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Tetraaquabis(2,4-dicarboxybenzoato)zinc(II) dihydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.102
Data-to-parameter ratio = 12.2

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

In the complex molecule of the title compound, $[Zn(C_9H_5O_6)_2(H_2O)_4]\cdot 2H_2O$, zinc(II) is six-coordinated by two O atoms from two monodentate 2,4-dicarboxybenzoate ligands and four O atoms from water molecules. The complex possesses a crystallographically imposed centre of symmetry. In the crystal packing, complex molecules and water molecules are connected by strong intermolecular O—H···O hydrogen bonds, resulting in an extended three-dimensional network. A zigzag chain of hydrogen-bonded water molecules running along the c axis is observed.

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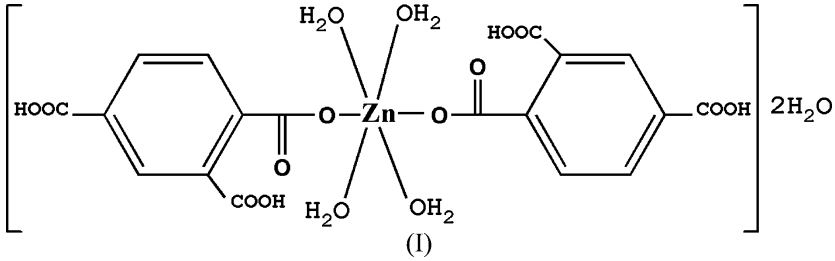
Comment

In recent years, considerable attention has been paid to the investigation of structures and properties of complexes or salts containing benzenepolycarboxylate ligands because of their potential technological importance. While symmetrical polycarboxylate ligands, such as 1,4-benzenedicarboxylate, 1,3,5-benzenetricarboxylate and 1,2,4,5-benzenetetracarboxylate, are well documented in the literature, compounds containing the unsymmetrical 1,2,4-benzenetricarboxylate ligand (btc) are relatively scarce. Among these, the polymeric structures of transition metal complexes of manganese (Li *et al.*, 2004; Plater *et al.*, 2001), iron (Riou-Cabellec *et al.*, 2003), cadmium (Wang *et al.*, 2005; Xia *et al.*, 2004; Zheng *et al.*, 2003; Fan *et al.*, 2003), cobalt (Lu *et al.*, 2003; Plater *et al.*, 2001; Ren *et al.*, 2002; Hao *et al.* 2003; Yan *et al.*, 2003), copper (Qin, Wang, Wang *et al.*, 2004*a*; Fan *et al.*, 2004) and zinc (Qin, Wang, Wang *et al.*, 2004*b*; Qin, Wang, Carlucci *et al.*, 2004; Zheng *et al.*, 2003; Wang *et al.*, 2004; Yan *et al.*, 2003) have been reported. Rare earth complexes containing the H_2btc^- anion were also reported (Jin *et al.*, 1990; Wei *et al.*, 1992). To our knowledge, monomeric complexes including the 1,2,4-benzenetricarboxylate ligand have been reported only by Fan *et al.* (2004) and Hao *et al.* (2004). We report here the structure of a new zinc(II) complex, $[Zn(H_2btc)_2(H_2O)_4]$, which cocrystallized with water molecules in a 1:2 molar ratio to give crystals of the title compound, (I).



(I)

The complex molecule of (I) possesses a crystallographically imposed centre of symmetry (Fig. 1). The

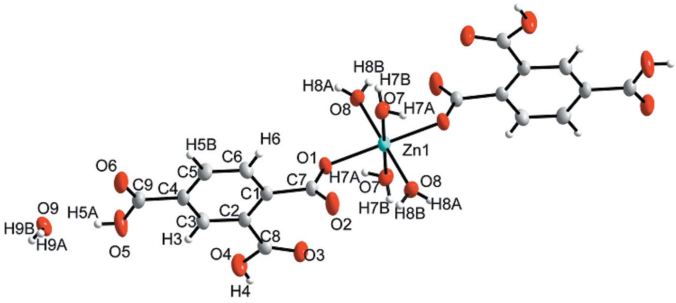


Figure 1
A view of the structure showing the atom-labelling scheme and 50% probability displacement ellipsoids. Unlabelled atoms are related to labelled atoms by the symmetry code $(1-x, 1-y, 1-z)$.

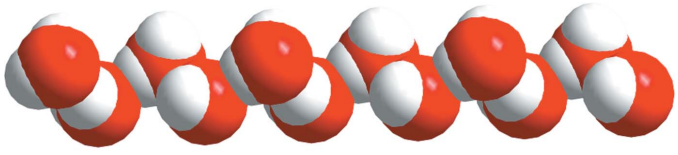


Figure 2
The chain of hydrogen-bonded water molecules running along the *c* axis.

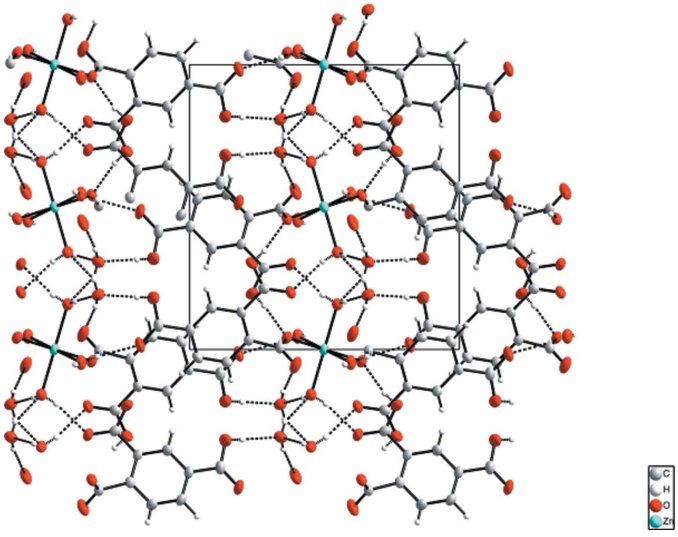


Figure 3
Packing diagram of the title compound, viewed along the *c* axis. Hydrogen-bonding interactions are shown as dashed lines.

zinc(II) metal exhibits an octahedral geometry defined by the O atoms from two monodentate *trans*-arranged H_2btc^- ligands and four water molecules. The Zn—O7 and Zn—O8 (Table 1) bond lengths involving the water molecules are significantly different, reflecting the different role played by the water molecules in the formation of intermolecular hydrogen bonds. All O atoms of the H_2btc^- anions and water molecules are linked by strong hydrogen-bonding interactions (Table 2), resulting in a complex three-dimensional supramolecular network (Fig. 3). Moreover, the O7 and O9 water molecules are linked by O—H···O hydrogen interactions to generate a zigzag chain running along the *c* axis (Fig. 2).

Experimental

1,2,4-Benzenetricarboxylic acid anhydride (0.5 mmol) and $ZnSO_4{\cdot}7H_2O$ (0.5 mmol) were dissolved in hot water (15 ml). The resulting solution was stirred for two hours. The pH value was adjusted to 2.5 with 2*M* NaOH solution. This mixture was cooled to room temperature and filtered. Colourless crystal of the title compound suitable for X-ray analysis grew from the solution after standing for several days at room temperature.

Crystal data

$[Zn(C_9H_5O_6)_2(H_2O)_4]{\cdot}2H_2O$
$M_r = 591.73$
Monoclinic, $P2_1/c$
$a = 12.3211\ (7)$ Å
$b = 12.6398\ (9)$ Å
$c = 7.5043\ (5)$ Å
$\beta = 103.597\ (3)^\circ$
$V = 1135.94\ (13)$ Å^3
$Z = 2$
$D_x = 1.730$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8978 reflections
$\theta = 2.4$–27.5°
$\mu = 1.17$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.36 × 0.35 × 0.31 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
$\omega/2\theta$ scans
Absorption correction: multi-scan (*RAPID-AUTO*; Rigaku Corporation, 1998)
$T_{min} = 0.556$, $T_{max} = 0.691$
10257 measured reflections
2598 independent reflections
1836 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.5^\circ$
$h = -15 \rightarrow 15$
$k = -16 \rightarrow 16$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.102$
$S = 1.01$
2598 reflections
213 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O8	2.050 (2)	O4—C8	1.310 (3)
Zn1—O1	2.0927 (17)	O5—C9	1.314 (4)
Zn1—O7	2.101 (2)	O2—C7	1.226 (3)
O1—C7	1.274 (3)	O6—C9	1.204 (3)
O3—C8	1.209 (3)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O9	0.78 (4)	1.83 (4)	2.603 (3)	179 (5)
O8—H8*A*···O6^{i}	0.77 (4)	2.00 (4)	2.751 (3)	165 (4)
O7—H7*A*···O3^{ii}	0.78 (3)	2.01 (3)	2.775 (3)	168 (4)
O9—H9*A*···O2^{iii}	0.76 (4)	1.96 (4)	2.709 (3)	171 (4)
O9—H9*B*···O7^{iv}	0.76 (2)	2.02 (3)	2.722 (3)	154 (4)
O4—H4···O1^{v}	0.79 (4)	1.88 (4)	2.654 (3)	166 (4)
O7—H7*B*···O9^{i}	0.75 (4)	1.99 (4)	2.735 (4)	174 (4)

Symmetry codes: (i) $x+1, y, z$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x, -y+1, -z+2$; (iv) $x-1, -y+\frac{1}{2}, z+\frac{1}{2}$; (v) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

All H atoms were found in difference Fourier maps and refined isotropically [C—H = 0.88 (3)–1.02 (3) Å and O—H = 0.75 (4)–0.79 (4) Å].

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL97-2* (Sheldrick, 1997).

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