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catena-Poly[bis[bis(1*H*-benzotriazole)zinc(II)]-μ_4-benzene-1,2,4,5-tetracarboxylato], a one-dimensional coordination polymer with double chains

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Key indicators

Single-crystal X-ray study
T = 283 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.086
Data-to-parameter ratio = 14.3

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

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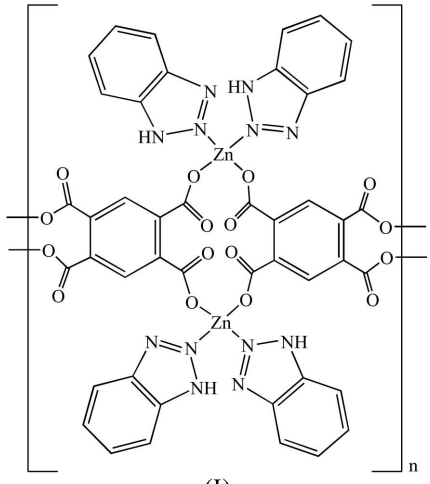
In the title compound, $[Zn_2(C_{10}H_2O_8)(C_6H_5N_3)_4]_n$, the Zn^{II} atom has a distorted tetrahedral coordination geometry, defined by two N atoms and two carboxyl O atoms from two benzotriazole ligands and a benzene-1,2,4,5-tetracarboxylate ligand. The structure exhibits one-dimensional double chains running along the [100] direction, which further extend into a three-dimensional supramolecular network by π–π stacking.

Comment

The rational design and synthesis of supramolecular complexes is of current interest in the field of supramolecular chemistry and crystal engineering. Benzotriazole (BTAH) is an attractive choice for multifunctional linking groups and has been investigated in the construction of metal-organic frameworks. Some structures of metal-organic polymers containing BTAH have been reported previously (Yuan & Zhou, 2004; Hu *et al.*, 2005; Jones, Brechin, Collison, Raftery & Teat, 2002; Jones, Brechin, Collison, Harrison *et al.*, 2002; Low *et al.*, 2003; Meng *et al.*, 2004). We present here the crystal structure of the title compound, (I), which is a new example with a one-dimensional polymeric structure.



(I)

As shown in Fig. 1, the asymmetric unit of (I) contains one Zn^{II} atom, two benzotriazole (BTAH) ligands and one-half of a benzene-1,2,4,5-tetracarboxylate (BTC) ligand. The Zn^{II} atom is coordinated by two O atoms from two BTC ligands and two N atoms from two BTAH ligands, showing a distorted tetrahedral geometry. The Zn—O bond distances are 1.9469 (17) and 1.9572 (18) Å, while the Zn—N bond distances are 2.006 (2) and 2.038 (2) Å. Each BTC ligand is coordinated to four Zn^{II} atoms and each BTAH ligand is

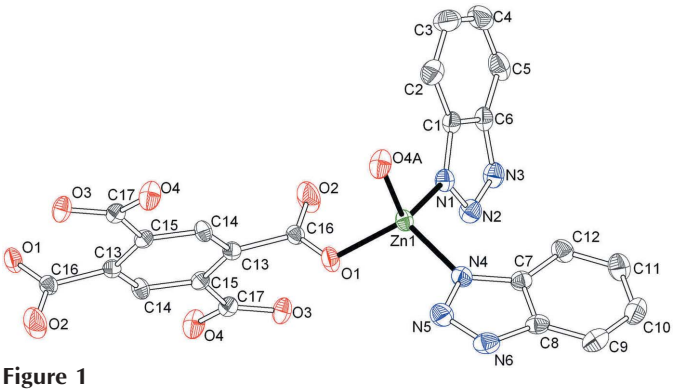


Figure 1
Part of the polymeric structure of (I) with 50% probability displacement ellipsoids [symmetry code: (A) $-x+1, -y, -z+1$]. H atoms have been omitted.

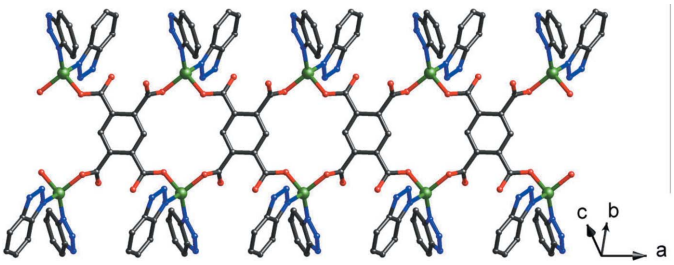


Figure 2
A view of the one-dimensional double chains running along the [100] direction. H atoms have been omitted.

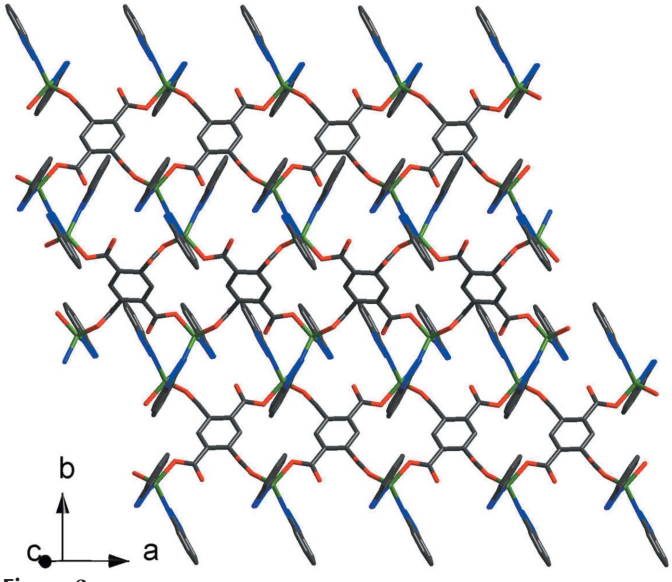


Figure 3
Packing model of the three-dimensional supramolecular network. H atoms have been omitted.

coordinated to one Zn^{II} atom. The dihedral angle between the planes of the two BTAH ligands is 61.739 (3)°.

Adjacent $[Zn(BTAH)_2]$ units are linked by the BTC ligands to form one-dimensional double chains running along the [100] direction like a molecular ladder (Fig. 2). The two BTAH ligands coordinated to one Zn^{II} atom are directed away from the double chains. This orientation plays an important role in packing as a three-dimensional network through π–π stacking interactions between BTAH ligands. Firstly, the adjacent double chains are extended into a two-dimensional layer parallel to the (001) plane, and then a three-dimensional supramolecular network is formed by π–π stacking interactions. The face-to-face distances between neighboring parallel BTAH planes are 3.436 (3) and 3.571 (3) Å (Fig. 3).

Experimental

Compound (I) was prepared by hydrothermal methods. A mixture of $Zn(NO_3)_2{\cdot}6H_2O$ (0.5 mmol), H_4BTC (0.6 mmol), benzotriazole (1.0 mmol) and water (12 ml) was stirred for 20 min in air. The mixture was then transferred to a 23 ml Teflon reactor and kept at 433 K for 72 h under autogenous pressure. Colorless single crystals of (I) suitable for X-ray analysis were obtained from the reaction mixture.

Crystal data

$[Zn_2(C_{10}H_2O_8)(C_6H_5N_3)_4]$
$M_r = 857.38$
Monoclinic, $P2_1/n$
$a = 7.7961$ (16) Å
$b = 19.346$ (4) Å
$c = 10.732$ (2) Å
$\beta = 101.78$ (3)°
$V = 1584.6$ (6) Å^3
$Z = 2$
$D_x = 1.797$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15373 reflections
$\theta = 3.1$–27.5°
$\mu = 1.59$ mm^{-1}
$T = 283$ (2) K
Block, colorless
0.26 × 0.22 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996; Blessing, 1995)
$T_{min} = 0.668$, $T_{max} = 0.764$
15373 measured reflections
3628 independent reflections
2924 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 27.5°$
$h = -10 \rightarrow 8$
$k = -25 \rightarrow 25$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.086$
$S = 1.05$
3628 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.7439P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and treated as riding atoms in the final cycles of refinement, with $U_{iso}(H) = 1.2U_{eq}$(carrier).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure and prepare material for publication: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998).

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