Crystal structure of catena-poly[dichlorido-(μ-ethane-1,2-diyl-bis-(pyridyl-4-carboxylate-κN:N′)mercury(II)], C\textsubscript{15}H\textsubscript{14}Cl\textsubscript{2}HgN\textsubscript{2}O\textsubscript{4}

Abstract

C\textsubscript{15}H\textsubscript{14}Cl\textsubscript{2}HgN\textsubscript{2}O\textsubscript{4}, triclinic, \textit{P}\textbar{}1, (no. 2), \(a = 7.8177(4)\) Å, \(b = 7.9757(4)\) Å, \(c = 15.2165(7)\) Å, \(\alpha = 76.444(2)^\circ\), \(\beta = 79.660(2)^\circ\), \(\gamma = 77.353(2)^\circ\), \(V = 891.71(8)\) Å\(^3\), \(Z = 2\), \(R_{gt}(F) = 0.0300\), \(wR_{ref}(F^2) = 0.041\), \(T = 297(2)\) K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

Single crystals of the title compound were obtained from a HgCl\textsubscript{2} solution (56 mg, 0.1 mmol) in H\textsubscript{2}O (3 mL), which was added to a CH\textsubscript{3}CN (3 mL) solution of ethane-1,2-diyl-bis(pyridyl-4-carboxylate) (L) (27 mg, 0.1 mmol). The clear solution was kept for many days at room temperature until crystals formed. Colorless crystals of [Hg(L)(Cl\textsubscript{2})] were collected with approximately 75% yield.

IR (KBr, cm\(^{-1}\)): 3454 (w), 3101 (w), 3070 (w), 2964 (w), 2375 (w), 1731 (s), 1598 (m), 1479 (m), 1112 (m), 780 (w), 720 (w), 700 (w).

Discussion

Coordination polymers containing metal nodes and organic ligands have attracted tremendous attention over the past 30 years because of their wide application as functional materials [1, 2]. The synthesis of coordination polymers by the judicious choice of organic spacers and metal centers can be an efficient method to obtain new types of luminescent materials, especially for d\textsuperscript{10} or d\textsuperscript{10}−d\textsuperscript{10} systems of metal centers [3, 4]. The most important motifs among one-dimensional...
coordination polymers are linear chains, zig-zag chains, double chains, ladder chains, fish-bone chains and helix and double helix chains. The group 12 elements are rather a special case when considering the chemistry of the main group elements. Supramolecular structures that contain mercury(II) seem to have much more in common with main group elements. Supramolecular structures that contain mercury(II) seem to have much more in common with main group elements.

This paper forms part of our continuing study on the synthesis, structural characterization and photo-physical properties of hybrid materials based on d^{10} ions and flexible ligands [8].

The coordination environment of the Hg(II) atom is depicted in the figure, showing a part of the crystal structure of the zig-zag chain along [001]. It can be clearly seen that each Hg(II) atom is four-coordinated and adopts a distorted tetrahedral geometry with two different N atoms of two symmetry related ligands and two chlorido ligands with Hg—Cl and Hg—N bond distances (mean) of 2.3840(10) and 2.4913(3) Å, respectively. The bond angles of Cl1—Hg—Cl2, Cl—Hg—N, N1—Hg—N2 (symmetry code: i = x, 1+y, −z+1) are in the range of 93.47(10)–157.69(4)°, in good agreement with those for other Hg(II) coordination polymers [9]. The Hg—Hg^II (symmetry code ii: x−y, 1+z) separation across (L) is 15.4357(7) Å. The dihedral angle between pyridine rings is 89.4(2). π–π stacking interactions are observed between neighboring chains Cg−Cg^iii = 3.804(2) Å (symmetry code iii: 2−x, 1−y, 1−z) (Cg = N1/C1−C5).

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References
versus coordination polymers based on Cu(I) and Ag(I) ions and flexible ligands: structural diversification and luminescent properties. Polymers 8 (2016) 2–16.


