Poly[[μ2-1,4-bis(4,5-dihydro-1,3-oxazol-2-yl)benzene-$\kappa^2N:N'$]di-μ2-chlorido-cadmium]

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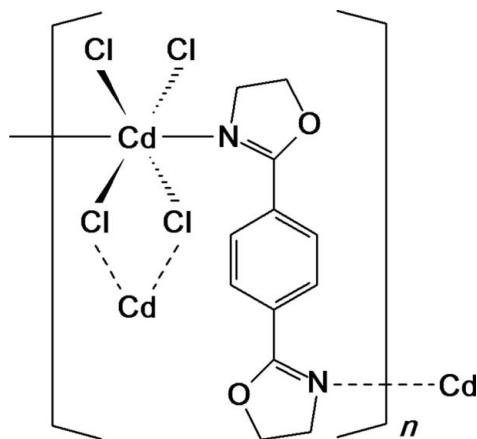Correspondence e-mail: sun@nanya.edu.tw

In the title coordination polymer, $[CdCl_2(C_{12}H_{12}N_2O_2)]_n$, the Cd^{II} ion, situated on an inversion center, is coordinated by four bridging Cl atoms and two N atoms from two 1,4-bis(4,5-dihydro-1,3-oxazol-2-yl)benzene (L) ligands in a distorted octahedral geometry. Each L ligand also lies across an inversion center and bridges two Cd^{II} ions, forming infinite two-dimensional rectangular layers running parallel to (010).

Related literature

For background to coordination polymers with organic ligands, see: Kitagawa *et al.* (2004); Chiang *et al.* (2008); Yeh *et al.* (2008, 2009); Hsu *et al.* (2009). For Cd^{II} coordination polymers, see Suen *et al.* (2007*a*,*b*). For related structures, see: Wang *et al.* (2008).

Experimental

Crystal data

$[CdCl_2(C_{12}H_{12}N_2O_2)]$	γ = 84.002 (2)°
M_r = 399.54	V = 311.30 (5) Å^3
Triclinic, $P\bar{1}$	Z = 1
a = 3.9242 (4) Å	Mo $K\alpha$ radiation
b = 8.0290 (8) Å	μ = 2.18 mm^{-1}
c = 10.0778 (10) Å	T = 297 K
α = 84.632 (2)°	0.50 × 0.50 × 0.07 mm
β = 81.458 (2)°	

Data collection

Bruker SMART CCD area-detector diffractometer	1779 measured reflections
	1209 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	1204 reflections with $I > 2\sigma(I)$
T_{min} = 0.319, T_{max} = 0.862	R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044	88 parameters
$wR(F^2)$ = 0.125	H-atom parameters constrained
S = 1.13	$\Delta\rho_{max}$ = 0.93 e Å^{-3}
1209 reflections	$\Delta\rho_{min}$ = −1.80 e Å^{-3}

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: DAIMOND (Brandenburg, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GW2103).

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supporting information

Poly[[*μ*₂-1,4-bis(4,5-dihydro-1,3-oxazol-2-yl)benzene-*κ²N*:*N′*]di-*μ*₂-chlorido-cadmium]

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S1. Comment

The synthesis of metal coordination polymers has been a subject of intense research due to their interesting structural chemistry and potential applications in gas storage, separation, catalysis, magnetism, luminescence, and drug delivery (Kitagawa *et al.*, 2004). Roles of anion, solvent and ligand comformations in self-assembly of coordination complexes containing polydentate nitrogen ligands are very intersting (Chiang *et al.*, 2008; Yeh *et al.*, 2008; Hsu *et al.*, 2009; Yeh *et al.*, 2009). The Cd^{II} complexes containing polydentate ligands showing various type frameworks are also reported (Suen *et al.*, 2007*a*,b). The Ag(I) complexes containing 1,4-bis(4,5-dihydro-2-oxazolyl)benzene (*L*) ligands has been reported, which show various two-dimensional networks (Wang *et al.*, 2008). The Cd^{2+} cations are sixcoordinated with four Cl atoms and two N atoms from two *L* ligands (Fig. 1). The Cd···Cd distances separated by the bridging *L* ligands and Cl atoms are 10.257 (1) and 3.924 (1) Å, while the ligands adopt the *anti* conformation in the structure (Fig. 2).

S2. Experimental

An aqueous solution (5.0 ml) of cadmium chloride (1.0 mmol) was layered carefully over a methanolic solution (5.0 ml) of 1,4-bis(4,5-dihydro-2-oxazolyl)benzene (1.0 mmol) in a tube. Colourless crystals were obtained after several weeks. These were washed with methanol and collected in 65.2% yield.

S3. Refinement

H atoms were constrained to ideal geometries, with C—H = 0.93 (phenyl) or 0.97 (methylene) Å and U_{iso}(H) = 1.2U_{eq}(C).
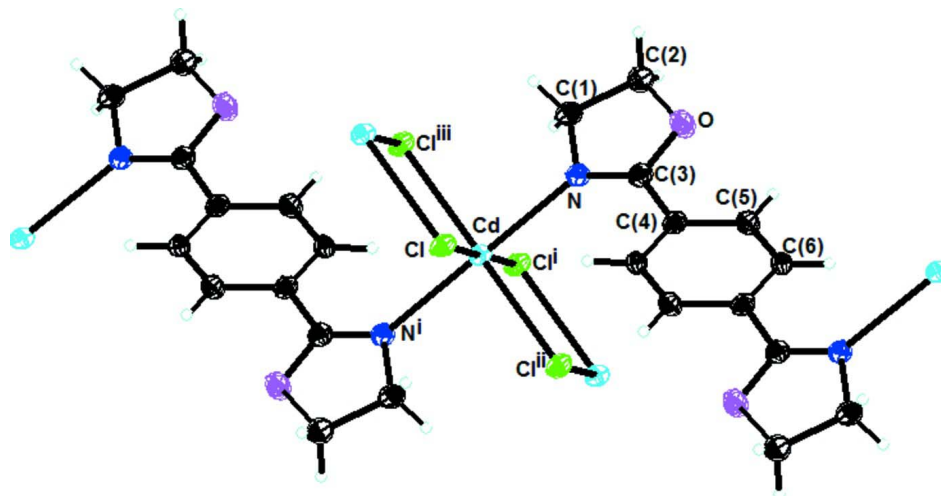
Figure 1

A portion of the two-dimensional net. Ellipsoids are drawn at 30% probability level, and H atoms of spheres of arbitrary radius. Symmetry codes: (i) $1 - x$, $1 - y$, $1 - z$; (ii) $x - 1$, y, z.
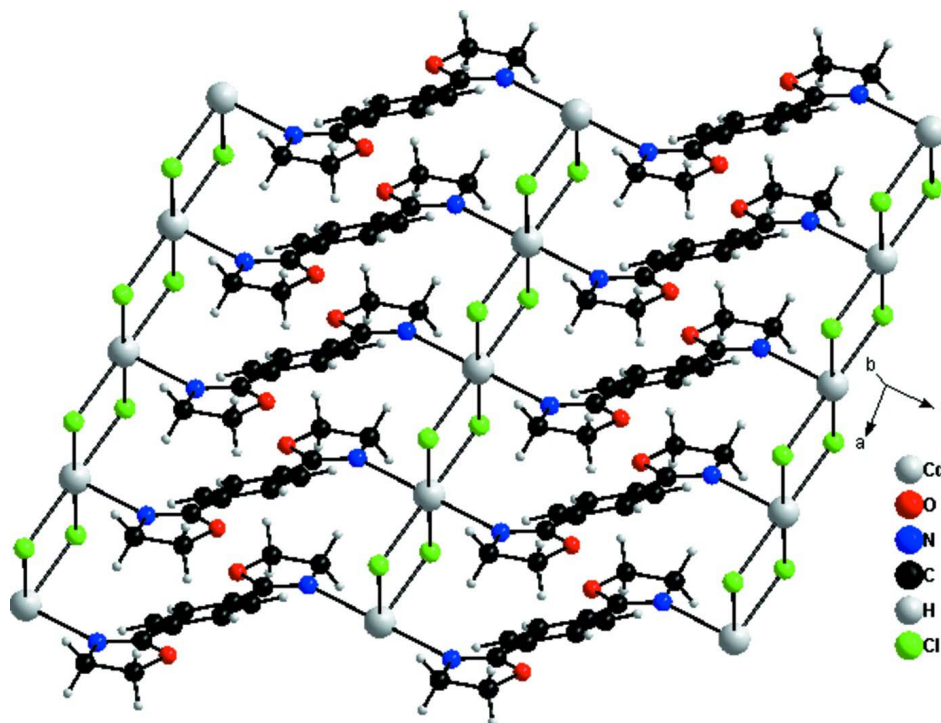
Figure 2

A drawing of the two-dimensional rectangular net.

Poly[[μ$_2$-1,4-bis(4,5-dihydro-1,3-oxazol-2-yl)benzene- κ^{2}N:N′]di-μ$_2$-chlorido-cadmium]

Crystal data

[CdCl$_2$(C$_{12}$H$_{12}$N$_2$O$_2$)]	Hall symbol: -P 1
$M_r = 399.54$	$a = 3.9242$ (4) Å
Triclinic, $P\overline{1}$	$b = 8.0290$ (8) Å

$c = 10.0778\ (10)$ Å

$\alpha = 84.632\ (2)°$

$\beta = 81.458\ (2)°$

$\gamma = 84.002\ (2)°$

$V = 311.30\ (5)$ Å^3

$Z = 1$

$F(000) = 196$

$D_x = 2.131$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 1711 reflections

$\theta = 2.6$–$26.0°$

$\mu = 2.18$ mm^{-1}

$T = 297$ K

Parallelepiped, colourless

$0.50 \times 0.50 \times 0.07$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 1997)

$T_{min} = 0.319$, $T_{max} = 0.862$

1779 measured reflections

1209 independent reflections

1204 reflections with $I > 2\sigma(I)$

$R_{int} = 0.029$

$\theta_{max} = 26.0°$, $\theta_{min} = 2.1°$

$h = -2\rightarrow4$

$k = -9\rightarrow9$

$l = -12\rightarrow12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.125$

$S = 1.13$

1209 reflections

88 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

$w = 1/[\sigma^2(F_o^2) + (0.110P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.93$ e Å^{-3}

$\Delta\rho_{min} = -1.80$ 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}
Cd	0.5000	0.5000	0.5000	0.0206 (2)
Cl	0.9164 (2)	0.67051 (12)	0.60009 (9)	0.0232 (3)
O	0.2884 (9)	0.1013 (4)	0.8636 (3)	0.0366 (7)
N	0.4705 (9)	0.2869 (4)	0.6933 (3)	0.0214 (6)
C1	0.6062 (11)	0.1199 (4)	0.6473 (4)	0.0276 (8)
H1A	0.8569	0.1106	0.6290	0.033*
H1B	0.5150	0.1001	0.5663	0.033*
C2	0.4811 (12)	−0.0049 (5)	0.7647 (4)	0.0319 (9)
H2A	0.3342	−0.0813	0.7368	0.038*

H2B	0.6751	−0.0698	0.8001	0.038*
C3	0.3089 (9)	0.2623 (4)	0.8112 (4)	0.0226 (7)
C4	0.1447 (9)	0.3868 (4)	0.9047 (3)	0.0207 (7)
C5	0.2302 (9)	0.5530 (4)	0.8878 (3)	0.0217 (7)
H5A	0.3857	0.5879	0.8141	0.026*
C6	0.0839 (9)	0.6652 (4)	0.9805 (3)	0.0217 (7)
H6A	0.1363	0.7764	0.9673	0.026*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd	0.0178 (3)	0.0218 (3)	0.0219 (3)	0.00137 (19)	−0.00280 (19)	−0.00334 (19)
Cl	0.0209 (5)	0.0258 (5)	0.0226 (5)	0.0017 (4)	−0.0016 (4)	−0.0068 (4)
O	0.051 (2)	0.0240 (13)	0.0264 (13)	0.0061 (13)	0.0120 (13)	0.0015 (10)
N	0.0240 (15)	0.0221 (15)	0.0168 (14)	0.0029 (11)	−0.0019 (11)	−0.0025 (11)
C1	0.031 (2)	0.0227 (17)	0.0263 (18)	0.0054 (14)	0.0015 (15)	−0.0046 (14)
C2	0.038 (2)	0.0235 (18)	0.0291 (19)	0.0043 (16)	0.0064 (16)	−0.0031 (15)
C3	0.0192 (17)	0.0231 (17)	0.0253 (17)	−0.0002 (13)	−0.0031 (13)	−0.0015 (12)
C4	0.0200 (17)	0.0240 (16)	0.0176 (15)	0.0024 (13)	−0.0023 (12)	−0.0044 (12)
C5	0.0225 (17)	0.0238 (16)	0.0167 (16)	0.0007 (14)	0.0000 (12)	0.0015 (12)
C6	0.0269 (19)	0.0183 (15)	0.0193 (17)	−0.0018 (13)	−0.0023 (13)	−0.0005 (12)

Geometric parameters (Å, º)

Cd—N^i	2.467 (3)	C1—H1A	0.9700
Cd—N	2.467 (3)	C1—H1B	0.9700
Cd—Cl	2.6035 (10)	C2—H2A	0.9700
Cd—Cl^i	2.6035 (10)	C2—H2B	0.9700
Cd—Cl^{ii}	2.6557 (9)	C3—C4	1.471 (5)
Cd—Cl^{iii}	2.6557 (9)	C4—C5	1.398 (5)
Cl—Cd^{iv}	2.6557 (9)	C4—C6^v	1.413 (5)
O—C3	1.355 (4)	C5—C6	1.380 (5)
O—C2	1.447 (4)	C5—H5A	0.9300
N—C3	1.269 (5)	C6—C4^v	1.413 (5)
N—C1	1.480 (4)	C6—H6A	0.9300
C1—C2	1.534 (5)		
N^i—Cd—N	180.000 (1)	C2—C1—H1A	110.9
N^i—Cd—Cl	87.04 (8)	N—C1—H1B	110.9
N—Cd—Cl	92.96 (8)	C2—C1—H1B	110.9
N^i—Cd—Cl^i	92.96 (8)	H1A—C1—H1B	108.9
N—Cd—Cl^i	87.04 (8)	O—C2—C1	103.7 (3)
Cl—Cd—Cl^i	180.000 (1)	O—C2—H2A	111.0
N^i—Cd—Cl^{ii}	87.28 (7)	C1—C2—H2A	111.0
N—Cd—Cl^{ii}	92.72 (7)	O—C2—H2B	111.0
Cl—Cd—Cl^{ii}	96.51 (3)	C1—C2—H2B	111.0
Cl^i—Cd—Cl^{ii}	83.49 (3)	H2A—C2—H2B	109.0
N^i—Cd—Cl^{iii}	92.72 (7)	N—C3—O	117.9 (3)

N—Cd—Cl^{iii}	87.28 (7)	N—C3—C4	128.7 (3)
Cl—Cd—Cl^{iii}	83.49 (3)	O—C3—C4	113.4 (3)
Cl^{i}—Cd—Cl^{iii}	96.51 (3)	C5—C4—C6^{v}	119.2 (3)
Cl^{ii}—Cd—Cl^{iii}	180.000 (1)	C5—C4—C3	121.3 (3)
Cd—Cl—Cd^{iv}	96.51 (3)	C6^{v}—C4—C3	119.3 (3)
C3—O—C2	106.9 (3)	C6—C5—C4	120.0 (3)
C3—N—C1	107.0 (3)	C6—C5—H5A	120.0
C3—N—Cd	140.4 (2)	C4—C5—H5A	120.0
C1—N—Cd	109.9 (2)	C5—C6—C4^{v}	120.8 (3)
N—C1—C2	104.5 (3)	C5—C6—H6A	119.6
N—C1—H1A	110.9	C4^{v}—C6—H6A	119.6

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*−1, *y*, *z*; (iii) −*x*+2, −*y*+1, −*z*+1; (iv) *x*+1, *y*, *z*; (v) −*x*, −*y*+1, −*z*+2.