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Poly[μ_4-benzene-1,3-dicarboxylato-di-μ_2-benzimidazolato-dizinc(II)]

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In the title compound, $[Zn_2(C_8H_4O_4)(C_7H_5N_2)_2]_n$, the Zn atom is four-coordinated by two O atoms from two benzene-1,3-dicarboxylate (1,3-BDC) ligands and two N atoms from two anionic benzimidazolate (bzim) ligands, resulting in a ZnN_2O_2 tetrahedron. The complete 1,3-BDC ligand is generated by crystallographic twofold rotation symmetry, with two C atoms lying on the rotation axis. Together, the 1,3-BDC and bzim ligands bridge the Zn atoms, forming an infinite three-dimensional structure containing one-dimensional channels.

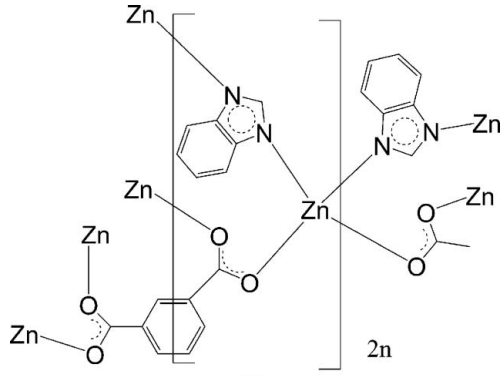
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
Some non-H atoms missing
R factor = 0.025
wR factor = 0.070
Data-to-parameter ratio = 16.4

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

Comment

Coordination polymers with a variety of supramolecular structures have been studied extensively because of their novel topologies and potential applications as functional materials (Eddaoudi *et al.*, 2002). However, compounds containing deprotonated benzimidazolate (bzim) ligands have been rarely studied (Huang *et al.*, 2003). We now report the title compound, (I), which is a new coordination polymer containing Zn^{2+} cations, bzim anions, and the benzene-1,3-dicarboxylate anion (1,3-BDC). These species combine in a 2:2:1 ratio to ensure charge balance.



(I)

In compond (I), the Zn atom is coordinated by two N atoms of two different bzim ligands and two O atoms from two different 1,3-BDC ligands in a slightly distorted tetrahedral geometry (Fig. 1). The bond lengths (Table 1) are normal (Allen *et al.*, 1987). The C—O bond lengths of the 1,3-BDC species imply charge delocalization.

The complete 1,3-BDC dianion is generated by crystallographic twofold rotation symmetry and serves to link four Zn^{2+} ions together. The bzim species acts as a bridge between two zinc ions. This connectivity results in a three-dimensional reticular coordination polymer containing honeycomb-like channels with dimensions of 5.9 × 4.0 Å along [100] (Fig. 2).

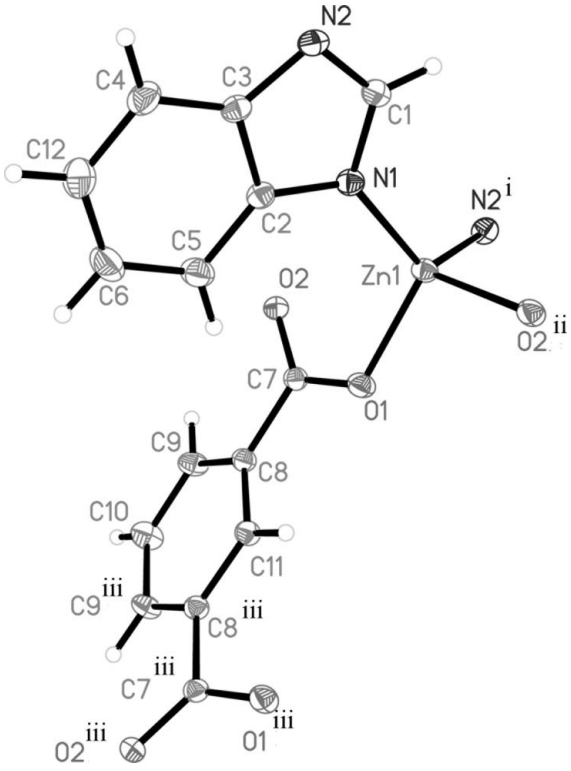


Figure 1
The asymmetric unit of (I), expanded to show the complete 1,3-BDC ligand and the Zn coordination. Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for the H atoms). [Symmetry codes: (i) $\frac{1}{2}-x, -y, \frac{1}{2}+z$; (ii) $\frac{1}{2}+x, +y, \frac{1}{2}-z$; (iii) $x, \frac{1}{2}-y, z$.]

Experimental

Benzimidazole (0.23 g, 2 mmol), 1,3-H_2BDC (0.17 g, 1 mmol) and zinc acetate dihydrate (0.44 g, 2 mmol) in water (18 ml) were stirred for 30 min, then the pH was adjusted to 8.0 with 0.1 *M* aqueous KOH. The mixture, with a total volume of 21 ml, was heated at 393 K for 8.5 d in a sealed 25 ml Teflon-lined stainless steel vessel under autogenous pressure. After the reaction mixture had been slowly cooled to room temperature at a rate of 4 K h^{-1}, yellow crystals of (I) were collected by filtration, washed with distilled water and dried in air (yield 23% based on Zn).

Crystal data

$[Zn_2(C_8H_4O_4)(C_7H_5N_2)_2]$
M_r = 529.12
Orthorhombic, *Pnma*
a = 8.8679 (6) Å
b = 22.2946 (15) Å
c = 10.1532 (7) Å
V = 2007.4 (2) Å^3
Z = 4
Mo *Kα* radiation
μ = 2.43 mm^{-1}
T = 293 (2) K
0.30 × 0.17 × 0.17 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.528, T_{max} = 0.689
11274 measured reflections
2430 independent reflections
2008 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

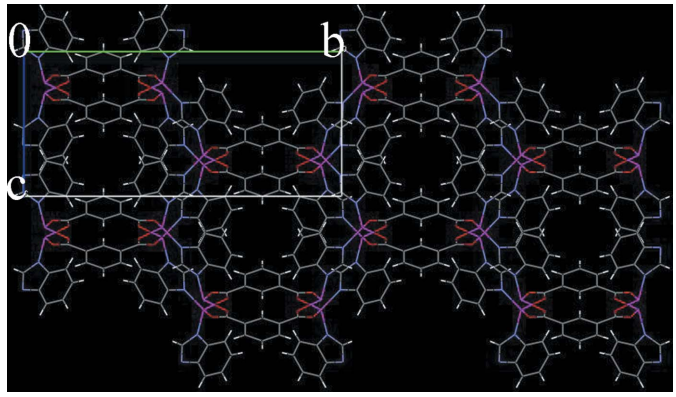


Figure 2
The honeycomb-like channels in the extended structure of (I), viewed along the *a* axis.

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.070
S = 1.01
2430 reflections
148 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—N1	1.9770 (16)	Zn1—O2^{ii}	2.0261 (14)
Zn1—N2^{i}	1.9674 (16)	C7—O2	1.260 (2)
Zn1—O1	1.9651 (14)	C7—O1	1.262 (2)

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

All H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding atoms, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXL97*.

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