CRYSTAL STRUCTURE OF A 3D COORDINATION POLMER:
ZINC TEREPHALATE HYDRATE

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Figure 1. ORTEP plot of a portion of the 1D zigzag chain formed in zinc terephthalate hydrate. The
diagram was drawn at the 50% probability level and hydrogen atoms have been omitted for clarity. Selected
bond distances and angles: Zn1-O1 1.9446(17), Zn1-O3 1.978(3), Zn1-O2b 2.1829(17) Å; O1-Zn1-O1a
138.68(12), O1-Zn1-O3 110.66(6), O1-Zn1-O2b 88.43(7), O3-Zn1-O2b 87.14(5), O1-Zn1-O2c 93.58(7),
O2b-Zn1-O2c 174.28(9)°. Symmetry transformation: a = -x, y, -z+1/2, b = x, -y+1, z+1/2, c = -x, -
y+1, -z+2.

Figure 2. ORTEP plot of the 3D structure of zinc terephthalate hydrate along c axis. The diagram was
drawn at the 30% probability level and the hydrogen atoms have been omitted for clarity.

Comment
Terephthalate, acting as an excellent multidentate ligand, has received great concern in the assembly of
metal-organic coordination polymers. Up till now, several coordination polymers have been constructed out
of zinc and terephthalate and, some of them show unique properties [1–4]. In this paper, we report an
example of 3D coordination polymer formed by zinc and terephthalate under hydrothermal conditions. The
crystallography shows that zinc atom in the title complex is five-coordinated by four oxygen atoms from
four carboxylic groups, that define a plane, and one oxygen atom of water molecule that occupies an apical
position in the square pyramidal geometry. The Zn-O3 (water) bond lies on C2 axis (b axis of the crystal)
while the four terephthalates stretch out to four directions in C2 symmetry. The pair of zinc atoms, bridged
by two of carboxylic groups, forms a binuclear unit. Connections between these units lead to the formation
of an infinite 1D zigzag chain along c axis, which, joined via zinc atoms, generates a 3D network. The
composition and structure of the title complex is different from other coordination polymers [1-3], including
the closely related zinc terephthalate dihydrate [4], this may be due to the different synthesis conditions.

**Experimental**
A mixture of Zn(NO3)2·6H2O (0.30g, 1.0 mmol), terephthalic acid (0.17g, 1.0 mmol) and NaOH (0.08g, 2.0
mmol) was stirred and transferred into a 20 ml Teflon-lined vessel, heated from room temperature to 200 °C
at the rate of 0.05°C/min, and kept at 200 °C for 100 h, followed by slow cooling to room temperature at the
rate of 0.1°C/min. Colorless plate-like crystals of the title complex separated upon cooling (0.09g, yield
36%) were filtrated, washed by distilled water and dried in air. Calc. (%) for C16H12O2Zn: C, 38.82; H, 2.44.
Found (%): C, 38.28; H, 2.39. IR (cm⁻¹): 3168s,br, 1591s, 1548s, 1502s, 1385vs, 1294w, 1254w, 1015m,
826m, 761s, 592m, 492m. A 0.47 × 0.18 × 0.07 mm crystal was used in the diffraction measurements. The
intensities were corrected for absorption effects [5].

**Acknowledgments**
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Province, P.R. China (E0110001).

**Table 1. Crystal data for zinc terephthalate hydrate**

<table>
<thead>
<tr>
<th>Empirical formula</th>
<th>C6H12O2Zn</th>
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<tr>
<td>Crystal system</td>
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<td>Space group</td>
<td>C2/c</td>
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<tr>
<td>Unit cell dimensions</td>
<td>a 17.978(4)</td>
<td>Volume, Å³</td>
<td>829.4(3)</td>
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<tr>
<td></td>
<td>b 6.3581(13)</td>
<td>Z</td>
<td>4</td>
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<td></td>
<td>c 7.2579(15) Å</td>
<td>Dcalc, g cm⁻³</td>
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<tr>
<td>μ (Mo-Kα), mm⁻¹</td>
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<td>θ range, °</td>
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<tr>
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<td>F(000)</td>
<td>496</td>
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<tr>
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<td>No. parameters refined</td>
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<tr>
<td>R (all data)</td>
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<td>Final R [θ&gt;2σ(θ)]</td>
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<tr>
<td>w</td>
<td>[w(Fo²)+0.0365P]²+0.9449P]⁻¹</td>
<td>wR²(all data)</td>
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<td>Goodness-of-fit on F²</td>
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<td>ρ, eÅ⁻³</td>
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* P = (Fo²+2Fc²)/3

**References**

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