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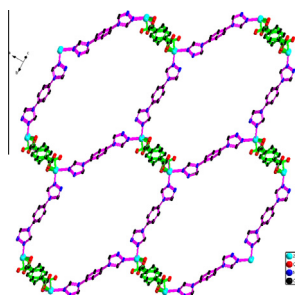
Tuning zinc coordination architectures by benzenedicarboxylate position isomers and bis(triazole)

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HIGHLIGHTS

- Three zinc coordination polymers based on benzenedicarboxylate position isomers were synthesized.
- A 5-fold interpenetrated three-dimensional diamondoid network.
- The luminescence and thermal stability.
- The rigid 4-substituted 1,2,4-triazole ligand 1,4-bis(1,2,4-triazol-4-yl)benzene.

GRAPHICAL ABSTRACT



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ABSTRACT

Three position isomers 1,2-, 1,3-, 1,4-benzenedicarboxylate and 1,4-bis(1,2,4-triazol-4-yl)benzene were used to assembly zinc(II) coordination polymers $\{[Zn_2(\text{btX})_{0.5}(1,2\text{-bdc})_2(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}\}_n$ (**1**), $\{[Zn(\text{btX})(1,3\text{-bdc})]\cdot 2\text{H}_2\text{O}\cdot(\text{DMF})\}_n$ (**2**) and $\{[Zn(\text{btX})(1,4\text{-bdc})]\cdot 3\text{H}_2\text{O}\}_n$ (**3**). **1** is a (3,4,4,4)-connected two-dimensional network with point symbol $(4^2\cdot 6)(4^4\cdot 6^2)(4^3\cdot 6^2\cdot 8)(4^2\cdot 6\cdot 10^3)$. **2** shows a two-dimensional (4,4) network. **3** exhibits a 5-fold interpenetrated three-dimensional diamondoid network. The structural versatility shows that the structures of coordination polymers can be tuned by the position isomers ligands. The luminescence and thermal stability were investigated.

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Introduction

The rational design and synthesis of coordination polymers is of great interest in modern inorganic chemistry stemming from their potential applications as functional materials such as luminescence, catalysis and gas absorption and their intriguing variety of topologies [1–13]. In order to get such intriguing topologies and functional materials, the crucial step is to employ appropriate

organic building blocks as well as metal ions. Because of the diversity of the coordination modes and high structural stability, polycarboxylate ligands are frequently used for the construction of MOFs. The position isomers 1,2-, 1,3-, 1,4-benzenedicarboxylate are rigid, planar molecules and well bridging ligands in the synthesis of novel MOFs [14–18].

In the other hand, flexible bidentate N-donors ligands such as bis(imidazole) [19,20] and 1-substituted bis(triazole) [21–24], and ligands are widely used to construct coordination polymers because flexible ligands can adopt different conformations according to the geometric needs of the different metal ions. In previous work, we synthesized a lot of coordination polymers using flexible

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1-substituted bis(triazole) building blocks, such as 1,2-bis(1,2,4-triazol-1-yl)ethane (bte) [25], 1,3-bis(1,2,4-triazol-1-yl)propane (btp) [26], 1,4-bis(1,2,4-triazol-1-yl)butane (btb) [27] and 1,4-bis(1,2,4-triazol-1-ylmethyl)benzene (bbtz) [28].

In contrast to 1-substituted-1,2,4-triazole derivatives, the research of coordination polymers based on 4-substituted-1,2,4-triazole derivatives is only just beginning [29–32]. We also achieved a series of fantastic frameworks based on flexible 4-substituted-1,2,4-triazole ligand 1,2-bis(1,2,4-triazol-4-yl)ethane (btre) [33,34], such as $\{[\text{Cd}(\text{btre})\text{Cl}]\cdot\text{OH}\}_n$, $\{[\text{Cd}(\text{btre})\text{Cl}][\text{CdCl}(\text{dca})_2]\cdot 0.5\text{H}_2\text{O}\}_n$ and $\{[\text{Zn}(\text{btre})_{0.5}(\text{OH}-\text{bdc})(\text{H}_2\text{O})_2]\cdot 1.5\text{H}_2\text{O}\}_n$. The 4-substituted-1,2,4-triazole bridging ligand 1,4-bis(1,2,4-triazol-4-yl)benzene (btx) should be a good rigid building block to construct coordination polymers with novel structures.

With this background information, we sought to investigate the role of three isomeric ligands 1,2-, 1,3-, 1,4-benzenedicarboxylate (1,2-bdc, 1,3-bdc, 1,4-bdc) and 1,4-bis(1,2,4-triazol-4-yl)benzene (btx) (Scheme 1) in the construction of zinc(II) coordination polymers. In the present work, three Zn(II) coordination polymers $\{[\text{Zn}_2(\text{btx})_{0.5}(1,2-\text{bdc})_2(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}\}_n$ (**1**), $\{[\text{Zn}(\text{btx})(1,3-\text{bdc})]\cdot 2\text{H}_2\text{O}\cdot(\text{DMF})\}_n$ (**2**) and $\{[\text{Zn}(\text{btx})(1,4-\text{bdc})]\cdot 3\text{H}_2\text{O}\}_n$ (**3**) were synthesized. **1** is a (3,4,4,4)-connected two-dimensional network. **2** shows a two-dimensional (4,4) network. **3** exhibits a 5-fold interpenetrated three-dimensional diamondoid network which is short communication [35]. The luminescence and thermal stability were investigated.

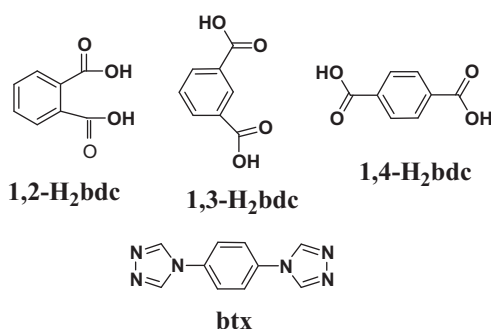
Experimental section

Materials and general methods

All reagents were of analytical grade and used without further purification. Elemental analyses for C, H and N were performed on a Perkin–Elmer 240C analyzer. IR spectra were obtained for KBr pellets on a Nicolet 170SX FT-IR spectrophotometer in the 4000–400 cm^{-1} region. The luminescence measurements were carried out in the solid state at room temperature and the spectra were collected with a Perkin–Elmer LS50B spectrofluorimeter. TGA was carried out using a Thermal Analyst 2100 TA Instrument and SDT 2960 Simultaneous TGA-DTA Instrument in flowing dinitrogen at a heating rate of 10 $^\circ\text{C}/\text{min}$.

Synthesis of $\{[\text{Zn}_2(\text{btx})_{0.5}(1,2-\text{bdc})_2(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}\}_n$ (**1**)

A solution of 1,2- H_2bdc (0.2 mmol) in 10 mL of H_2O was adjusted to pH 6 with 0.35 mL of a 1.0 M NaOH solution and $\text{Zn}(\text{NO}_3)_2\cdot 6\text{H}_2\text{O}$ (0.2 mmol) was added with stirring. Then 5 mL DMF solution of btx (0.1 mmol) was added and continuously stirred for 10 min. The mixture solution was filtered and stood for one month to give colorless single crystals of **1** (0.041 g, 68% yield). Anal. Calcd. for $\text{C}_{21}\text{H}_{16}\text{N}_3\text{O}_{10}\text{Zn}_2$ (**1**) C, 41.96; H, 2.68; N, 6.99.



Scheme 1. The Ligands 1,2- H_2bdc , 1,3- H_2bdc , 1,4- H_2bdc and btx.

Found: C, 41.82%; H, 2.61%; N, 6.91%. IR data (cm^{-1}): 3436 m, 1621s, 1542s, 1487w, 1447w, 1408s, 1257w, 1087w, 1056w, 843w, 758 m, 710w, 661w, 503w.

Synthesis of $\{[\text{Zn}(\text{btx})(1,3-\text{bdc})]\cdot 2\text{H}_2\text{O}\cdot(\text{DMF})\}_n$ (**2**)

A solution of 1,3- H_2bdc (0.2 mmol) in 10 mL of H_2O was adjusted to pH 6 with 0.35 mL of a 1.0 M NaOH solution and $\text{Zn}(\text{NO}_3)_2\cdot 6\text{H}_2\text{O}$ (0.2 mmol) was added with stirring. Then 5 mL DMF solution of btx (0.2 mmol) was added and continuously stirred for 10 min. The mixture solution was filtered and stood for one month to give colorless single crystals of **2** (0.067 g, 61% yield). Anal. Calcd. for $\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_7\text{Zn}$ (**2**) C, 45.79; H, 4.21; N, 7.80. Found: C, 45.65%; H, 4.13%; N, 7.72%. IR data (cm^{-1}): 3382s, 3164m, 1621s, 1566s, 1448w, 1384s, 1244w, 1156w, 1099w, 1044w, 849w, 747w, 722m, 637w, 540w.

Synthesis of $[\text{Zn}(\text{btx})(1,4-\text{bdc})]\cdot 3\text{H}_2\text{O}$ (**3**)

A solution of 1,4- H_2bdc (0.2 mmol) in 10 mL of H_2O was adjusted to pH 6 with 0.35 mL of a 1.0 M NaOH solution and $\text{Zn}(\text{NO}_3)_2\cdot 6\text{H}_2\text{O}$ (0.2 mmol) was added with stirring. Then 5 mL DMF solution of btx (0.2 mmol) was added and continuously stirred for 10 min. The mixture solution was filtered and stood for one month to give colorless single crystals of **3** (0.064 g, 65% yield). Anal. Calcd. for $\text{C}_{18}\text{H}_{18}\text{N}_6\text{O}_7\text{Zn}$ (**3**) C, 43.61; H, 3.66; N, 16.96. Found: C, 43.52%; H, 3.60%; N, 16.89%. IR data (cm^{-1}): 3430s, 1572s, 1542s, 1437w, 1390s, 1318w, 1257w, 1099m, 1050w, 1013w, 837m, 752m, 625w, 528w.

X-ray crystallography

Suitable single crystals of **1**, **2** and **3** were carefully selected under an optical microscope and glued to thin glass fibers. The diffraction data were collected on the Rigaku Mercury CCD diffractometers with graphite monochromated Mo K α radiation. Intensities were collected by the ω scan technique. The structures were solved by direct methods and refined with full-matrix least-squares technique (SHELXTL-97) [36]. The positions of hydrogen atoms of organic ligands were placed in their geometrically idealized positions and constrained to ride on their parent atoms. The parameters of the crystal data collection and refinement of **1**, **2** and **3** are given in Table 1. Selected bond lengths and bond angles are given in Table 2.

Results and discussion

Crystal structures

Single-crystal X-ray analysis revealed that **1** crystallizes in the monoclinic system with C2/c space group. The asymmetric unit of **1** consists of two Zn(II) atoms, half btx, two 1,2-bdc, one coordination water and disordered lattice water molecules. The Zn1(II) atom is five-coordinated and surrounded by three carboxylate oxygen atoms from three 1,2-bdc, one oxygen atom from coordination water and one triazole nitrogen atom from btx ligand in a distorted trigonalbipyramidal geometry (ZnO_4N) (Fig. 1a). The Zn2(II) atom is four-coordinated and surrounded by four carboxylate oxygen atoms from four 1,2-bdc ligands in a distorted tetrahedral geometry (ZnO_4). There are two kinds of 1,2-bdc ligands. One carboxylate group (O1O2) of one 1,2-bdc ligand shows bidentate coordination mode and coordinates two Zn(II) atoms. The other carboxylate group (O3O4) acts as monodentate coordination mode and links one Zn(II) atom. Two carboxylate groups (O5O6 and O7O8) of the other 1,2-bdc ligand both show bidentate coordination mode and

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