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Poly[μ_2-4-aminobenzoato-aqua-μ_2-nitrato-zinc]

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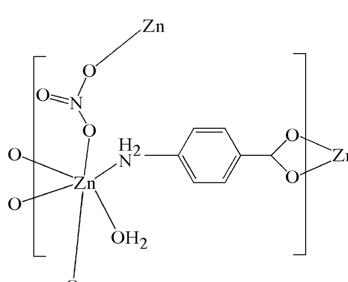
In the title compound, $[Zn(C_7H_6NO_2)(NO_3)(H_2O)]_n$, the Zn atom is coordinated by two nitrate ions, one aqua molecule and two 4-aminobenzoate ions in a distorted octahedral geometry. The structure of the compound exhibits a two-dimensional layer, which is formed by the interconnection of $[Zn(C_7H_6NO_2)(H_2O)]_n$ chains *via* μ_2-nitrate bridges or by the interconnection of $[Zn(NO_3)(H_2O)]_n$ chains *via* μ_2-4-aminobenzoate bridges.

Comment

Metal–organic framework materials have made rapid progress in recent years because this class of materials may have interesting physicochemical properties and potential applications such as adsorption, ion exchange and shape-selective catalysis, and as nonlinear optical and magnetic materials. A number of rigid or flexible bridging ligands have been employed to construct metal–organic materials, including one-, two- or three-dimensional frameworks. Generally, the construction of frameworks can be achieved using either covalent bonds or weaker intermolecular forces, *e.g.* hydrogen bonds, aryl–aryl interactions, *etc.*



(I)

As a bifunctional organic ligand, 4-aminobenzoic acid (4-abaH) has been reported in coordination chemistry because of the richness of its coordination modes. Firstly, 4-abaH can act as a carboxylic acid synthon and also as a good monodentate ligand through the amine group (Le Fur & Masse, 1996; Chen & Chen, 2002). Secondly, deprotonated 4-aminobenzoic acid can act as a monodentate ligand through a carboxylate O atom (Sundberg *et al.*, 1998; Chandrasekhar *et al.*, 1988; Amiraslanov *et al.*, 1979), chelating and/or bridging ligands through its amide and/or carboxylate groups (Zheng *et al.*, 2001; Rzaezynska & Belskii, 1994; Hauptmann *et al.*, 2000). Finally, 4-abaH may be protonated to form organic cation templating agents (Wang *et al.*, 2002). Recently, a compound containing mixed 4-aminobenzoate and another nitrogen-donor ligand has been synthesized in our group (Zhang & Lu, 2005). As part of our continuing investigation of this type of compound, we report here the synthesis and characterization of the title complex, (I).

As shown in Fig. 1, the Zn atom of (I) is coordinated by two chelating carboxylate O atoms from one 4-aminobenzoate ion, two bridging nitrate O atoms, an N atom from another 4-aminobenzoate ion and one coordinated water molecule in a distorted octahedral geometry. The two nitrate O atoms [O4 and O5^{ii}; symmetry code: (ii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$] are at the apical positions [Zn—O = 2.124 (2) and 2.333 (2) Å, and O—Zn—O = 165.97 (8)°], while the two carboxylate O atoms [O1^{i} and O2^{i}; symmetry code: (i) $-\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$], the amine N atom (N1) and the water O atom (O3) define the equatorial plane (mean deviation = 0.224 Å). The Zn atom is raised above the equatorial plane by 0.284 Å towards the apical atom O4.

The 4-aminobenzoate ligand adopts a chelating/bridging coordination mode (Wang *et al.*, 2002), linking two neighbouring Zn coordination centres to form a one-dimensional chain, $[Zn(H_2O)(C_7H_6NO_2)]_n$, with a Zn—N—C bond angle of 115.9 (2)° and a Zn···Zn separation of 9.40 (2) Å. Similarly, the nitrate ion acts as a μ_2-bridge (Huang *et al.*, 2004; Ling *et al.*, 2004), linking two neighbouring metal centres to form another one-dimensional chain, $[Zn(NO_3)(H_2O)]_n$, with Zn—O—N bond angles of 112.5 (2) and 124.9 (2)°, and a Zn···Zn separation of 5.74 (3) Å. Thus, compound (I) exhibits a two-dimensional layer-like structure (Fig. 2), which is formed by the interconnection of neighbouring $[Zn(H_2O)(C_7H_6NO_2)]_n$ chains *via* μ_2-nitrate bridges or by the interconnection of neighbouring $[Zn(NO_3)(H_2O)]_n$ chains *via* μ_2-4-aminobenzoate bridges. The two-dimensional layer consists of rectangular grids with dimensions of 9.40 (2) × 5.74 (3) Å, based on the Zn···Zn distances.

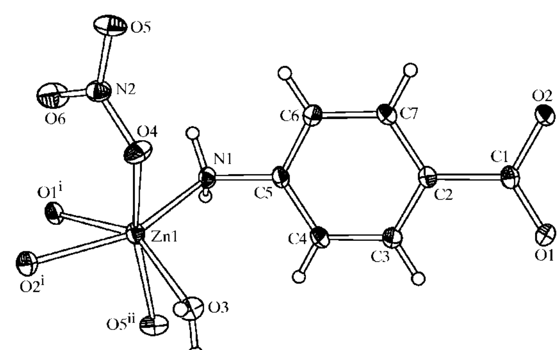


Figure 1
A locally expanded unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $-\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$; (ii) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$.]

It is noteworthy that there is hydrogen bonding in the title compound. One weak interaction occurs between the layers. The water ligand forms hydrogen bonds with the carboxylate O atoms of the 4-aminobenzoate, with O—H···O distances of 2.720 (3) and 2.721 (3) Å (Table 2). Such hydrogen-bonding interactions consolidate the structural architecture and further extend the two-dimensional layers into a three-dimensional framework.

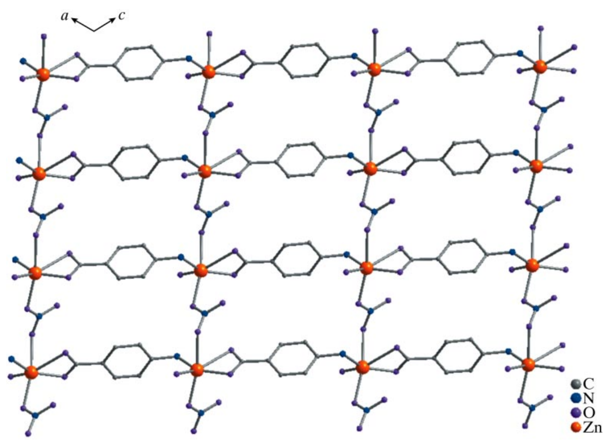


Figure 2
The two-dimensional structure of (I). All H atoms have been omitted for clarity.

Experimental

An ethanol solution (8 ml) of 2,2′-bipyridine (1.2 mmol) and 4-aminobenzoic acid (1.6 mmol) was added slowly to an aqueous solution (10 ml) of $Zn(NO_3)_2{\cdot}6H_2O$ (1 mmol) with continuous stirring for 30 min. The reaction mixture was then allowed to stand at room temperature undisturbed for two weeks, resulting in colourless crystals of (I) (yield 71%). Analysis calculated for $C_7H_8N_2O_6Zn$: C 29.86, H 2.86, N 9.95%; found: C 29.81, H 2.71, N 9.89%.

Crystal data

$[Zn(C_7H_6NO_2)(NO_3)(H_2O)]$
M_r = 281.52
Monoclinic, $P2_1/n$
a = 10.6087 (16) Å
b = 9.4342 (10) Å
c = 11.1367 (19) Å
β = 118.000 (6)°
V = 984.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.51 mm^{-1}
T = 293 (2) K
0.20 × 0.16 × 0.08 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.760, T_{max} = 1.000 (expected range = 0.621–0.818)
7449 measured reflections
2256 independent reflections
1864 reflections with $I > 2\sigma(I)$
R_{int} = 0.044

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.092
S = 1.11
2256 reflections
153 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

The H atoms of the coordinated water molecule were located in a difference Fourier map and refined isotropically. The remaining H atoms were constrained to an ideal geometry, with N—H = 0.90 Å and C—H = 0.93 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N).

Table 1
Selected geometric parameters (Å, °).

Zn1—O2^{i}	1.998 (2)	Zn1—O4	2.124 (2)
Zn1—O3	2.009 (2)	Zn1—O5^{ii}	2.333 (2)
Zn1—N1	2.045 (3)	Zn1—O1^{i}	2.470 (2)
O2^{i}—Zn1—O3	105.20 (9)	O3—Zn1—O5^{ii}	78.81 (10)
O2^{i}—Zn1—N1	143.27 (9)	N1—Zn1—O5^{ii}	87.07 (10)
O3—Zn1—N1	109.52 (10)	O4—Zn1—O5^{ii}	165.97 (8)
O2^{i}—Zn1—O4	99.50 (9)	O3—Zn1—O1^{i}	148.46 (9)
O3—Zn1—O4	87.83 (10)	N1—Zn1—O1^{i}	86.17 (8)
N1—Zn1—O4	93.47 (10)	O4—Zn1—O1^{i}	119.26 (8)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3B···O2^{iii}	0.83 (4)	1.89 (4)	2.720 (3)	177 (4)
O3—H3C···O1^{iv}	0.85 (5)	1.88 (5)	2.721 (3)	171 (5)

Symmetry codes: (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+2, -y+1, -z+1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV3098). Services for accessing these data are described at the back of the journal.

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