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catena-Poly[[aqua(pyridine *N*-oxide-κO)-cadmium(II)]-di-μ-chloro]

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Key indicators

Single-crystal X-ray study
T = 268 K
Mean σ(C–C) = 0.017 Å
R factor = 0.049
wR factor = 0.167
Data-to-parameter ratio = 19.4

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

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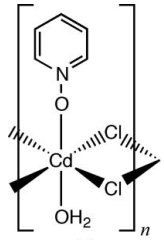
The title compound, $[CdCl_2(C_5H_5NO)(H_2O)]_n$, represents a chain polymer. Cadmium centers are coordinated in a pseudo-octahedral fashion by four bridging chloro ligands, a pyridine *N*-oxide ligand and a water molecule.

Comment

The title coordination polymer, (I), extends in the crystallographic [010] direction (Fig. 1). Neighbouring Cd atoms are almost symmetrically bridged by two chloro ligands in either direction, and the octahedral coordination is completed by the O atom of a pyridine *N*-oxide and an aqua ligand in *trans* positions.



(I)

The metal–metal distance along the resulting chain of edge-sharing octahedra is 3.708 (2) Å, slightly shorter than in related chain polymers of cadmium with two pyridine-type ligands (Hu & Englert, 2002; Hu *et al.*, 2003). Two classical

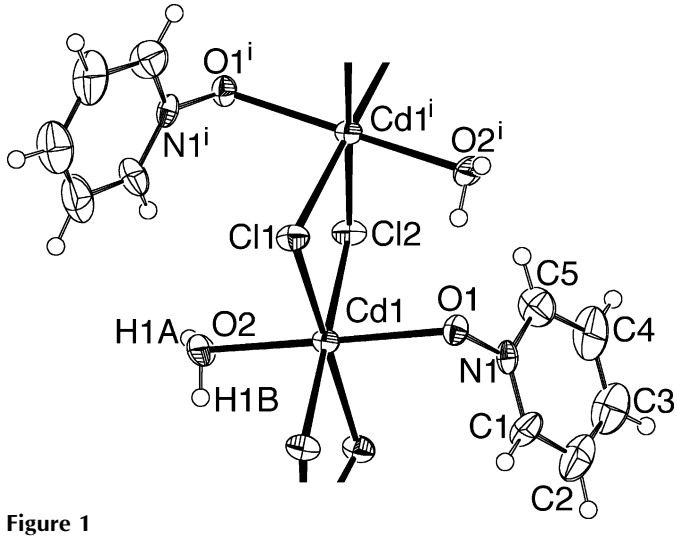


Figure 1
Displacement ellipsoid plot (50% probability and H atoms with arbitrary radii) of a section of the coordination polymer. The view direction is slightly tilted with respect to [100] and the chain extends along the *b*-axis direction. [Symmetry code: (i) $2-x, \frac{1}{2}+y, \frac{3}{2}-z$.]

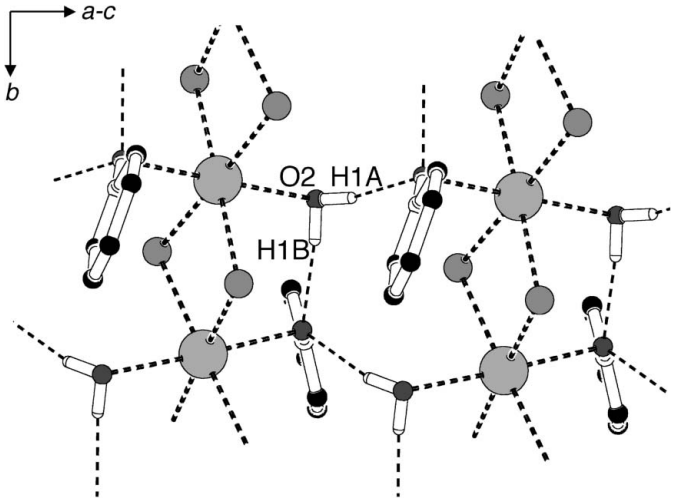


Figure 2
Two adjacent polymer strands, linked *via* a classical hydrogen bond. H atoms of pyridine have been omitted.

hydrogen bonds occur: (i) an intrachain bond exists between atom H1*B* of the aqua ligand and the N-bonded O atom of the neighbouring pyridine ligand, and (ii) perpendicular to the chain, in the [100] direction, adjacent polymer strands are linked, *via* atom H1*A*, into two-dimensional layers. A two-dimensional network of cadmium cations bridged by μ_3-chloro and μ_2-pyridine *N*-oxide ligands has been reported by Nieuwenhuyzen *et al.* (1991).

Experimental

Crystals were obtained from an aqueous solution. 1 equivalent of cadmium chloride was added to 2 equivalents of pyridine *N*-oxide in water. After stirring for 5 min, the solution was kept at room temperature for 20 d. The crystals grew as colourless platelets with dominant {010} faces.

Crystal data

$[CdCl_2(C_5H_5NO)(H_2O)]$
M_r = 296.42
Orthorhombic, $P2_12_12_1$
a = 6.3241 (9) Å
b = 7.415 (4) Å
c = 19.243 (6) Å
V = 902.4 (6) Å^3
Z = 4
D_x = 2.182 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 8.3–13.9°
μ = 2.96 mm^{-1}
T = 268 (2) K
Platelet, colourless
0.35 × 0.3 × 0.1 mm

Data collection

Bruker SMART diffractometer
ω scans
Absorption correction: analytical (*PLATON*; Spek, 2003)
T_{min} = 0.3, T_{max} = 0.79
8540 measured reflections
1937 independent reflections
1782 reflections with $I > 2\sigma(I)$
R_{int} = 0.118
θ_{max} = 27.0°
$h = -7 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.167
S = 1.12
1937 reflections
100 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0964P)^2 + 3.5458P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 3.56 e Å^{-3}
$\Delta\rho_{min}$ = −1.55 e Å^{-3}
Absolute structure: Flack (1983), 760 Friedel pairs
Flack parameter: −0.01 (15)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1A···O1^{i}	0.85	1.97	2.794 (8)	167
O2—H1B···O1^{ii}	0.85	2.02	2.827 (8)	159

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

All H atoms were introduced in idealized positions (C—H = 0.93 Å and O—H = 0.85 Å) and refined as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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