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$[Cd(phen)_2\{MoO_4\}]\cdot H_2O$, a one-dimensional coordination polymer with bridging molybdate groups

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In the title compound, *catena*-poly[[bis(1,10-phenanthroline)-cadmium(II)]-μ-tetraoxomolybdato], $\{[CdMoO_4(C_{12}H_8N_2)_2]\cdot H_2O\}_n$, the Cd^{II} ion has a distorted octahedral geometry, defined by four N atoms of two chelating phen (phenanthroline) ligands and two O atoms from two MoO_4 tetrahedra. The Mo^{VI} atom has a distorted tetrahedral geometry, defined by two terminal O atoms and two bridging (to Cd) O atoms. The compound exhibits a one-dimensional corrugated chain structure, and is further extended into a three-dimensional inorganic–organic hybrid compound *via* hydrogen-bonding and weaker π–π bonding interactions.

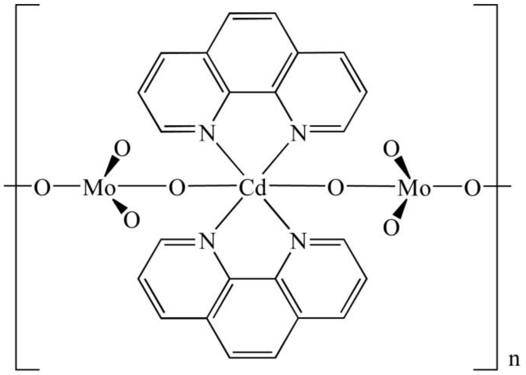
Key indicators

Single-crystal X-ray study
T = 283 K
Mean σ(C–C) = 0.007 Å
R factor = 0.038
wR factor = 0.128
Data-to-parameter ratio = 15.9

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

Comment

In the past decade, organic–inorganic hybrid materials have attracted extensive attention due to their potential applications in catalysis, magnetism, electron conductivity and photochemistry as well as their interesting structural features (Gouzerh & Proust, 1998; Hagrman *et al.*, 1999; Hagrman & Zubieta, 1999). Hydrothermal methods are a key technique for preparing such materials (Yaghi & Li, 1995).



(I)

One topic of interest to us is the integration of metal–organic complexes with molybdenum oxide moieties into a single hybrid structure. A variety of such phases have been prepared and characterized including $[Mn(phen)(H_2O)MoO_4]\cdot H_2O$ (phen is 1,10-phenanthroline; Zhang *et al.*, 2004), $[Cu(phen)MoO_4]\cdot H_2O$ (Hagrman & Zubieta, 1999) and [FeCl(2,2′-bpy)MoO_4] (2,2′-bpy is 2,2′-bipyridine; Zapf *et al.*, 1998). In these complexes, the organonitrogen components act not only as charge compensators and space-filling constituents, but also as ligands bonded directly to a secondary metal center. We report here the synthesis and structure of the title compound, (I), a new one-dimensional coordination polymer containing $\{MoO_4\}$ tetrahedra and $[Cd(phen)_2O_2]$ octahedra.

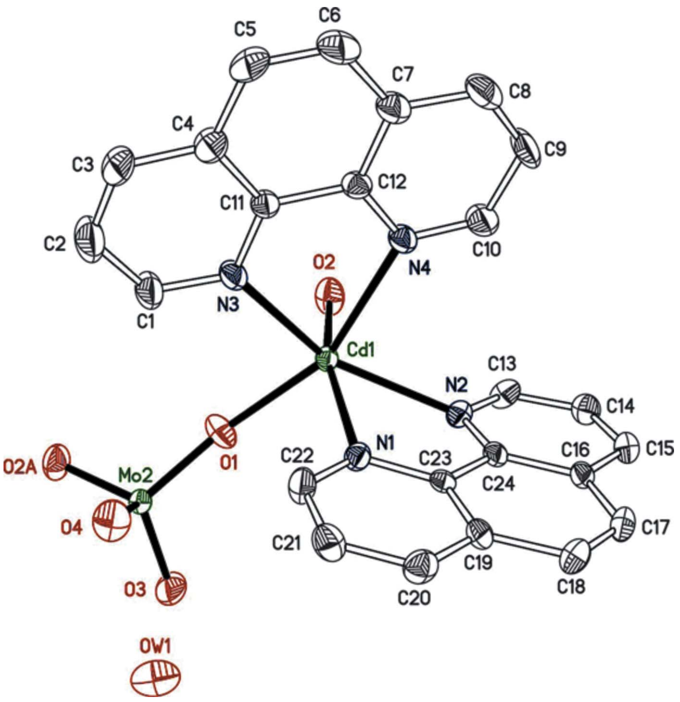


Figure 1
A view of the building units of (I), showing 50% probability displacement ellipsoids (H atoms omitted for clarity). Atom O2*A* is generated by the symmetry code ($x, \frac{1}{2} - y, z - \frac{1}{2}$). H atoms have been omitted.

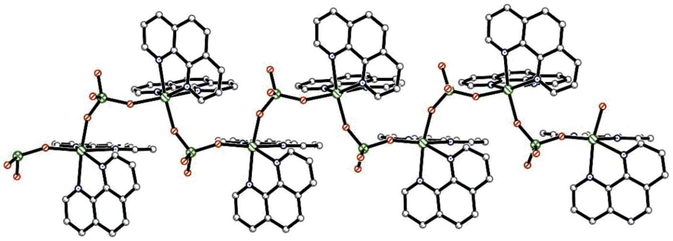


Figure 2
A view of the one-dimensonal chain formed by alternating {MoO_4} tetrahedra and [CdN_2O_2] units. H atoms have been omitted.

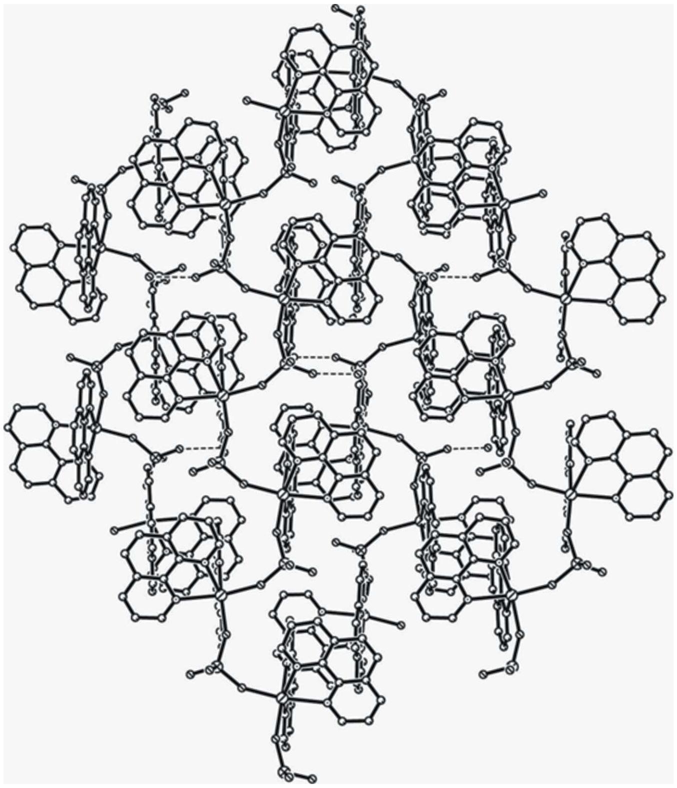


Figure 3
A view of the packing arrangement of the three-dimensional network of (I), with dashed lines indicating the O$\cdots$O hydrogen-bond contacts. H atoms have been omitted.

As shown in Fig. 1, there is one crystallographically independent Cd center and one Mo atom in the asymmetric unit. The octahedral coordination environment about Cd is defined (Table 1) by four N atoms from two chelating phen ligands, and two O atoms from two {MoO_4} tetrahedra. The average Cd—N distance is 2.400 (4) Å, and the Cd—O bond lengths are 2.211 (3) and 2.191 (3) Å. The Mo atom, residing in a tetrahedral environment, is coordinated by two terminal O atoms and two bridging O atoms, with Mo—O bond lengths in the range 1.731 (4)0–1.762 (3) Å. The {CdO_2N_4} octahedra and {MoO_4} tetrahedra are connected by corner-sharing O atoms to form a one-dimensional chain, which is similar to the nickel–molybdate chains in [Ni(3,4′-bipyridine)$_2$MoO$_4$]·3H$_2$O (LaDuca *et al.*, 2002). In (I), adjacent chains are held together *via* two types of supramolecular interactions. One involves O—H$\cdots$O hydrogen bonds arising from the non-coordinated water molecule (Table 2). The other involves weak aromatic π—π stacking of the phen groups; the close contact distance between adjacent aromatic rings of phen is 3.841 Å. (I) is finally extended into a three-dimensional structure by these weak interactions (Fig. 3).

Experimental

A mixture of Cd(NO$_3$)$_2$·8H$_2$O (0.5 mmol), Na$_2$MoO$_4$·2H$_2$O (0.5 mmol), 1,10-phenanthroline (0.6 mmol) and water (10 ml) was stirred for 20 min in air. The mixture was then transferred to a 23 ml Teflon reactor and kept at 433 K for 72 h under autogenous pressure. Crystals of (I) suitable for X-ray analysis were obtained after the reactor had been cooled and opened.

Crystal data

[CdMoO$_4$(C$_{12}$H$_8$N$_2$)$_2$]·H$_2$O
$M_r = 650.76$
Monoclinic, $P2_1/c$
$a = 13.901$ (3) Å
$b = 15.370$ (3) Å
$c = 10.742$ (2) Å
$\beta = 101.61$ (3)°
$V = 2248.2$ (8) Å^3
$Z = 4$

$D_x = 1.923$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20706 reflections
$\theta = 3.0$–27.5°
$\mu = 1.55$ mm^{-1}
$T = 283$ (2) K
Block, colorless
0.34 × 0.28 × 0.26 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
oscillation scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.611$, $T_{\max} = 0.668$
20706 measured reflections

5060 independent reflections
4251 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.047$
$\theta_{\max} = 27.5°$
$h = -18 \rightarrow 16$
$k = -19 \rightarrow 19$
$l = -13 \rightarrow 13$

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Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.128$
$S = 1.01$
5060 reflections
318 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.09P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.98$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Cd1—O2	2.191 (3)	Cd1—N4	2.457 (4)
Cd1—O1	2.211 (3)	Mo2—O3	1.730 (3)
Cd1—N2	2.374 (4)	Mo2—O4	1.746 (3)
Cd1—N3	2.375 (4)	Mo2—O2^{i}	1.762 (3)
Cd1—N1	2.390 (4)	Mo2—O1	1.763 (3)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1W—H1$\cdots$O4	0.85	1.91	2.743 (5)	165
O1W—H2$\cdots$O3^{ii}	0.85	1.93	2.739 (6)	158

Symmetry code: (ii) $-x+2, -y, -z$.

C-bound H atoms were placed in idealized positions (C—H = 0.93 Å) and refined as riding with the constraint U_{iso}(H) = 1.2U_{eq} applied. The water H atoms were positioned geometrically (O—H = 0.85 Å) and refined as riding, with U_{iso}(H) values freely refined.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXL97*.

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