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catena-Poly[cadmium(II)-di-*μ*-chloro-*μ*-4-1*H*-pyridone-*κO*:*κO*]

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Key indicators

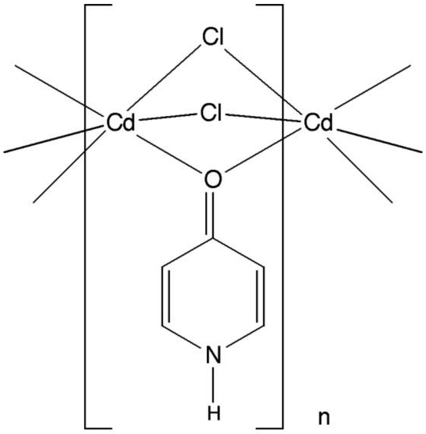
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.021
wR factor = 0.064
Data-to-parameter ratio = 19.7

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

The crystal structure of the title compound, $[CdCl_2(C_5H_5NO)]_n$, is reported. The asymmetric unit consits of one-half of a pyridone ligand which is located on a twofold axis, one cadmium cation which occupies a centre of inversion and one chloro ligand in a general position. This one-dimensional polymer represents a rare example of a structure with an oxygen-bonded bridging 4-pyridone ligand.

Comment

The title polymer, (I), consists of infinite chains of face-sharing cadmium-centred octahedra with a metal–metal distance of 3.3404 (9) Å. For coordination polymers based on Cd this type of connectivity is much less common than edge-sharing (Hu & Englert, 2002; Hu *et al.*, 2003). A comparable Cd···Cd distance occurs in a chain polymer described by Puget *et al.* (1991). Neighbouring Cd atoms are bridged by two chloro and one oxygen-bonded pyridone ligands. Closest contacts between adjacent polymer strands are due to CH···Cl interactions at a distance of 2.74 Å; no classical hydrogen bonds are involved. The metal centres occupy inversion centres; the bridging O atoms, C3, N1 and the H atom attached to the latter are located on twofold axes in space group *I*2/*a*. We are aware of only one previous example of a bridging pyridone ligand (Gao *et al.*, 2005).



(I)

Experimental

Single crystals were obtained from an aqueous solution. One equivalent of $CdCl_2$ was added to two equivalents of 4-hydroxypyridine in water. After stirring for 5 min, the solution was left to stand for 9 d at 315 K. The crystals are colourless platelets with dominant {010} faces.

Crystal data

$[CdCl_2(C_5H_5NO)]$
$M_r = 278.42$
Monoclinic, $I2/a$
$a = 7.510$ (2) Å
$b = 15.531$ (4) Å
$c = 6.6809$ (18) Å
$\beta = 98.057$ (5)°
$V = 771.6$ (4) Å^3
$Z = 4$
$D_x = 2.397$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3571 reflections
$\theta = 2.6$–28.4°
$\mu = 3.45$ mm^{-1}
$T = 293$ (2) K
Platelet, colourless
0.47 × 0.40 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: analytical (*SHELXTL*; Sheldrick, 1998)
$T_{\min} = 0.23$, $T_{\max} = 0.79$
5114 measured reflections
967 independent reflections
916 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.032$
$\theta_{\max} = 28.4$°
$h = -10 \rightarrow 10$
$k = -20 \rightarrow 20$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.064$
$S = 1.40$
967 reflections
49 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.47$ e Å^{-3}
$\Delta\rho_{\min} = -0.57$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O1	2.3351 (14)	O1—C1	1.286 (3)
Cd1—Cl1$^{\rm i}$	2.5922 (9)	C1—C2	1.417 (2)
Cd1—Cl1	2.6288 (8)	C2—C3	1.352 (3)
Cd1···Cd1$^{\rm i}$	3.3404 (10)	C3—N1	1.343 (3)
O1$^{\rm ii}$—Cd1—Cl1	102.33 (3)	Cd1$^{\rm i}$—Cl1—Cd1	79.55 (3)
O1—Cd1—Cl1	77.67 (3)	Cd1$^{\rm i}$—O1—Cd1	91.33 (7)
Cl1$^{\rm i}$—Cd1—Cl1	85.67 (3)		

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

All H atoms were introduced in idealized positions (C—H = 0.93 Å and N—H = 0.86 Å) and were refined using a riding model, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C, N})$. The setting $I2/a$ for space group 15 was preferred over $C2/c$ because the very obtuse monoclinic angle in the latter resulted in correlations between x and z parameters in the refinement matrix.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; 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: *SHELXL97*.

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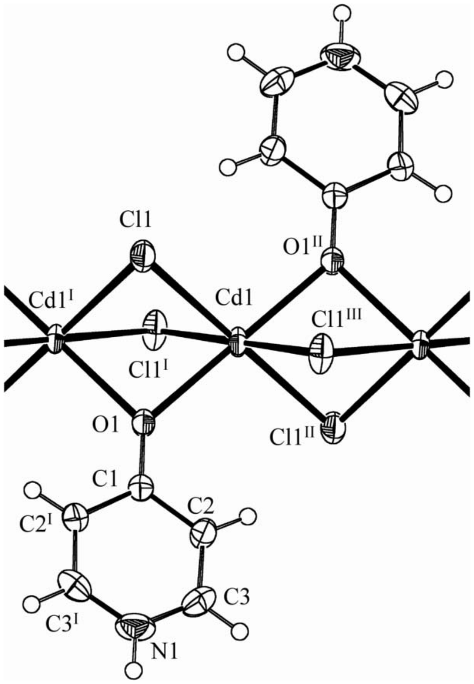

Figure 1
Displacement ellipsoid plot (50% probability level, H atoms with arbitrary radii) of a section of the coordination polymer. The chain extends along c. [Symmetry operations: (I) $\frac{1}{2}-x, y, -z$; (II) $\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z$; (III) $x, \frac{1}{2}-y, \frac{1}{2}+z$.]

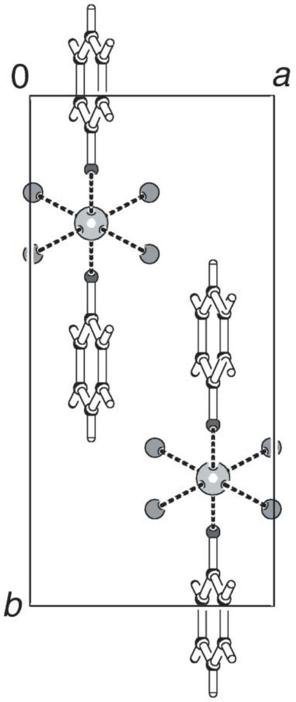

Figure 2
Packing diagram of two polymer chains in the unit cell. The view is in the chain direction, along c.

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