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Dichloro(*N,N*-dimethylethylenediamine)-cadmium(II): a novel two-dimensional chloro-bridged coordination polymer

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.015 Å
R factor = 0.046
wR factor = 0.124
Data-to-parameter ratio = 18.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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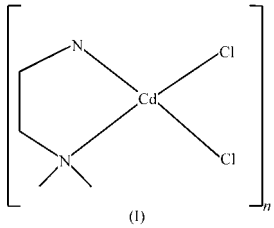
Polymeric dichloro(*N,N*-dimethylethylenediamine)cadmium-(II), $[CdCl_2(C_4H_{12}N_2)]_n$, has been synthesized and characterized by single-crystal X-ray diffraction. The two-dimensional polymeric sheet structure involves 12-membered zigzag rings formed by chloro bridges.

Comment

With the development of the inorganic coordination chemistry of supramolecular and polymeric networks, there has been a growing interest in the synthesis of coordination polymers, using various ligands which can provide inner cavities or networks of a desired size (Jung *et al.*, 1998; Tapas *et al.*, 2001; Gable *et al.*, 1990). As a terminal ligand, *N,N*-dimethylethylenediamine can form supramolecular complexes with other bridging ligands, such as azide and thiocyanate (Mondal *et al.*, 2000).



(I)

In this paper, we describe the chloro-bridged two-dimensional polymeric sheet structure of the cadmium complex polymeric dichloro(*N,N*-dimethylethylenediamine)cadmium-(II), (I).

The structure of (I) is shown in Fig. 1. Tables 1 and 2 list selected geometrical and hydrogen-bond data. The Cd atom in the polymer is in a distorted octahedral environment, coordinated by one bidentate amine ligand and four Cl atoms. Each unit of the complex consists of a $[Cd(dmen)]^{2+}$ cation (dmen is *N,N*-dimethylethylenediamine) with two monochloro and one dichloro bridging groups. Cd—Cd distances of 4.800 (3) and 3.873 (3) Å strongly suggest that no direct Cd—Cd bond interaction is present in this structure. The Cd—Cl distances are in the range 2.533 (3)–2.748 (3) Å. The two-dimensional polymeric sheets of the complex are shown in Fig. 2. The dimeric subunit that is formed by a dichloro bridge is further linked to neighbouring molecules by two monochloro bridges. Because of the difference between the chloro bridges, a 12-membered zigzag ring, as well as a four-membered ring, are formed (Fig. 3). There are three real Cd···Cd diagonals dividing the rings exactly into two halves, the longer diagonal is 10.015 Å (Cd1*B*···Cd1*E*) and two shorter ones are 6.821 (Cd1···Cd1*D*) and 8.607 Å (Cd1*A*···Cd1*C*). There is a hydrogen bond of length 3.300 (8) Å involving N1 of the

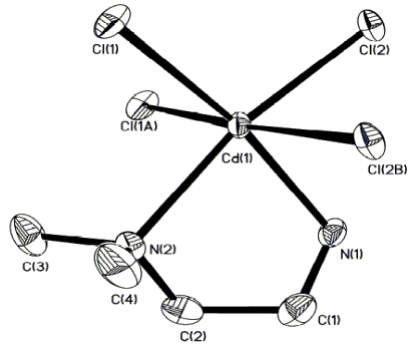


Figure 1
A view of the molecular structure of the title complex, with the atom-numbering scheme and 30% displacement ellipsoids. H atoms are not shown.

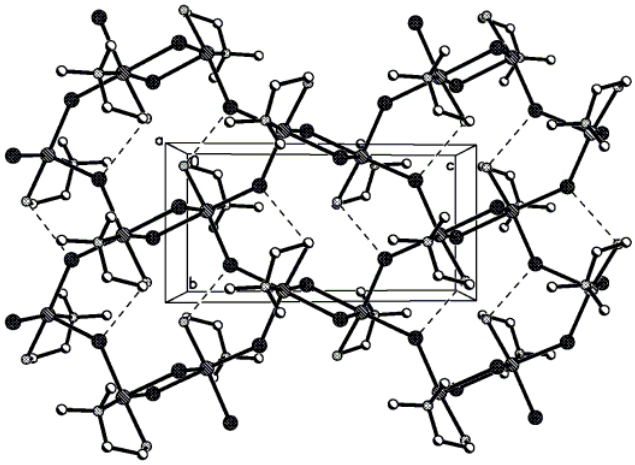


Figure 2
The two-dimensional polymeric sheet of the title complex.

terminal ligand as donor and Cl1^{iii} as acceptor. The second H atom on N1 does not participate in any hydrogen bonding.

Experimental

Dmen (0.5 mmol) in 10 ml MeOH was added to a solution of $CdCl_2{\cdot}2.5H_2O$ (0.5 mmol) in 5 ml MeOH and 1 ml H_2O. Colourless single crystals suitable for X-ray analysis were separated after several weeks.

Crystal data

$[CdCl_2(C_4H_{12}N_2)]$
M_r = 271.46
Monoclinic, $P2_1/c$
a = 9.455 (9) Å
b = 6.731 (6) Å
c = 13.399 (12) Å
β = 97.002 (15)°
V = 846.3 (13) Å^3
Z = 4
D_x = 2.130 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3239 reflections
θ = 2.2–25.0°
μ = 3.13 mm^{-1}
T = 293 (2) K
Rhombic block, colourless
0.25 × 0.20 × 0.15 mm

Data collection

Bruker SMART 1K CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.508, T_{max} = 0.651
3239 measured reflections
1484 independent reflections
1172 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 25.0°
$h = -11 \rightarrow 11$
$k = -8 \rightarrow 7$
$l = -8 \rightarrow 15$

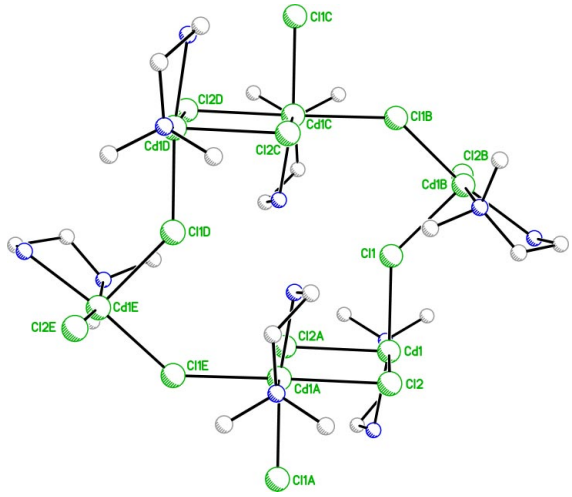


Figure 3
A view of the structure of the title complex, showing the 12-membered and four-membered rings that form the polymer.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.125
S = 1.10
1484 reflections
82 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0724P)^2 + 0.5378P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.013
$\Delta\rho_{max}$ = 1.01 e Å^{-3}
$\Delta\rho_{min}$ = −1.33 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—N1	2.294 (7)	Cd1—Cl2	2.553 (3)
Cd1—N2	2.417 (7)	Cd1—Cl1^{i}	2.643 (3)
Cd1—Cl1	2.533 (3)	Cd1—Cl2^{ii}	2.748 (3)
N1—Cd1—N2	76.3 (2)	Cl1—Cd1—Cl1^{i}	90.32 (6)
N1—Cd1—Cl1	164.5 (2)	Cl2—Cd1—Cl1^{i}	91.28 (8)
N2—Cd1—Cl1	90.96 (17)	N1—Cd1—Cl2^{ii}	83.71 (19)
N1—Cd1—Cl2	92.67 (19)	N2—Cd1—Cl2^{ii}	92.61 (17)
N2—Cd1—Cl2	168.96 (17)	Cl1—Cd1—Cl2^{ii}	88.24 (8)
Cl1—Cd1—Cl2	99.96 (7)	Cl2—Cd1—Cl2^{ii}	86.20 (8)
N1—Cd1—Cl1^{i}	98.33 (19)	Cl1^{i}—Cd1—Cl2^{ii}	176.83 (7)
N2—Cd1—Cl1^{i}	90.24 (18)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*C*···Cl1^{iii}	0.90	2.43	3.300 (8)	163

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

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.97 Å for CH_2, C—H = 0.96 Å for CH_3 and N—H = 0.90 Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT* and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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