Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[bis(μ_3-3-amino-1,2,4-triazolato)-(μ_2-glutarato)dizinc(II)]

Zhi-Qiang Zheng,* Chong-Wu Liu and Bin Lin

Affil Ated Stomatological Hospital, Fujian Medical University, Fuzhou, Fujian 350002, People's Republic of China

Correspondence e-mail: oliverzq@hotmail.com

Received 20 February 2007
Accepted 27 March 2007

In the title compound, $[Zn_2(C_5H_6O_4)(C_2H_3N_4)_2]_n$, one of the Zn atoms is four-coordinated by three N atoms from three 3-amino-1,2,4-triazolate ligands and one O atom from the glutarate ligand, while the other Zn atom is five-coordinated by three N atoms from three 3-amino-1,2,4-triazolate ligands and two O atoms from the glutarate ligand. The binuclear unit interacts through glutarate and 3-amino-1,2,4-triazolate ligands, leading to a polymeric three-dimensional structure.

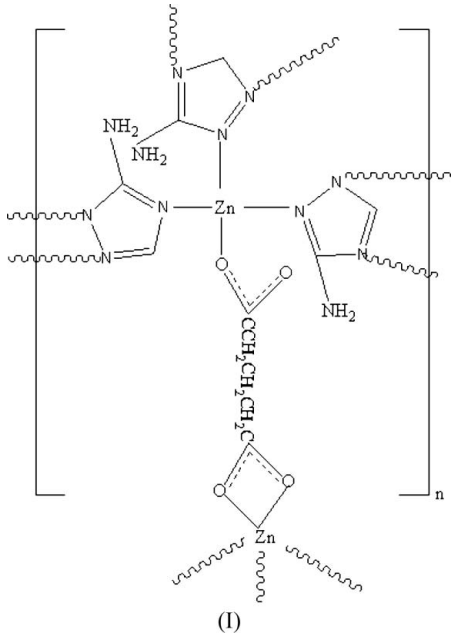
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.035
wR factor = 0.091
Data-to-parameter ratio = 17.5

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

Comment

The design and synthesis of inorganic coordination polymeric complexes have been extensively studied due not only to their intriguing structural topologies, but also to their unexpected properties as functional materials (Noro *et al.*, 2000; Yaghi *et al.*, 1998). Accordingly, the design of ligands is crucial to the construction of specific inorganic coordination polymeric complexes. This concept has been demonstrated by a great variety of structural topologies of discrete supramolecular complexes or infinite supramolecular arrays, such as molecular racks and grids as well as helicates. In general, (i) the multiple coordination sites of the ligand can form structures of higher dimensions and (ii) the high symmetry of the ligand may result in novel structures. Based on the above considerations, we chose glutaric acid and 3-amino-1,2,4-triazole ligands as bridging ligands. Thus, a Zn complex, (I), with a polymeric structure has been obtained.



(I)

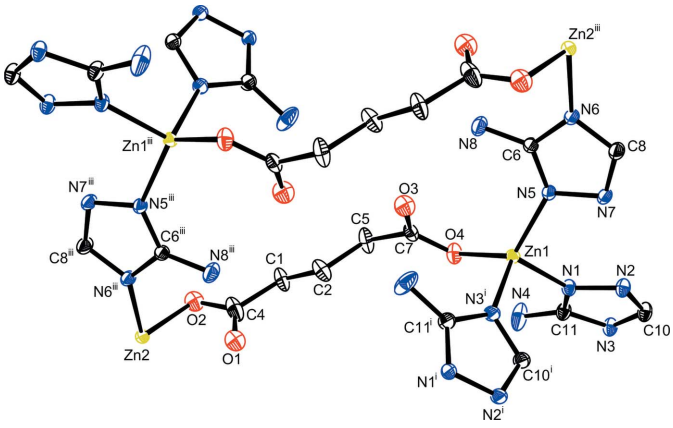


Figure 1
A portion of the polymeric structure, showing two connected dinuclear units with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $y-\frac{3}{4}, \frac{5}{4}-x, z-\frac{3}{4}$; (iii) $1-x, 2-y, 2-z$.]

The asymmetric unit of (I) is built up from two Zn(II) ions, two 3-amino-1,2,4-triazolate ligands and one glutarate ligand. The Zn1 ion is four-coordinated (distorted tetrahedral coordination geometry) by three N atoms from three 3-amino-1,2,4-triazolate ligands and one O atom from the glutarate ligand, while the Zn2 ion is five-coordinated (nearly square-pyramidal geometry) by three N atoms from three 3-amino-1,2,4-triazolate ligands and two O atoms from the glutarate ligand (Fig. 1), with the Zn—N bond lengths ranging from 1.991 (2) to 2.028 (2)Å and Zn—O bond lengths ranging from 1.958 (2) to 2.385 (3)Å. The glutarate ligands in this structure have two coordination modes; one carboxylate group is linked to Zn in a monodentate mode while the other carboxylate is linked to Zn in a bidentate mode. The 3-amino-1,2,4-triazolate ligand connects three Zn atoms. The distance between the two Zn atoms is 3.548 (1)Å, indicating no metal–metal interaction. Finally, the binuclear units interact through glutarate and 3-amino-1,2,4-triazolate ligands, giving a three-dimensional supramolecular structure.

Experimental

A solution (15 ml, H_2O–CH_3OH, 1:1) containing $Zn(OAc)_2$ (0.5 mmol), NaOH (0.2 mmol), glutaric acid (0.5 mmol) and 3-amino-1,2,4-triazole (1 mmol) was stirred at room temperature for 24 h and then filtered. The filtrate was kept at room temperature in the dark for several weeks to give white crystals of (I).

Crystal data

$[Zn_2(C_5H_6O_4)(C_2H_3N_4)_2]$
M_r = 427.05
Tetragonal, $I4_1/a$
a = 19.734 (3) Å
c = 16.293 (5) Å
V = 6345 (2) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 3.06 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.10 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2000)
T_{min} = 0.469, T_{max} = 0.728
22369 measured reflections
3646 independent reflections
3582 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.091
S = 1.07
3646 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.00 e Å^{-3}
$\Delta\rho_{min}$ = −0.98 e Å^{-3}

All H atoms were positioned geometrically and treated as riding, with C—H = 0.93 (aromatic) or 0.97Å (methylene), N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N). The highest residual density peak is located at (0.5612, 1.2190, 1.5396).

Data collection: *CrystalClear* (Rigaku, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

This work was supported by the Youth Natural Science Foundation of Fujian Sanitary Office under Project No. 2006–1–20.

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