Poly[\(\mu_4\)-5-(3-carboxylatophenyl)-1\(H\)-tetrazolato-zinc(II)]

The title compound, [\(\text{Zn(C}_8\text{H}_4\text{N}_4\text{O}_2)\)]\(_n\), is a coordination polymer prepared by the hydrothermal reaction of zinc chloride and 3-(1\(H\)-tetrazol-5-yl)benzoic acid. The zinc cation is tetrahedrally coordinated by two N atoms and two O atoms from four ligands, resulting in a three-dimensional framework encapsulating one-dimensional channels.

Comment

Coordination frameworks with channels or pores have received much attention over the past decade because of their potential applications in catalysis (Seo et al., 2000), separation (Uemura et al., 2002), ion exchange (Yaghi & Li, 1995) and gas storage (Rosi et al., 2003). Multifunctional organic ligands are necessary for constructing such frameworks. Among a variety of organic ligands used, 5,5\(^0\)--(1,4-phenylene)bis(1\(H\)-tetrazole) (PBT) is one of the most important (Xiong et al., 2002; Xue et al., 2002; Tao et al., 2004).

We report here the synthesis and crystal structure of the title compound, (I), a new coordination polymer of zinc and 3-(1\(H\)-tetrazol-5-yl)benzoic acid, which is a ligand related to PBT with two different functional groups; viz. one carboxylate group and one tetrazolate ring. Compound (I) was obtained by the hydrothermal reaction of zinc chloride and 3-(1\(H\)-tetrazol-5-yl)benzoic acid.

In the structure of (I), the Zn cation is tetrahedrally coordinated (Table 1) by two N atoms and hydroxyl and carbonyl O atoms from four different ligands (Fig. 1), resulting in a three-dimensional framework with two types of channels propagating along the \(a\) axis (Fig. 2). These channels are too small to have any content.

Experimental

Zinc chloride (0.5 mmol, 0.068 g) and 3-(1\(H\)-tetrazol-5-yl)benzoic acid (0.5 mmol, 0.110 g) were dissolved in water (8 ml) with stirring. The solution was transferred into a Teflon-lined stainless steel auto-
clave and heated to 433 K for 5 d, then cooled to room temperature. Colorless block-shaped crystals of (I) suitable for diffraction were recovered.

**Crystal data**

\[\text{Zn(C_8H_4N_4O_2)}\]

- \(M_r = 253.52\)
- Monoclinic, \(P_2_1/c\)
- \(a = 4.9026 (5) \text{ Å}\)
- \(b = 17.0331 (16) \text{ Å}\)
- \(c = 10.479 (1) \text{ Å}\)
- \(\beta = 97.880 (2)^\circ\)
- \(V = 866.80 (15) \text{ Å}^3\)
- \(Z = 4\)

**Refinement**

- 1943 reflections with \(I > 2\sigma(I)\)
- \(R_{\text{int}} = 0.036\)
- \(\theta_{\text{max}} = 27.5^\circ\)
- \(k = -6 \rightarrow 6\)
- \(l = -13 \rightarrow 13\)

**Table 1**

<table>
<thead>
<tr>
<th>Bond Distance (Å)</th>
<th>Symmetry Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zn1−O2(^{\text{ii}})</td>
<td>1.945 (3)</td>
</tr>
<tr>
<td>Zn1−N1(^{\text{ii}})</td>
<td>1.974 (3)</td>
</tr>
<tr>
<td>O2−Zn1−O1</td>
<td>108.28 (12)</td>
</tr>
<tr>
<td>O2−Zn1−N4(^{\text{ii}})</td>
<td>113.96 (14)</td>
</tr>
<tr>
<td>O1−Zn1−N4(^{\text{ii}})</td>
<td>103.90 (14)</td>
</tr>
<tr>
<td>O1−Zn1−N1(^{\text{ii}})</td>
<td>104.33 (14)</td>
</tr>
</tbody>
</table>

**Figure 1**

A fragment of (I), showing the zinc cation environment, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) \(-x, y + \frac{1}{2}, -z + \frac{1}{2}\); (ii) \(-x, -y, -z\); (iii) \(-x, -y, \frac{1}{2} - z\)]

**Figure 2**

Packing diagram of (I), showing the channels along the \(a\) axis.

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**References**


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