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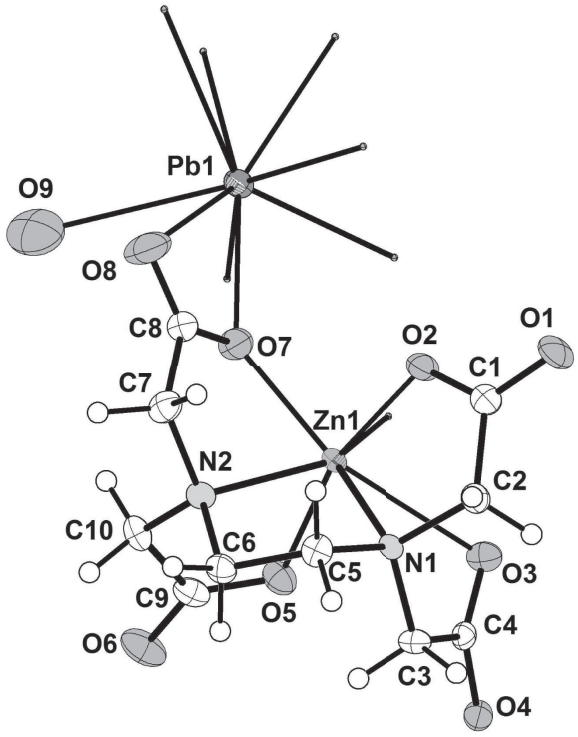
Crystal structure of poly[aqua-ethylenediaminetetraacetatolead(II)zinc(II)]



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Abstract

$C_{10}H_{14}N_2O_9PbZn$, triclinic, $P\bar{1}$ (no. 2), $a = 7.4992(6)$ Å, $b = 8.2890(7)$ Å, $c = 11.8236(10)$ Å, $\alpha = 101.604(1)°$, $\beta = 106.540(1)°$, $\gamma = 98.931(1)°$, $V = 672.25(10)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.019$, $wR_{ref}(F^2) = 0.044$, $T = 296(2)$ K.

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The crystal structure is shown in the figure. Tables 1–3 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Colorless, prism
Size:	0.050×0.050×0.200 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	143.45 cm^{-1}
Diffractometer, scan mode:	Bruker smart APEX II CCD, ω scans
$2\theta_{max}$:	56.59°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	8308, 3290
$N(param)_{refined}$:	208
Programs:	SHELX [7]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	Site	x	y	z	U_{iso}
H(2A)	2*i*	0.5059	0.5384	0.5922	0.024
H(2B)	2*i*	0.6290	0.6891	0.7046	0.024
H(3A)	2*i*	0.2998	0.3638	0.7643	0.021
H(3B)	2*i*	0.4579	0.3559	0.7017	0.021
H(5A)	2*i*	0.5359	0.7831	0.8631	0.022
H(5B)	2*i*	0.5795	0.6118	0.8879	0.022
H(6A)	2*i*	0.2891	0.5419	0.9214	0.023
H(6B)	2*i*	0.3992	0.7216	1.0076	0.023
H(7A)	2*i*	0.3501	0.9604	0.9152	0.026
H(7B)	2*i*	0.1996	0.9514	0.9841	0.026
H(10A)	2*i*	−0.0875	0.7289	0.8783	0.026
H(10B)	2*i*	0.0315	0.6403	0.9690	0.026
H(9A)	2*i*	−0.3372	0.1816	0.7916	0.069
H(9B)	2*i*	−0.5364	0.0739	0.7302	0.069

Source of material

A mixture of ethylenediaminetetraacetic acid (H_4EDTA) (0.1 mmol), $ZnCl_2$ (0.1 mmol), $PbCl_2$ (0.1 mmol), DMF (5 ml) and water (5 ml) whose pH value was adjusted to 4 by NaOH, was placed in a 30-mL Teflon-lined stainless steel autoclave. Then the autoclave was sealed, heated to 160 °C under autogenous pressure for 48 h. After slowly cooled to room temperature at a rate of 5 °C/h, a few colorless prismatic crystals were recovered by filtration, washed by distilled water, and air dried.

Discussion

In recent years, study of coordination polymers has gained great recognition as an important interface between synthetic

Table 3: Atomic displacement parameters (Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Pb(1)	2*i*	−0.17742(2)	1.07232(2)	0.60183(2)	0.01834(7)	0.02046(7)	0.01884(7)	0.00540(4)	0.00700(5)	0.00834(5)
Zn(1)	2*i*	0.09668(5)	0.65477(4)	0.65987(3)	0.0158(2)	0.0166(2)	0.0150(2)	0.0017(1)	0.0049(1)	0.0058(1)
C(1)	2*i*	0.4241(5)	0.7591(4)	0.5827(3)	0.018(2)	0.017(2)	0.017(2)	−0.001(1)	0.004(1)	0.002(1)
C(2)	2*i*	0.5000(5)	0.6365(4)	0.6504(3)	0.021(2)	0.021(2)	0.022(2)	0.006(1)	0.011(1)	0.008(1)
C(3)	2*i*	0.3420(5)	0.3952(4)	0.6999(3)	0.019(2)	0.013(1)	0.019(2)	0.003(1)	0.004(1)	0.006(1)
C(4)	2*i*	0.1896(4)	0.3102(4)	0.5778(3)	0.015(1)	0.015(1)	0.018(2)	0.003(1)	0.009(1)	0.003(1)
C(5)	2*i*	0.4786(4)	0.6659(4)	0.8538(3)	0.014(1)	0.020(2)	0.016(2)	0.001(1)	0.001(1)	0.001(1)
C(6)	2*i*	0.3365(5)	0.6584(4)	0.9230(3)	0.020(2)	0.024(2)	0.016(2)	0.008(1)	0.004(1)	0.009(1)
C(7)	2*i*	0.2177(5)	0.9157(4)	0.9056(3)	0.023(2)	0.019(2)	0.019(2)	0.005(1)	0.002(1)	0.001(1)
C(8)	2*i*	0.0886(5)	0.9858(4)	0.8124(3)	0.025(2)	0.021(2)	0.023(2)	0.008(1)	0.011(1)	0.008(1)
C(9)	2*i*	−0.0975(4)	0.4824(4)	0.7959(3)	0.014(2)	0.024(2)	0.024(2)	0.004(1)	0.004(1)	0.013(1)
C(10)	2*i*	0.0000(5)	0.6539(4)	0.8865(3)	0.021(2)	0.027(2)	0.019(2)	0.004(1)	0.010(1)	0.008(1)
O(1)	2*i*	0.5134(4)	0.8145(3)	0.5190(2)	0.024(1)	0.029(1)	0.034(1)	0.005(1)	0.017(1)	0.018(1)
O(2)	2*i*	0.2725(3)	0.8030(3)	0.5935(2)	0.022(1)	0.023(1)	0.028(1)	0.0083(9)	0.013(1)	0.014(1)
O(3)	2*i*	0.1281(3)	0.3983(3)	0.5085(2)	0.021(1)	0.019(1)	0.019(1)	0.0037(9)	0.001(1)	0.0050(9)
O(4)	2*i*	0.1328(3)	0.1506(3)	0.5580(2)	0.021(1)	0.015(1)	0.023(1)	−0.0004(9)	0.011(1)	0.0026(9)
O(5)	2*i*	−0.0602(3)	0.4511(3)	0.6967(2)	0.023(1)	0.023(1)	0.020(1)	−0.0012(9)	0.006(1)	0.006(1)
O(6)	2*i*	−0.2128(4)	0.3880(3)	0.8246(3)	0.023(1)	0.037(2)	0.041(2)	−0.002(1)	0.011(1)	0.021(1)
O(7)	2*i*	−0.0121(4)	0.8795(3)	0.7108(2)	0.034(1)	0.024(1)	0.016(1)	0.011(1)	0.003(1)	0.004(1)
O(8)	2*i*	0.0892(5)	1.1379(3)	0.8366(3)	0.055(2)	0.021(1)	0.039(2)	0.016(1)	0.008(2)	0.006(1)
O(9)	2*i*	−0.4051(6)	0.0657(4)	0.7786(3)	0.073(2)	0.032(2)	0.051(2)	−0.001(2)	0.007(2)	0.002(2)
N(1)	2*i*	0.3837(4)	0.5804(3)	0.7226(2)	0.019(1)	0.013(1)	0.012(1)	0.002(1)	0.005(1)	0.003(1)
N(2)	2*i*	0.1748(4)	0.7305(3)	0.8665(2)	0.014(1)	0.017(1)	0.016(1)	0.003(1)	0.004(1)	0.006(1)

chemistry and material science not only because of their fascinating topology and intriguing architectures, also due to their potential applications in magnetism, luminescence, ion exchange, electronic apparatus, and catalysis etc. [1–4]. The selection of suitable organic ligands are crucial for constructing extended coordination frameworks. As one of a fascinating ligands, ethylenediaminetetraacetic acid (H_4EDTA) is selected as a cluster ligand for several reasons. On one hand, the EDTA ligand, as one of the most fascinating ligands, can act as a tetradentate, pentadentate or hexadentate ligand to form a six-coordinate octahedron, seven-coordinate distorted monocapped trigonal prism or pentagonal bipyramid [5, 6]. With the aim to understand the interesting chemistry, we studied its assembly reaction of H_4EDTA with Zn (II) and Pb (II) ions under hydrothermal condition and afforded a new coordination polymer PbZn(EDTA)·H_2O.

Structure solution revealed that there are one Pb^{2+} cation, one Zn^{2+} cation, one deprotonated EDTA ligand and one water molecule in the asymmetric unit of title structure. Each Zn(1) cation is 7-coordinated by five carboxylate oxygens and two amido nitrogen atoms from two EDTA ligands with the Zn–O bond distances ranging from 2.083(2) to 2.190(2) Å and the Zn–N bond distances is 2.272(3) and 2.291(3). The Pb(1) atom is nine-coordinated by eight carboxylate oxygen atoms from five different EDTA ligands and one water ligand to form a distorted pentagonal bipyramid (see the figure). With the Pb–O bond distances ranging from 2.499(2) to 3.054(2) Å. On the other hand, each EDTA ligand adopts μ_7-coordination model, linking to five Pb^{2+} cations and two Zn^{2+} cations, in such a way to form the 3D framework.

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