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Transition metal coordination complexes based on V-shaped bis-triazole ligand: Syntheses, structures and properties

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Hydrothermal reactions of 1,3-bis(1,2,4-triazol-1-yl)benzene (btb) and M(NO₃)₂ (M = Co²⁺ (1), Cu²⁺ (2)) afforded two new coordination polymers, $[Co(btb)_2(NO_3)(H_2O)]_n \cdot NO_3 \cdot H_2O$ (1) and $[Cu(btb)_2(NO_3)_2]_n$ (2), respectively. Single-crystal X-ray diffraction reveals that 1 crystallizes in the space group P2₁/m and 2 crystallizes in the space group Pī, both showing a double-stranded chain structure. The 1D chains are interconnected via $\pi \cdots \pi$ interactions to lead to 2D ladder-like supramolecular architectures. In addition, magnetic behavior and thermal stability of 1 and 2 have been investigated. For 1, weak antiferromagnetic interactions are observed at low temperature, and the data obey the Curie–Weiss law $\chi_M = C/(T-\theta)$, with C = 3.22 cm³·mol⁻¹·K and $\theta = -10.39$ K. For 2, the decrease of the $\chi T vs$. T curve at low temperature is the result of intermolecular antiferromagnetic magnetic interactions.

Keywords: Crystal structure; 1,3-Bis(1,2,4-triazol-1-yl)benzene; Transition metal; Thermal stability; Magnetic property

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1. Introduction

Coordination polymers have attracted extensive interest not only due to the structural diversity but also due to their fascinating properties, such as luminescence, chemical sensing, magnetism, gas storage and separation, and catalysis [1-12]. The main step for preparing polymeric coordination complexes with versatile topologies and fascinating properties is to select multidentate organic ligands as building blocks [13-17]. A number of N-donor ligands (such as pyridyl-type ligands and azole-type ligands) have been used to build coordination polymers with attractive architectures and functional properties [18-25]. Among the various N-donor bridging ligands, 1,2,4-triazole and its derivatives have proven to be good candidates for the construction of coordination polymers with varied topologies and functional properties because of their versatile bridging feature [26-29]. 1,3-Bis(1,2,4-triazol-1-yl)benzene (abbreviated as btb) is a rigid ligand, which contains two 1,2,4-triazole rings and can act as a multidentate bridging ligand. In this contribution, two new complexes, [Co(btb)₂(NO₃)(H₂O)]_n·NO₃·H₂O (1) and [Cu(btb)₂(NO₃)₂]_n (2), were isolated by reactions of btb with MNO₃·3H₂O (M = Co, Cu). In addition, the structural character, magnetic behavior and thermal stability of 1 and 2 have been investigated.

2. Experimental

2.1. General considerations

Triazole and Cul were purchased from Tianjin Heowns Biochem LLC and 1,3-dibromobenzene from Meryer Chemical Technology Co., Ltd. The solvent (CH₃)₂SO for the reaction was dried over 4 Å molecular sieve and distilled under reduced pressure. The elemental analyses (C, H and N) were carried out on a Perkin–Elmer elemental analyzer. The ¹H NMR spectrum was recorded with Bruker 400 MHz spectrometer instruments in CDCl₃. Powder X-ray diffraction measurements were recorded on a D/Max-2500 X-ray diffractometer using Cu-Ka radiation. Thermogravimetric experiments were performed on a NETZSCH TG 209 instrument with a heating rate of 10 °C·min⁻¹ under nitrogen conditions. Direct-current (dc) magnetic susceptibilities of crystalline samples were measured on an MPMS-7 SQUID magnetometer. The data were corrected for the diamagnetism of the samples using Pascal constants. Alternatingcurrent (ac) susceptibilities were performed on the same magnetometer.

2.2. Synthesis of ligand 1,3-bis(1,2,4-triazol-1-yl)benzene (btb)

Triazole (2.18 g, 12.8 mmol), 1,3-dibromobenzene (0.75 g, 3.2 mmol), K₂CO₃ (2.96 g, 21.0 mmol), CuI (0.03 g, 0.13 mmol) and 7 drops of N,N'-dimethylethanamine were mixed in 15 ml dry DMSO solution and heated at 150 °C for 36 h under a nitrogen atmosphere. Then the mixture was cooled to room temperature, filtered and the solid was washed with a few milliliters of DMSO. The filtrate was distilled under reduced pressure to remove the solvent and the residue was extracted with CH_2Cl_2 (6×30 mL). The organic layer was dried over magnesium sulfate and the solvent removed using a rotary evaporator to give the crude product, which was further separated under column chromatography to give 0.54 g of btb. Yield: 79%; ¹H NMR [CDCl₃]: 8.61 (s, 2H), 8.09 (s, 3H), 7.68 (t, 1H), 7.66 (d, 1H), 7.60 (dd, 1H) ppm; elemental analysis calcd (%) for $C_{10}H_8N_6$: C, 56.59; H, 3.80; N, 39.61. Found: C, 56.37; H, 3.68; N, 39.42. The ¹H NMR spectrum is shown in the Supporting Information section as figure S1.

2.3. Synthesis of $[Co(btb)_2(NO_3)(H_2O)]_n \cdot NO_3 \cdot H_2O$ (di-1,3-bis(1,2,4-triazol-1yl)benzenemonoaquamononitratocobalt(II)monoaquanitrate (1))

A mixture of Co(NO₃)₂·6H₂O (29 mg, 0.1 mmol), btb (21 mg, 0.1 mmol), H₂O (4 mL) and CH₃OH (2 mL) was added to a Parr Teflon-lined stainless steel vessel, and then the vessel was sealed and heated to 120 °C for 3 days. After that the autoclave was cooled to room temperature at a rate of 1.5 °C/h⁻¹, the mixture was filtered, and a pink crystalline product **1** (30.24 mg) was obtained by evaporating the filtrate for about a week (yield 47% based on Co). Anal. Calc. for $C_{20}H_{20}CoN_{14}O_8$ (643.43): C, 43.55; H, 3.13; N, 19.31. Found: C, 43.26; H, 3.32; N, 19.18%.

2.4. Synthesis of $[Cu(btb)_2(NO_3)_2]_n$ (di-1,3-bis(1,2,4-triazol-1-yl)benzenedinitratocopper(II) (2))

Blue crystals of **2** (27.54 mg) were obtained by adopting the same synthetic procedure as **1** only with the use of $Cu(NO_3)_2 \cdot 4H_2O$ instead of $Co(NO_3) \cdot 6H_2O$. Yield: 45% (based on Cu). Anal. Calc. for $C_{20}H_{16}CuN_{14}O_6$ (612): C, 39.25; H, 2.61; N, 32.05. Found: C, 39.08; H, 2.44; N, 31.88%.

2.5. X-ray crystallography

Single-crystal X-ray diffraction measurements for **1** and **2** were carried out on a Bruker Smart CCD diffractometer with a graphite crystal monochromator situated in the incident beam for data collection at 296(2) K. Semi-empirical multiscan absorption corrections were applied by SCALE3 ABSPACK, and the programs CrysAlisPro were used for integration of the diffraction profiles [30, 31]. Structures were solved by direct methods and refined with the full-matrix leastsquares technique using the ShelXT and ShelXL programs for **1** [32-34] and the SHELXS-97 and SHELXL-97 programs for **2** [35]. Anisotropic thermal parameters were assigned to all nonhydrogen atoms, and hydrogens were located and refined isotropically. Crystallographic data for **1** and **2** are summarized in table 1.

3. Results and discussion

3.1. Crystal structure of [Co(btb)₂(NO₃)(H₂O)]_n·NO₃·H₂O (1)

Single-crystal X-ray diffraction analyses show that 1 belongs to the monoclinic $P2_1/m$ space group with Z = 2. As shown in figure 1, the asymmetric unit contains one crystallographically unique Co^{2+} ion, two btb ligands, a terminally coordinated NO₃ anion, a coordinated water molecule, one free NO₃ anion and one crystal lattice water molecule. Each Co^{II} ion lies on a crystallographic inversion center and adopts a slightly distorted octahedral {CoN₄O₂} environment involving four nitrogen atoms from four btb ligands, one oxygen atom from a monodentate nitrate and one oxygen atom from one aqua ligand. The Co–O bond distances are in the range of 2.053(10)–2.136(10) Å, and the Co–N bond lengths are 2.149(5) and 2.142(6) Å, respectively. The Co^{II} nodes are connected to each other to form an infinite 1D chain that consists of a 20-membered bimetallic macrocycle building block, in which the free water guest molecules and NO₃⁻ anions are located. The Co^{...}Co separation across the bridging btb ligand is 10.945(2) Å. Along the *b* direction, the $\pi \cdots \pi$ (3.547 Å, the distance between the two centers of the benzene rings) interactions with a slip angle of 6.43° help to generate an extended 2D framework (figure 1(c)). In addition, C1–H1···O4, C8–H8···O8, C1–H1···O4, C5–H5···O4 or C5–H5···O6 non-classical hydrogen-bonding interactions from NO₃⁻ and aqua oxygen atoms connect the chains to give a 3D supramolecular framework (figure S2). The crystal packing figure is shown in the Supporting Information and the chains are parallel to each other in *a* and *b* directions. The shortest distance of the Co^{II}···Co^{II} between the chains is 8.951 Å. The coordinated NO₃⁻ anions are disordered.

3.2. Crystal structure of $[Cu(btb)_2(NO_3)_2]_n$ (2)

Complex **2** crystallizes in the triclinic crystal system, space group Pī (table 1). As depicted in figure 2, Cu1 is six-coordinate with four nitrogen atoms, and two NO₃⁻ oxygen atoms, forming a distorted octahedral geometry. Every btb adopts a μ_2 -bridging mode and the dihedral angles between the benzene ring and the two triazole rings are 22.08 and 66.28°, respectively, which shows a certain degree of distortion. Acting as a bidentate bridging ligand, a pair of btb ligands chelate the Cu1 centers by triazolyl N donors with the Cu…Cu separation being 10.588(3) Å, which leads to a double-stranded chain (figure 2b). In the *bc* plane, the $\pi \dots \pi$ (3.588 Å, the distance between the two centers of the benzene rings) interactions with a slip angle of 9.90° help to generate an extended 2D framework. The chains are interlocked to each other through NO₃⁻ and crosslinked by weak hydrogen bond interactions (C1–H2…O1, C2–H2…O2, C6–H6…O2) to give 3D supramolecular structures as shown in figure S3. The shortest Cu…Cu distance between the nearest chains is 7.376 Å.

Only one bis-imidazole benzene coordination polymer has been reported [36]. Li *et al.* synthesized [Zn(dib)(CH₃COO)₂]·2H₂O (dib, 1,4-di(1H-imidazol-1-yl)benzene) with a 1-D onestranded chain structure. In the compound, though the coordinating mode of the dib ligand is bisconnected, the structure of the compound is different from 1 and 2 because of the angle of the two imidazoles in the dib is 180° .

3.3. Magnetic properties of 1

The magnetic susceptibilities of 1 were measured under 1 kOe in the 2-300 K range and the magnetic behaviors are shown in figure 3. At room temperature, the value of $\chi_M T$ $(3.12 \text{ cm}^3 \cdot \text{mol}^{-1} \cdot \text{K})$ is considerably higher than the spin-only value of $1.87 \text{ cm}^3 \cdot \text{mol}^{-1} \cdot \text{K}$ for one $S = 3/2 \text{ Co}^{II}$ ion, which is due to the spin-orbit coupling of high-spin Co^{II} ions in an octahedral surrounding. Upon cooling, the $\chi_M T$ product decreases slowly and reaches the value of 2.88 cm³·mol⁻¹·K at 120 K. With further cooling, $\chi_M T$ decreases linearly to 1.81 cm³·mol⁻¹·K at 2 K. The data in the range of 2–300 K obey the Curie–Weiss law $\chi_M = C/(T-\theta)$, with C = 3.22 cm³·mol⁻¹·K and $\theta = -10.39$ K. The strong spin-orbital coupling of Co^{II} itself can lead to a negative θ value and a decrease of $\chi_M T$ at higher temperature, therefore the negative θ does not necessarily indicate dominant antiferromagnetic interaction between the metal centers. In the low temperature region, the rapid decrease of the value of $\chi_{\rm M}$ T is ascribed to the weak antiferromagnetic intermolecular interaction through supramolecular contacts (stacking contacts or H bonds). The M vs. H plot for 1 is shown in figure 3(b). M increases rapidly at low field, and reaching about 2.07 NB at 20 kOe. In the high field region, the increase of magnetization is slow, reaching 2.43 NB at 70 kOe, which is a little smaller than the value of 3 NB anticipated for one independent Co^{II} with S = 3/2 ground state. In order to probe the magnetic dynamics behavior for 1, alternating current (ac) magnetic susceptibilities were measured. As shown in figure 4, the out-of-phase signals did not show frequency dependence and maximum, which excluded the occurrence of magnetic ordering above 2.0 K.

3.4. Magnetic properties of 2

The room temperature value of $\chi_M T$ is 0.381 cm³·mol⁻¹·K (figure 5(a)), which coincides with the spin-only value of 0.375 cm³·mol⁻¹·K for one S = 1/2 Cu^{II} ion. As the temperature is lowered, the $\chi_M T$ product remains basically the same. The Cu···Cu distance across the long btb ligand is 10.59 Å, the magnetic interaction through btb bridge is expected to be very weak, so the complex exhibits no obvious magnetic interaction at the high temperature. In the low temperature, the abrupt fall of the value $\chi_M T$ is ascribed to the weak antiferromagnetic interaction. The variation of the magnetization (M) *vs*. the field (H) at 2 K in figure 5(b) further confirms the nature of the ground state in **2**.

3.5. The thermal analyses of 1 and 2

The thermal behaviors of **1** and **2** were studied by thermogravimetric analysis (TGA) under a nitrogen atmosphere in the temperature range of 0–800 °C. The experimental curves are shown in figure 6. The TGA result of **1** displays two step weight losses. The first weight loss of 4.9% from 90 to 125 °C should be attributed to the loss of free and coordinated water (calcd. 5.59%), and the second weight loss is ascribed to the loss of btb ligands and the nitrate ligand when the temperature is above 265 °C. The TG curve for **2** indicates that it is stable up to 275 °C. Under further heating, a rapid weight loss occurs, which is due to the departure of organic ligands and nitrate ligand.

4. Conclusion

Two new metal–organic frameworks have been constructed from btb and divalent transition metals. Both **1** and **2** exhibit one-dimensional double-stranded chains. In both of the complexes, the 1D chains assembled into 2D step-ladder supramolecular architectures interconnected by $\pi \cdots \pi$ interactions, which are further constructed into 3D supramolecular structures by weak hydrogen bond interactions. In both of the complexes, weak intermolecular antiferromagnetic interactions exist at low temperature.

Supplementary material

CCDC 1587236 (2) and 1587237 (1) contain the supplementary crystallographic data. These data can be obtained free of charge via www.ccdc.can.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Centre, 12 Union Road, Cambridge CB2 1EZ, UK; Fax: (+44) 1223-336033; or E-mail: deposit@ccdc.cam.ac.uk).

Acknowledgements

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Figure 1. (a) Coordination environments of Co^{II} ions in 1. (b) The 1D double chain of 1, encapsulating free NO₃⁻ anions and water as guest molecules. (c) Partial view of the 2D supramolecular network.



Figure 2. (a) Coordination environments of Cu^{II} ions in 2. (b) Partial view of the 1D doublestranded chain. (c) Packing in polymer direction along [001]. Hydrogens have been omitted for clarity.



Figure 3. (a) Temperature dependence of $\chi_M T$ for 1 at 1000 Oe. The curve of $\chi_M^{-1} vs$. T; the solid line is the linear fitting of the Curie–Weiss law. (b) The M vs. H plot for 1 measured at 2 K.



Figure 4. Temperature dependence of the imaginary of the in-phase (χ') and out-of-phase (χ'') components of the AC magnetic susceptibility for 1 in a zero DC field with an oscillation of 3.5 Oe.



Figure 5. (a) Temperature dependence of $\chi_M T$ for 2 at 1000 Oe. (b) The M vs. H plot for 2 measured at 2 K.



Figure 6. TGA curve for **1** and **2**. The sample was heated to 800 °C at the heating rate of 1.5 °C/min.

	1	2
Formula	$C_{20}H_{20}CoN_{14}O_8$	$C_{20}H_{16}CuN_{14}O_{6}$
Mr	643.43	612.01
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/m$	Pī
<i>a</i> (Å)	7.0754(5)	7.376(2)
<i>b</i> (Å)	16.9645(11)	8.719(3)
<i>c</i> (Å)	10.9454(6)	9.581(3)
α (°)	90	81.683(5)
β (°)	107.999(7)	74.957(5)
γ (°)	90	81.811(4)
$V(Å^3)$	1249.49(14)	585.2(3)
Ζ	2	2
ρ calc (Mg/m ³)	1.710	1.737
μ (mm ⁻¹)	6.093	1.006
<i>F</i> (000)	658	311
θ range (°)	4.247 - 67.076	2.215 - 26.498
Limiting indices	$-6 \le h \le 8$	$-9 \le h \le 9$
	$-20 \le k \le 20$	$-10 \le k \le 10$
	-13 ≤1 ≤ 12	$-5 \le l \le 12$
Reflns. collected	4743	3414
GOF on F^2	1.032	1.095
$R_{I}/wR_{2}\left[I > 2\sigma(I)\right]$	$R_1 = 0.0764,$	$R_1 = 0.0344,$
	$wR_2 = 0.1920$	$wR_2 = 0.0942$
R_1/wR_2 (all data)	$R_1 = 0.1050,$	$R_1 = 0.0360,$
))	$wR_2 = 0.2159$	$wR_2 = 0.0956$

Table 1. Crystallographic data and structure refinement details for 1 and 2.