Di-µ-chlorido-bis{[1,2-bis(pyridin-2-ylmethoxy)benzene-$\kappa^4 N,O,O',N'$]-chloridocadmium}

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In centrosymmetric dinuclear title compound, [Cd₂Cl₄-(C₁₈H₁₆N₂O₂)₂], the Cd^{II} atom is seven-coordinated in a pentagonal–bipyramidal environment defined by two N atoms and two O atoms from one ligand and three Cl⁻ anions, two of which are bridging. A π–π interaction between adjacent pyridine rings [centroid–centroid distance = 3.773 (1) Å] further stablizes the dimer.

Related literature

For general background to flexible bipyridyl-based ligands, see: Wang *et al.* (2004); Oh *et al.* (2005). For the synthesis of the ligand, see: Liu *et al.* (2010a,b). For a related structure, see: Liu *et al.* (2011).
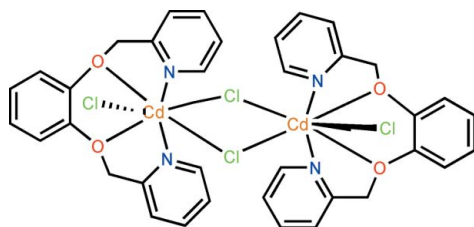
Experimental

Crystal data

[Cd₂Cl₄(C₁₈H₁₆N₂O₂)₂] $M_r = 951.26$

Monoclinic, $P2_1/c$
$a = 10.833$ (2) Å
$b = 10.968$ (2) Å
$c = 16.095$ (3) Å
$\beta = 109.14$ (3)°
$V = 1806.6$ (6) Å³

$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.52$ mm⁻¹
$T = 293$ K
$0.23 \times 0.22 \times 0.20$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.722$, $T_{max} = 0.751$

17295 measured reflections
4128 independent reflections
3686 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.048$
$S = 1.05$
4128 reflections

226 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.36$ e Å⁻³
$\Delta\rho_{min} = -0.24$ e Å⁻³

Table 1
Selected bond lengths (Å).

Cd1—N2	2.3920 (15)	Cd1—Cl1	2.6197 (6)
Cd1—N1	2.3958 (15)	Cd1—O2	2.6288 (14)
Cd1—Cl2	2.5103 (6)	Cd1—Cl1^i	2.6873 (11)
Cd1—O1	2.6197 (14)		

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); 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: *SHELXL97*.

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supporting information

Di-*μ*-chlorido-bis{[1,2-bis(pyridin-2-ylmethoxy)benzene-*κ*⁴*N,O,O′,N′*]chloridocadmium}

Jin-Sheng Gao, Ying-Hui Yu, Ying Liu and Guang-Feng Hou

S1. Comment

Aromatic molecules containing two pyridyl groups have been widely used as building blocks for new supramolecular architectures in recent years. Compared with rigid bridging ligands, flexible bipyridine ligands are able to generate some unusual frameworks (Wang *et al.*, 2004; Oh *et al.*, 2005). In continuation of previous works (Liu *et al.*, 2010*a*; 2010*b*), we report the crystal structure of the title compound.

In centrosymmetric dinuclear [CdCl2(C18H16N2O2)]2, the CdII atom is seven-coordinated in a pentagonal bipyramidal environment defined by two N atoms and two O atoms from one ligand and three chlorides. Two of chlorides serve are bridging. A π—π interaction between adjacent pyridine rings [center to center distance 3.773?(1)?Å] further stablizes the dimer (Fig. 1, Table 1).

S2. Experimental

The 1,2-bis(pyridin-2-ylmethoxy)benzene ligand was synthesized according to a literature method (Liu *et al.*,2010*a*). A solution of CdCl2·5H2O (0.2 mmol,0.0456 g) in water (2 ml) was added to a solution of the ligand (0.2 mmol, 0.0584 g) in 5 ml methanol under constant stirring; the solution was stirred for about 1 hour and then filted. The filtate was maintained for about one week under room temperature to give colorless block-like crystals.

S3. Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic); C—H = 0.97 Å (methylene), and with U_{iso}(H) = 1.2U_{eq}(C).
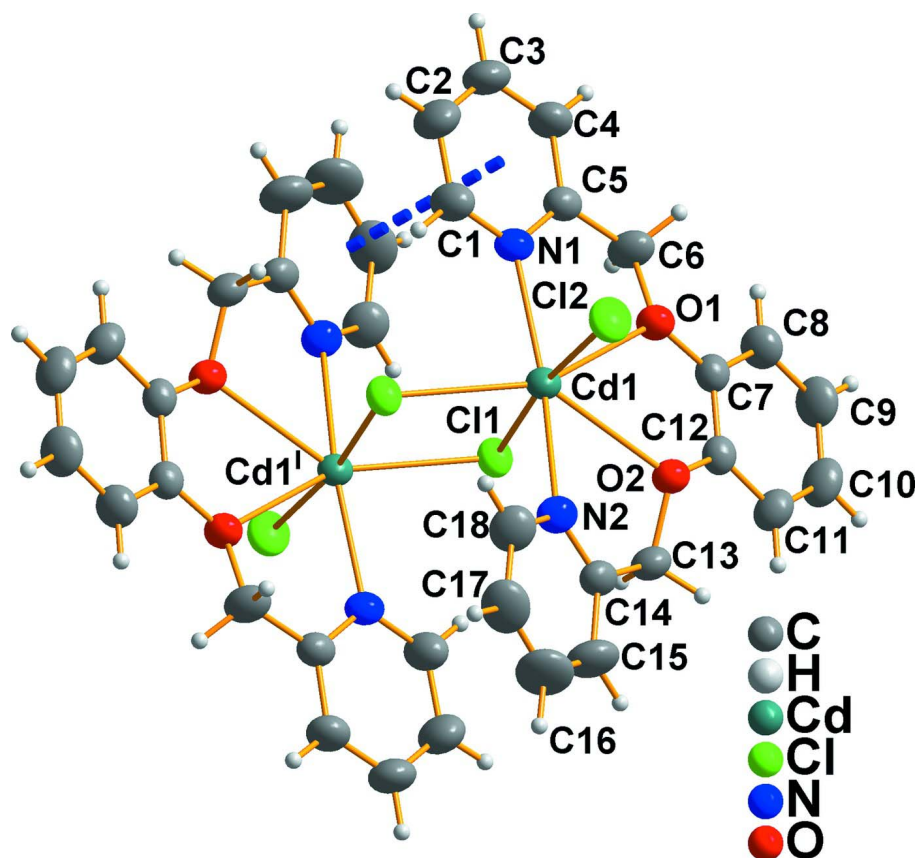
Figure 1

The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level for non-H atoms. Symmetry codes: (I) -x+1,-y+1,1-z.

Di-*µ*-chlorido-bis{[1,2-bis(pyridin-2-ylmethoxy)benzene- *κ*⁴*N*,*O*,*O′*,*N′*]chloridocadmium}

Crystal data

[Cd₂Cl₄(C₁₈H₁₆N₂O₂)₂]	$F(000) = 944$
$M_r = 951.26$	$D_x = 1.749$ Mg m⁻³
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 15418 reflections
$a = 10.833$ (2) Å	$\theta = 3.3–27.5°$
$b = 10.968$ (2) Å	$\mu = 1.52$ mm⁻¹
$c = 16.095$ (3) Å	$T = 293$ K
$\beta = 109.14$ (3)°	Bolck, colorless
$V = 1806.6$ (6) Å³	$0.23 × 0.22 × 0.20$ mm
$Z = 2$	

Data collection

Rigaku R-AXIS RAPID diffractometer	17295 measured reflections
Radiation source: fine-focus sealed tube	4128 independent reflections
Graphite monochromator	3686 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.021$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
	$h = −14{\rightarrow}13$
$T_{min} = 0.722$, $T_{max} = 0.751$	$k = −14{\rightarrow}14$
	$l = −20{\rightarrow}20$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.019$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.048$	
$S = 1.05$	H-atom parameters constrained
4128 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0229P)^2 + 0.5495P]$ where $P = (F_o^2 + 2F_c^2)/3$
226 parameters	
0 restraints	$(\Delta/\sigma)_{max} = 0.002$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.36$ e Å^{-3}
	$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.6708 (2)	0.4345 (2)	0.34515 (14)	0.0565 (5)
H1	0.5939	0.4787	0.3220	0.068*
C2	0.7136 (2)	0.3659 (3)	0.28896 (15)	0.0679 (7)
H2	0.6668	0.3642	0.2291	0.081*
C3	0.8267 (2)	0.2998 (2)	0.32244 (16)	0.0660 (6)
H3	0.8573	0.2515	0.2859	0.079*
C4	0.8935 (2)	0.3064 (2)	0.41076 (15)	0.0546 (5)
H4	0.9708	0.2631	0.4350	0.065*
C5	0.84454 (17)	0.37838 (17)	0.46357 (13)	0.0406 (4)
C6	0.9171 (2)	0.3807 (2)	0.55999 (13)	0.0516 (5)
H6A	0.8960	0.3081	0.5870	0.062*
H6B	1.0103	0.3801	0.5696	0.062*
C7	0.93736 (16)	0.48931 (16)	0.69088 (11)	0.0376 (4)
C8	1.0417 (2)	0.41839 (18)	0.73965 (14)	0.0507 (5)
H8	1.0810	0.3649	0.7111	0.061*
C9	1.0880 (2)	0.4263 (2)	0.83053 (15)	0.0565 (5)
H9	1.1587	0.3788	0.8628	0.068*
C10	1.0299 (2)	0.5037 (2)	0.87260 (13)	0.0554 (5)
H10	1.0605	0.5081	0.9337	0.066*
C11	0.9252 (2)	0.57610 (18)	0.82491 (13)	0.0473 (4)
H11	0.8860	0.6286	0.8542	0.057*
C12	0.87928 (17)	0.57023 (15)	0.73393 (12)	0.0367 (4)
C13	0.68776 (19)	0.68425 (18)	0.72191 (12)	0.0440 (4)
H13A	0.7328	0.7322	0.7736	0.053*
H13B	0.6476	0.6149	0.7404	0.053*

C14	0.58438 (17)	0.76039 (16)	0.65859 (12)	0.0417 (4)
C15	0.5092 (3)	0.8376 (2)	0.69083 (17)	0.0681 (7)
H15	0.5224	0.8415	0.7508	0.082*
C16	0.4150 (3)	0.9084 (2)	0.6327 (2)	0.0826 (9)
H16	0.3629	0.9600	0.6529	0.099*
C17	0.3989 (2)	0.9021 (2)	0.5454 (2)	0.0685 (7)
H17	0.3379	0.9513	0.5052	0.082*
C18	0.4747 (2)	0.82148 (18)	0.51789 (16)	0.0546 (5)
H18	0.4632	0.8167	0.4581	0.066*
Cd1	0.660311 (11)	0.587855 (10)	0.515336 (7)	0.03233 (5)
Cl1	0.57974 (4)	0.42461 (4)	0.60476 (3)	0.03852 (9)
Cl2	0.76064 (5)	0.75247 (5)	0.44987 (3)	0.05070 (12)
N1	0.73405 (15)	0.44122 (14)	0.43174 (10)	0.0401 (3)
N2	0.56444 (15)	0.74944 (13)	0.57321 (10)	0.0410 (3)
O1	0.88495 (11)	0.48583 (11)	0.60035 (8)	0.0393 (3)
O2	0.77949 (11)	0.64229 (11)	0.68148 (8)	0.0375 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0481 (11)	0.0767 (15)	0.0439 (11)	0.0117 (11)	0.0142 (9)	−0.0047 (10)
C2	0.0637 (14)	0.0959 (18)	0.0434 (12)	0.0060 (14)	0.0166 (10)	−0.0174 (12)
C3	0.0620 (13)	0.0842 (17)	0.0582 (13)	0.0049 (13)	0.0282 (11)	−0.0254 (12)
C4	0.0476 (11)	0.0610 (12)	0.0578 (12)	0.0089 (10)	0.0210 (10)	−0.0143 (10)
C5	0.0395 (9)	0.0410 (9)	0.0452 (10)	−0.0007 (8)	0.0190 (8)	−0.0059 (8)
C6	0.0551 (12)	0.0526 (11)	0.0460 (11)	0.0186 (10)	0.0150 (9)	−0.0048 (9)
C7	0.0344 (8)	0.0401 (9)	0.0367 (9)	−0.0027 (7)	0.0097 (7)	0.0005 (7)
C8	0.0434 (10)	0.0517 (11)	0.0524 (11)	0.0103 (9)	0.0095 (9)	0.0008 (9)
C9	0.0483 (11)	0.0593 (13)	0.0507 (12)	0.0091 (10)	0.0012 (9)	0.0092 (10)
C10	0.0581 (12)	0.0618 (13)	0.0368 (10)	−0.0025 (11)	0.0027 (9)	0.0034 (9)
C11	0.0530 (11)	0.0480 (10)	0.0374 (9)	−0.0011 (9)	0.0099 (8)	−0.0043 (8)
C12	0.0348 (8)	0.0355 (8)	0.0373 (9)	−0.0031 (7)	0.0085 (7)	0.0007 (7)
C13	0.0471 (10)	0.0507 (10)	0.0361 (9)	0.0023 (9)	0.0160 (8)	−0.0081 (8)
C14	0.0413 (9)	0.0377 (9)	0.0487 (10)	−0.0033 (8)	0.0184 (8)	−0.0117 (8)
C15	0.0770 (16)	0.0662 (14)	0.0667 (15)	0.0145 (13)	0.0311 (13)	−0.0216 (12)
C16	0.0782 (18)	0.0681 (16)	0.104 (2)	0.0297 (14)	0.0327 (17)	−0.0219 (15)
C17	0.0594 (14)	0.0456 (12)	0.0910 (19)	0.0189 (11)	0.0119 (13)	−0.0043 (12)
C18	0.0595 (12)	0.0414 (10)	0.0585 (12)	0.0116 (10)	0.0132 (10)	0.0016 (9)
Cd1	0.03316 (7)	0.03389 (7)	0.03234 (7)	0.00016 (5)	0.01399 (5)	0.00062 (5)
Cl1	0.0354 (2)	0.0422 (2)	0.0366 (2)	−0.00347 (17)	0.00993 (16)	0.00500 (17)
Cl2	0.0531 (3)	0.0566 (3)	0.0449 (2)	−0.0115 (2)	0.0195 (2)	0.0106 (2)
N1	0.0396 (8)	0.0453 (8)	0.0383 (8)	0.0041 (7)	0.0168 (6)	−0.0027 (6)
N2	0.0439 (8)	0.0360 (7)	0.0436 (8)	0.0059 (7)	0.0148 (7)	−0.0010 (6)
O1	0.0369 (6)	0.0421 (6)	0.0380 (6)	0.0080 (5)	0.0109 (5)	−0.0019 (5)
O2	0.0389 (6)	0.0393 (6)	0.0345 (6)	0.0039 (5)	0.0124 (5)	−0.0020 (5)

Geometric parameters (Å, º)

C1—N1	1.338 (3)	C11—H11	0.9300
C1—C2	1.368 (3)	C12—O2	1.381 (2)
C1—H1	0.9300	C13—O2	1.431 (2)
C2—C3	1.373 (3)	C13—C14	1.497 (3)
C2—H2	0.9300	C13—H13A	0.9700
C3—C4	1.369 (3)	C13—H13B	0.9700
C3—H3	0.9300	C14—N2	1.325 (2)
C4—C5	1.387 (3)	C14—C15	1.388 (3)
C4—H4	0.9300	C15—C16	1.376 (4)
C5—N1	1.330 (2)	C15—H15	0.9300
C5—C6	1.492 (3)	C16—C17	1.360 (4)
C6—O1	1.422 (2)	C16—H16	0.9300
C6—H6A	0.9700	C17—C18	1.376 (3)
C6—H6B	0.9700	C17—H17	0.9300
C7—O1	1.380 (2)	C18—N2	1.339 (3)
C7—C8	1.385 (3)	C18—H18	0.9300
C7—C12	1.396 (2)	Cd1—N2	2.3920 (15)
C8—C9	1.385 (3)	Cd1—N1	2.3958 (15)
C8—H8	0.9300	Cd1—Cl2	2.5103 (6)
C9—C10	1.362 (3)	Cd1—O1	2.6197 (14)
C9—H9	0.9300	Cd1—Cl1	2.6197 (6)
C10—C11	1.391 (3)	Cd1—O2	2.6288 (14)
C10—H10	0.9300	Cd1—Cl1[i]	2.6873 (11)
C11—C12	1.385 (3)	Cl1—Cd1[i]	2.6873 (11)
N1—C1—C2	123.4 (2)	C15—C14—C13	119.04 (19)
N1—C1—H1	118.3	C16—C15—C14	119.0 (2)
C2—C1—H1	118.3	C16—C15—H15	120.5
C1—C2—C3	118.9 (2)	C14—C15—H15	120.5
C1—C2—H2	120.6	C17—C16—C15	119.3 (2)
C3—C2—H2	120.6	C17—C16—H16	120.3
C4—C3—C2	118.7 (2)	C15—C16—H16	120.3
C4—C3—H3	120.7	C16—C17—C18	118.5 (2)
C2—C3—H3	120.7	C16—C17—H17	120.8
C3—C4—C5	119.2 (2)	C18—C17—H17	120.8
C3—C4—H4	120.4	N2—C18—C17	123.0 (2)
C5—C4—H4	120.4	N2—C18—H18	118.5
N1—C5—C4	122.40 (18)	C17—C18—H18	118.5
N1—C5—C6	119.51 (16)	N2—Cd1—N1	169.53 (5)
C4—C5—C6	118.06 (17)	N2—Cd1—Cl2	86.19 (4)
O1—C6—C5	111.39 (16)	N1—Cd1—Cl2	88.69 (4)
O1—C6—H6A	109.3	N2—Cd1—O1	124.10 (5)
C5—C6—H6A	109.3	N1—Cd1—O1	65.35 (5)
O1—C6—H6B	109.3	Cl2—Cd1—O1	94.05 (3)
C5—C6—H6B	109.3	N2—Cd1—Cl1	91.55 (4)
H6A—C6—H6B	108.0	N1—Cd1—Cl1	94.72 (4)

O1—C7—C8	124.05 (17)	Cl2—Cd1—Cl1	171.978 (16)
O1—C7—C12	116.44 (15)	O1—Cd1—Cl1	80.84 (3)
C8—C7—C12	119.51 (17)	N2—Cd1—O2	64.32 (5)
C7—C8—C9	120.6 (2)	N1—Cd1—O2	125.51 (5)
C7—C8—H8	119.7	Cl2—Cd1—O2	97.34 (3)
C9—C8—H8	119.7	O1—Cd1—O2	60.22 (4)
C10—C9—C8	119.8 (2)	Cl1—Cd1—O2	74.77 (3)
C10—C9—H9	120.1	N2—Cd1—Cl1ⁱ	82.91 (4)
C8—C9—H9	120.1	N1—Cd1—Cl1ⁱ	89.09 (4)
C9—C10—C11	120.51 (19)	Cl2—Cd1—Cl1ⁱ	100.64 (2)
C9—C10—H10	119.7	O1—Cd1—Cl1ⁱ	150.24 (3)
C11—C10—H10	119.7	Cl1—Cd1—Cl1ⁱ	86.69 (2)
C12—C11—C10	120.13 (19)	O2—Cd1—Cl1ⁱ	141.26 (3)
C12—C11—H11	119.9	Cd1—Cl1—Cd1ⁱ	93.31 (2)
C10—C11—H11	119.9	C5—N1—C1	117.47 (16)
O2—C12—C11	123.89 (16)	C5—N1—Cd1	123.73 (12)
O2—C12—C7	116.75 (15)	C1—N1—Cd1	118.10 (13)
C11—C12—C7	119.34 (17)	C14—N2—C18	118.17 (17)
O2—C13—C14	110.24 (15)	C14—N2—Cd1	121.82 (12)
O2—C13—H13A	109.6	C18—N2—Cd1	119.42 (13)
C14—C13—H13A	109.6	C7—O1—C6	115.30 (14)
O2—C13—H13B	109.6	C7—O1—Cd1	121.99 (10)
C14—C13—H13B	109.6	C6—O1—Cd1	115.63 (11)
H13A—C13—H13B	108.1	C12—O2—C13	115.29 (13)
N2—C14—C15	121.80 (19)	C12—O2—Cd1	121.12 (10)
N2—C14—C13	119.12 (15)	C13—O2—Cd1	110.67 (10)

Symmetry code: (i) −x+1, −y+1, −z+1.