_{14}N_4)_2]_n$, has a slightly distorted octahedral coordination geometry, formed by four N atoms from 1,4-bis(imidazol-1-ylmethyl)benzene ligands and two Cl atoms, giving a two-dimensional network. The Cd atom lies on a centre of inversion.

Related literature

For related literature, see: Zhou & Du (2007).



Experimental

Crystal data

$[CdCl_2(C_{14}H_{14}N_4)_2]$
M_r = 659.88
Monoclinic, $P2_1/c$
a = 7.7983 (3) Å
b = 12.8274 (6) Å
c = 14.4190 (6) Å
β = 105.642 (1)°
V = 1388.94 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.01 mm^{-1}
T = 293 (2) K
0.32 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SAINT*; Bruker, 2001)
T_{min} = 0.74, T_{max} = 0.78
7453 measured reflections
2728 independent reflections
2331 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.058
S = 1.00
2728 reflections
178 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1^{i}	2.3546 (17)	Cd1—N3^{i}	2.3561 (15)
Cd1—N1	2.3546 (17)	Cd1—Cl1^{i}	2.6248 (5)
Cd1—N3	2.3561 (15)	Cd1—Cl1	2.6248 (5)
N1^{i}—Cd1—N1	180	N1—Cd1—Cl1	90.04 (4)
N1^{i}—Cd1—N3	94.57 (6)	N3—Cd1—Cl1	89.60 (4)
N1—Cd1—N3	85.43 (6)	N3^{i}—Cd1—Cl1	90.40 (4)
N3—Cd1—N3^{i}	180	Cl1^{i}—Cd1—Cl1	180
N1—Cd1—Cl1^{i}	89.96 (4)		

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: SG2246).

References

Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhou, H. & Du, S. W. (2007). *Chin. J. Struct. Chem.* **26**, 711–716.

supporting information

Acta Cryst. (2008). E**64**, m973 [doi:10.1107/S1600536808018990]

Poly[bis[μ-1,4-bis(imidazol-1-ylmethyl)benzene]dichloridocadmium(II)]

Yu Ding, Genwen Zheng, Zhengbing Fu and Xinliang Hu

S1. Comment

The self-assembly reactions of $M^{II}Cl_2$ (M = Ni, Co) with the flexible bix ligand with 2D network $[Ni(bix)_2Cl_2]_n$ and a 1D chain $[Co(bix)Cl_2]_n$ had been reported (Zhou *et al.*, 2007). Here we report a new polymer. The Cd(II) center is coordinated by four nitrogen atoms from four bix ligands and two Cl atoms to furnish a slightly distorted octahedral. Four nitrogen atoms (N1, N1^i, N3, and N3^i) [symmetry code: (i) -*x*,-*y* + 1,-*z*] occupy the equatorial positions. The axial positions are occupied by two Cl donors. Each Cd(II) ion is linked by four μ2-birdging bix ligands to its four neighboring Cd(II) ions, thus affording two-dimensional grid layers (Fig. 2) in the direction of *b* axis. There are two different types of μ^2-bridging bix ligands in the compound.

The ring centriods distances and displacement angles of of *Cg*1···*Cg*1^i is 1.573 Å and 0.03° [*Cg*1 is N1—C1 ring centroid; symmetry code: (i) -*x*,-*y* + 1,-*z*], suggesting significant π-π interactions. which are the factors that stabilized the crystal structure.

S2. Experimental

Compound (I) was was prepared as follows: to a solution of bix dihydrate 0.14 g(0.5 mmol) and water (8 mL) was added $CdCl_2$ (0.092 g, 0.5 mmol). The mixture was sealed in a stainless steel reactor with a Teflon liner, and was heated to 393 K for two days. After slow cooling to room temperature, colourless block-shaped crystals of (I) were obtained.

S3. Refinement

The H atoms bonded to C atoms were introduced at calculated positions and refined using a riding model, with U_{iso}(H) = 1.2Ueq(C) and U_{iso}(H) = 1.5Ueq(C), and C–H distances of 0.93–0.96 Å.

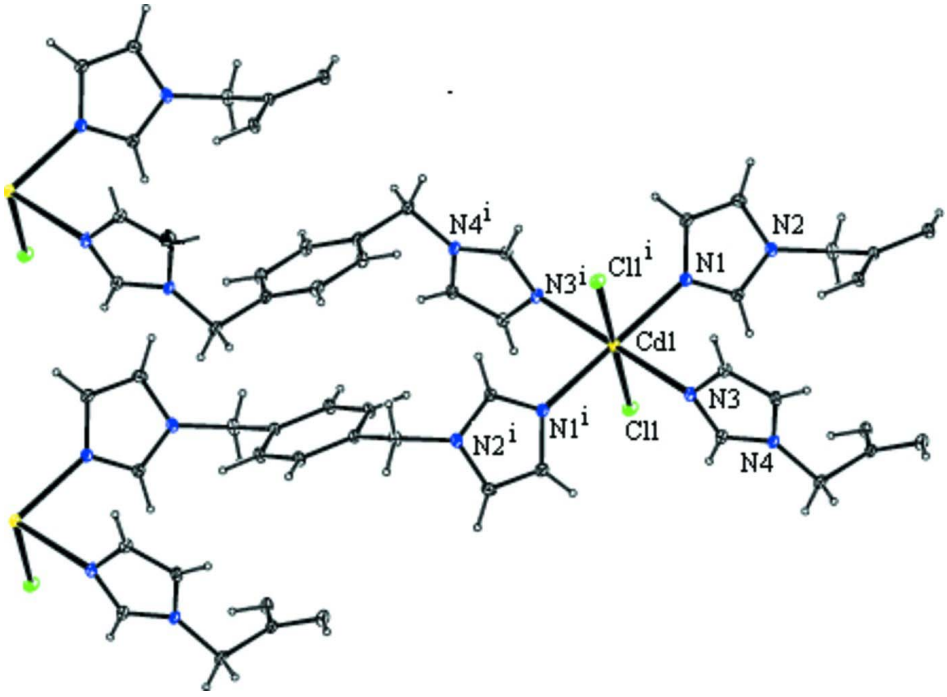

Figure 1

The molecular structure of (I), showing ellipsoids at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i)-*x*,-*y* + 1,-*z*]

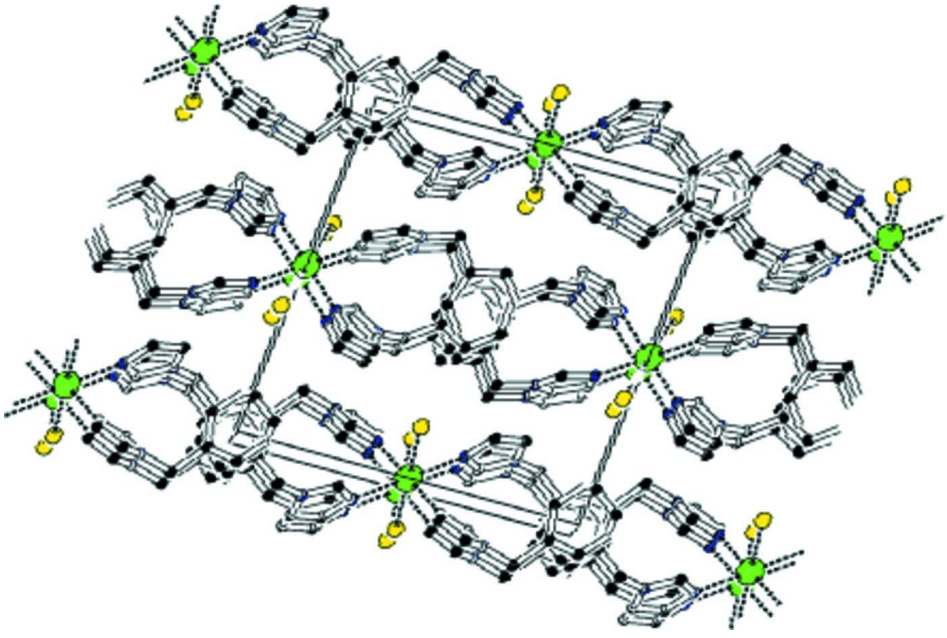

Figure 2

The molecular packing diagram of (I), with hydrogen bonds shown as dashed lines.

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$c = 14.4190$ (6) Å
$\beta = 105.642$ (1)°
$V = 1388.94$ (10) Å^3
$Z = 2$
$F(000) = 668$
$D_x = 1.578$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4013 reflections
$\theta = 2.7$–$28.3°$
$\mu = 1.01$ mm^{-1}
$T = 293$ K
Block, colourless
0.32 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SAINT*; Bruker, 2001)
$T_{min} = 0.74$, $T_{max} = 0.78$
7453 measured reflections
2728 independent reflections
2331 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.2°$
$h = -9 \rightarrow 6$
$k = -15 \rightarrow 14$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.058$
$S = 1.01$
2728 reflections
178 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
$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.34$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cd1	0.0000	0.5000	0.0000	0.02725 (8)
C1	0.3962 (3)	0.60574 (17)	0.12383 (16)	0.0408 (5)
H1	0.4470	0.5971	0.0729	0.049*
C2	0.2078 (3)	0.60595 (15)	0.20672 (14)	0.0323 (5)

H2	0.1033	0.5975	0.2253	0.039*
C3	0.4819 (3)	0.64371 (17)	0.21155 (16)	0.0418 (5)
H3	0.5999	0.6653	0.2321	0.050*
C4	0.3888 (3)	0.67235 (16)	0.36600 (15)	0.0411 (5)
H4A	0.2794	0.7003	0.3757	0.049*
H4B	0.4784	0.7268	0.3818	0.049*
C5	0.4493 (3)	0.58124 (15)	0.43373 (14)	0.0300 (4)
C6	0.3967 (3)	0.47986 (15)	0.40840 (16)	0.0367 (5)
H6	0.3268	0.4656	0.3465	0.044*
C7	0.4469 (3)	0.39939 (16)	0.47405 (15)	0.0353 (5)
H7	0.4103	0.3317	0.4559	0.042*
C8	0.0724 (3)	0.33407 (15)	0.18324 (15)	0.0351 (5)
H8	0.1700	0.3061	0.1665	0.042*
C9	0.0320 (3)	0.31662 (16)	0.26739 (15)	0.0361 (5)
H9	0.0957	0.2760	0.3186	0.043*
C10	−0.1663 (3)	0.41959 (15)	0.17628 (14)	0.0340 (5)
H10	−0.2654	0.4624	0.1550	0.041*
C11	−0.2121 (3)	0.38072 (18)	0.33871 (15)	0.0434 (6)
H11A	−0.2346	0.3118	0.3606	0.052*
H11B	−0.3260	0.4149	0.3132	0.052*
C12	−0.1024 (3)	0.44253 (16)	0.42282 (14)	0.0338 (5)
C13	−0.0831 (3)	0.54885 (18)	0.41550 (15)	0.0413 (5)
H13	−0.1394	0.5825	0.3582	0.050*
C14	−0.0181 (3)	0.39392 (18)	0.50832 (14)	0.0401 (5)
H14	−0.0296	0.3223	0.5146	0.048*
Cl1	−0.23305 (7)	0.63726 (4)	0.02514 (4)	0.04181 (14)
N1	0.2237 (2)	0.58192 (13)	0.12087 (12)	0.0331 (4)
N2	0.3585 (2)	0.64392 (12)	0.26426 (12)	0.0330 (4)
N3	−0.0517 (2)	0.39902 (12)	0.12627 (12)	0.0338 (4)
N4	−0.1214 (2)	0.37075 (13)	0.26207 (11)	0.0327 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.03452 (13)	0.02730 (12)	0.02127 (12)	0.00197 (8)	0.00982 (9)	0.00096 (8)
C1	0.0377 (13)	0.0508 (13)	0.0369 (12)	0.0034 (11)	0.0151 (10)	0.0020 (10)
C2	0.0337 (12)	0.0325 (11)	0.0313 (11)	0.0002 (9)	0.0098 (9)	0.0016 (9)
C3	0.0301 (12)	0.0469 (13)	0.0461 (14)	−0.0008 (10)	0.0066 (11)	0.0077 (11)
C4	0.0568 (15)	0.0319 (11)	0.0292 (11)	−0.0001 (10)	0.0025 (11)	−0.0002 (9)
C5	0.0343 (11)	0.0285 (10)	0.0257 (10)	−0.0028 (8)	0.0058 (9)	0.0005 (8)
C6	0.0433 (13)	0.0334 (12)	0.0261 (11)	−0.0056 (9)	−0.0030 (10)	−0.0027 (9)
C7	0.0459 (13)	0.0266 (11)	0.0292 (10)	−0.0076 (9)	0.0029 (9)	−0.0031 (9)
C8	0.0409 (13)	0.0314 (11)	0.0353 (11)	0.0025 (9)	0.0140 (10)	0.0016 (9)
C9	0.0439 (13)	0.0341 (11)	0.0279 (11)	−0.0023 (10)	0.0057 (10)	0.0046 (9)
C10	0.0409 (12)	0.0328 (11)	0.0295 (11)	−0.0005 (9)	0.0120 (10)	−0.0002 (9)
C11	0.0512 (14)	0.0534 (14)	0.0322 (12)	−0.0177 (11)	0.0226 (11)	−0.0107 (10)
C12	0.0410 (13)	0.0368 (12)	0.0281 (11)	−0.0056 (10)	0.0171 (10)	−0.0057 (9)
C13	0.0535 (15)	0.0399 (13)	0.0289 (11)	0.0021 (11)	0.0081 (11)	0.0056 (10)

C14	0.0607 (16)	0.0270 (11)	0.0348 (12)	−0.0030 (10)	0.0169 (11)	0.0005 (9)
Cl1	0.0455 (3)	0.0355 (3)	0.0504 (3)	0.0090 (2)	0.0233 (3)	−0.0009 (2)
N1	0.0341 (10)	0.0366 (10)	0.0293 (9)	0.0022 (8)	0.0098 (8)	−0.0002 (7)
N2	0.0393 (10)	0.0302 (9)	0.0265 (9)	−0.0012 (8)	0.0035 (8)	0.0031 (7)
N3	0.0437 (11)	0.0325 (9)	0.0276 (9)	0.0018 (8)	0.0139 (8)	0.0038 (7)
N4	0.0427 (11)	0.0347 (9)	0.0235 (9)	−0.0087 (8)	0.0139 (8)	−0.0030 (7)

Geometric parameters (Å, º)

Cd1—N1^{i}	2.3546 (17)	C6—H6	0.9300
Cd1—N1	2.3546 (17)	C7—C5^{ii}	1.380 (3)
Cd1—N3	2.3561 (15)	C7—H7	0.9300
Cd1—N3^{i}	2.3561 (15)	C8—C9	1.352 (3)
Cd1—Cl1^{i}	2.6248 (5)	C8—N3	1.370 (3)
Cd1—Cl1	2.6248 (5)	C8—H8	0.9300
C1—C3	1.352 (3)	C9—N4	1.367 (3)
C1—N1	1.369 (3)	C9—H9	0.9300
C1—H1	0.9300	C10—N3	1.317 (2)
C2—N1	1.314 (2)	C10—N4	1.346 (2)
C2—N2	1.335 (3)	C10—H10	0.9300
C2—H2	0.9300	C11—N4	1.469 (2)
C3—N2	1.378 (3)	C11—C12	1.507 (3)
C3—H3	0.9300	C11—H11A	0.9700
C4—N2	1.468 (3)	C11—H11B	0.9700
C4—C5	1.514 (3)	C12—C13	1.379 (3)
C4—H4A	0.9700	C12—C14	1.380 (3)
C4—H4B	0.9700	C13—C14^{iii}	1.379 (3)
C5—C7^{ii}	1.380 (3)	C13—H13	0.9300
C5—C6	1.383 (3)	C14—C13^{iii}	1.379 (3)
C6—C7	1.384 (3)	C14—H14	0.9300
N1^{i}—Cd1—N1	180.00 (7)	C6—C7—H7	119.7
N1^{i}—Cd1—N3	94.57 (6)	C9—C8—N3	109.92 (19)
N1—Cd1—N3	85.43 (6)	C9—C8—H8	125.0
N1^{i}—Cd1—N3^{i}	85.43 (6)	N3—C8—H8	125.0
N1—Cd1—N3^{i}	94.57 (6)	C8—C9—N4	106.13 (18)
N3—Cd1—N3^{i}	180.00 (6)	C8—C9—H9	126.9
N1^{i}—Cd1—Cl1^{i}	90.04 (4)	N4—C9—H9	126.9
N1—Cd1—Cl1^{i}	89.96 (4)	N3—C10—N4	111.30 (19)
N3—Cd1—Cl1^{i}	90.40 (4)	N3—C10—H10	124.3
N3^{i}—Cd1—Cl1^{i}	89.60 (4)	N4—C10—H10	124.3
N1^{i}—Cd1—Cl1	89.96 (4)	N4—C11—C12	111.53 (17)
N1—Cd1—Cl1	90.04 (4)	N4—C11—H11A	109.3
N3—Cd1—Cl1	89.60 (4)	C12—C11—H11A	109.3
N3^{i}—Cd1—Cl1	90.40 (4)	N4—C11—H11B	109.3
Cl1^{i}—Cd1—Cl1	180.00 (2)	C12—C11—H11B	109.3
C3—C1—N1	110.09 (19)	H11A—C11—H11B	108.0
C3—C1—H1	125.0	C13—C12—C14	118.68 (18)

N1—C1—H1	125.0	C13—C12—C11	120.56 (19)
N1—C2—N2	112.35 (18)	C14—C12—C11	120.8 (2)
N1—C2—H2	123.8	C14^{iii}—C13—C12	121.08 (19)
N2—C2—H2	123.8	C14^{iii}—C13—H13	119.5
C1—C3—N2	105.90 (19)	C12—C13—H13	119.5
C1—C3—H3	127.0	C13^{iii}—C14—C12	120.2 (2)
N2—C3—H3	127.0	C13^{iii}—C14—H14	119.9
N2—C4—C5	113.02 (17)	C12—C14—H14	119.9
N2—C4—H4A	109.0	C2—N1—C1	105.06 (18)
C5—C4—H4A	109.0	C2—N1—Cd1	124.26 (14)
N2—C4—H4B	109.0	C1—N1—Cd1	130.41 (14)
C5—C4—H4B	109.0	C2—N2—C3	106.59 (17)
H4A—C4—H4B	107.8	C2—N2—C4	126.14 (18)
C7^{ii}—C5—C6	118.61 (17)	C3—N2—C4	127.12 (19)
C7^{ii}—C5—C4	118.82 (18)	C10—N3—C8	105.51 (16)
C6—C5—C4	122.48 (19)	C10—N3—Cd1	126.54 (13)
C5—C6—C7	120.8 (2)	C8—N3—Cd1	123.87 (13)
C5—C6—H6	119.6	C10—N4—C9	107.12 (16)
C7—C6—H6	119.6	C10—N4—C11	126.32 (19)
C5^{ii}—C7—C6	120.60 (19)	C9—N4—C11	126.38 (18)
C5^{ii}—C7—H7	119.7		

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