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# **One-Pot Synthesis, Crystal Structures and Topology Analysis** of Two Nickel(II) Complexes Based on 1,3,5-Benzenetricarboxylic Acid

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**Abstract** The one-pot solvothermal reaction of Ni(NO<sub>3</sub>)<sub>2</sub> with 1,3,5-benzenetricarboxylic acid (H<sub>3</sub>btc) and 4,4'-bis(imidazol-1-yl)benzene (bibp) affords two coordination compounds. The H<sub>3</sub>btc ligand is deprotonated step-by-step, and connects Ni<sup>II</sup> ions into two different valence-bonded structures (the binuclear molecule and 2D (4,4) grid) under the cooperation of bibp. Hydrogen bonds have been deeply investigated, and yield an interpenetrating binodal (3,5)-connected supramolecular network with the Schäfli symbol of  $[4^2.6] \cdot [4^2.6^5.8^3]$  and interdigitating binodal (4,6)-connected supramolecular network with the Schäfli symbol of  $[4^4.5^2] \cdot [4^4.5^6.6^4.7]$ , respectively.

**Keywords** Complexes · One-pot synthesis · Topology analysis · Supramolecular network

### Introduction

The rational design and synthesis of coordination polymer have currently attracted extensive attention, which is propelled by the aesthetic architecture as well as their tremendous potential applications in functional materials [1–4]. The observation of coordination polymers derived from organic ligands and metal ions through a selfassembly route has been explored intensively, and many efforts have been devoted to use of N- and O-donor organic ligands as co-ligands to bridge metal ions to form infinite network structures, such as one-dimensional (1D) chain structures and 2- or 3-D frameworks [5]. However, it is still a great challenge in crystal engineering to obtain designed and predictable frameworks with potential properties assembled by coordination bonds and/or supramolecular interactions such as hydrogen bonds,  $\pi$ - $\pi$  stacking, and charge-transfer interactions, etc. [6–10].

The combination of carboxylic acid and neutral imidazole-containing ligand offers a facile strategy to construct mixed-ligand frameworks [11, 12]. 1,3,5-benzenetricarboxylic acid (H<sub>3</sub>btc) has been extensively used in the selfassembly of coordination polymer due to the versatile coordination character [13]. This Y-shaped ligand presents many potential coordination sites, which is just beneficial to elucidate the multi-step process of deprotonation and coordination, resulting into the polymorphism. On the other hand, the coordination chemistry of rigid bis (imidazole) ligands has been deeply explored in our group, and they are good candidates for the construction of mixedligand frameworks owing to the stronger coordination ability and linear feature [14]. In this paper,  $Ni(NO_3)_2$ ,  $H_3$ **btc**, and 4,4'-bis(imidazol-1-yl)biphenyl (**bibp**) have been introduced into a one-pot solvothermal reaction to afford two coordination compounds {[Ni(Hbtc)(bibp)<sub>1.5</sub>  $(H_2O)_3] \cdot (H_2O)_2\}_{\infty}$  (1) and  $[Ni(Hbtc)(bibp)(H_2O)]_{\infty}$  (2). The crystal structures and supramolecular network topologies have been discussed.

### Experimental

Materials and Physical Measurements

All solvents and reagents for synthesis were commercially available and used as received. The ligand bibp was synthesized according to the reported procedure [15]. Elemental

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analyses of C, H, and N were performed on a Perkin-Elmer 240C analyzer. IR spectra were measured on a TENSOR 27 (Bruker) FT-IR spectrometer with KBr pellets. Compounds 1 and 2 were further characterized by X-ray crystallographic analysis.

## Synthesis of $\{[Ni(Hbtc)(bibp)_{1.5}(H_2O)_3] \cdot (H_2O)_2\}_{\infty}$ (1) and $[Ni(Hbtc)(bibp)(H_2O)]_{\infty}$ (2)

Compounds 1–3 with the same ligand combination have different compositions (and structures) were synthesized from one-pot solvothermal reaction, however, the Ni(II) complex 3 {[Ni<sub>3</sub>(btc)<sub>2</sub>(bibp)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]·3(H<sub>2</sub>O)<sub>2</sub>} $_{\infty}$  had been reported by Zheng groups [13]. The suspension of Ni(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O (0.12 mmol, 35 mg), H<sub>3</sub>btc (0.15 mmol, 32 mg) and bibp (0.10 mmol, 28 mg) in 12 mL component solvent (H<sub>2</sub>O:CH<sub>3</sub>OH = 3:4) was sealed in a Teflon-lined autoclave and heated to 120 °C for 3 days. Three kinds of crystals with distinct differences in color (blue for 1, green for 2 and yellow-green for 3), were obtained after the autoclave was cooled to room temperature at 10°Ch<sup>-1</sup>. Approximate yields: ca. 5 % for 1, 5 % for 2, and 60 % for 3 based on bibp.

Anal. Calcd. for  $C_{72}H_{70}N_{12}N_{12}O_{22}$  (1): C, 54.98; H, 4.49; N, 10.69. Found: C, 54.74; H, 4.55; N, 10.77. IR (KBr) for 1: 3739w, 3253s, 1901w, 1678m, 1612m, 1572m, 1514s, 1431m, 1365s, 1300w, 1242m, 1184m, 1101w, 1061m, 962w, 814m, 723w, 648m, 517w.

Anal. Calcd. for  $C_{27}H_{20}N_4NiO_7$  (2): C, 56.78; H, 3.53; N, 9.81. Found: C, 56.61; H, 3.58; N, 9.90. IR (KBr) for 2: 3624m, 3433s, 3161s, 1720m, 1620s, 1579m, 1514s, 1456m, 1423w, 1373s, 1315m, 1242m, 1176w, 1119w, 1061m, 937w, 822m, 764w, 723m, 648w, 508w.

Anal. Calcd. for  $C_{54}H_{44}N_8Ni_3O_{17}$  (**3**): C, 51.76; H, 3.54; N, 8.94. Found: C, 51.53; H, 3.59; N, 9.03. IR (KBr) for **3**: 3616m, 3450s, 3120m, 1869w, 1612s, 1572m, 1514s, 1448m, 1365s, 1325m, 1257m, 1127w, 1068m, 930w, 822m, 771m, 731m, 658w, 517w, 442w.

Moreover, a series of solvothermal reactions have been carried out under different crystallization time and temperature (Table 1). Although the bulk products are cocrystallized in one-pot, the yield of **3** ( $\sim$ 60 %) is much higher than that of **1** and **2** (both  $\sim$ 5 %) when standing 3 days at 120 °C. However, a short time (1 day at 120 °C) leads to higher yields of **1** and **2** ( $\sim$ 50 and 20 % respectively) without visible **3**. It is also found that the yield of **3** is up to 75 % when standing 2 days at 140 °C, while compounds **1** and **2** are invisible at the 80× microscope. If the reaction standing 1 day at 140 °C, compounds **1** and **2** are overwhelming ( $\sim$ 35 and 30 % respectively), while the yield of **3** greatly decreases ( $\sim$ 10 %). Furthermore, compounds **1**–**3** are air-stable.

#### X-ray Crystallography

X-ray single-crystal diffraction data of 1-2 were collected on a Rigaku MM-007/Saturn 70 with graphite monochromatic Mo-K $\alpha$  radiation ( $\lambda = 0.71073$  Å). The program SAINT [16] was used for integration of the diffraction profiles. All the structures were solved by direct methods using the SHELXS program of the SHELXTL package and refined by full-matrix least-squares methods with SHELXL [17]. Metal atoms in each complex were located from the E-maps and other non-hydrogen atoms were located in successive difference Fourier syntheses and refined with anisotropic thermal parameters on F<sup>2</sup>. Hydrogen atoms of organic ligands were generated theoretically onto the specific atoms and refined isotropically. However, hydrogen atoms of water molecules were added by difference Fourier maps, and refined using a riding model. Mercury software offers a comprehensive range of tools for 3D structure visualization [18]. In the structure of 1, the two lattice water molecules are disordered, thus this structure was refined by the SQUEEZE routine of PLATON program [19]. Further details for structural analysis are summarized in Table 2, and selected bond lengths and angles are listed in Table 3.

#### **Results and Discussion**

Crystal structure of  $\{[Ni(Hbtc)(bibp)_{1.5}(H_2O)_3] \cdot (H_2O)_2\}_{\infty}$  (1)

Single-crystal X-ray diffraction analysis reveals that compound **1** crystallizes in the monoclinic space group  $P2_1/c$ . As shown in Fig. 1a, each Ni<sup>II</sup> ion is coordinated by two nitrogen atoms from individual bibp molecules and one Hbtc<sup>2–</sup> oxygen atom. The octahedral coordination geometry of Ni<sup>II</sup> node is completed by three water molecules. The Ni–N distances are 2.077(4) and 2.078(4) Å, and Ni–O bond lengths range from 2.055(3) to 2.096(3) Å, which are all in good agreement with those typically observed values [20]. The partially deprotonated ligand Hbtc<sup>2–</sup> coordinates

Table 1The yields of compounds 1-3 under different reaction timeand temperature

	Complex							
	1		2		3			
Time	120 °C	$140 ^\circ C^a$	120 °C	140 °C	120 °C	140 °C		
1 day	50 %	35 %	20 %	30 %	0 %	10 %		
2 days		0 %		$0 \ \%$		75 %		
3 days	5 %		5 %		60 %			

 $^a$  Solvethermal reaction under 120 and 140  $^{\circ}\mathrm{C}$  are shown by roman and italics, respectively

Table 2 Crystal data and structure refinement for 1 and 2

**Table 3** Selected bond lengths (Å) and angles (deg) for 1-2

Complex	1	2
Empirical formula	C <sub>72</sub> H <sub>70</sub> N <sub>12</sub> Ni <sub>2</sub> O <sub>22</sub>	C <sub>27</sub> H <sub>20</sub> N <sub>4</sub> NiO <sub>7</sub>
Formula weight	1572.82	571.18
Crystal size (mm <sup>3</sup> )	$0.25\times0.20\times0.18$	$0.25\times0.22\times0.18$
Crystal system	monoclinic	monoclinic
Space group	$P2_{1}/c$	$P2_{1}/c$
a (Å)	13.564(3)	10.515(2)
<i>b</i> (Å)	12.096(2)	10.101(2)
<i>c</i> (Å)	21.708(4)	22.705(5)
β (°)	93.86(3)	102.84(3)
$V(\text{\AA}^3)$	3553.6 (12)	2351.2(8)
Ζ	2	4
$D_{\text{calcd}} (\text{g.cm}^{-3})$	1.470	1.614
<i>F</i> (000), e	1636	1176
Refl. measured	29487	19889
Refl. unique	6261	4134
R <sub>int</sub>	0.0755	0.0296
Goodness-of-fit on $F^2$	1.191	1.119
Final <i>R</i> indices $[I > 2\sigma(I)]^{a}$	$R_1 = 0.0716,$ $wR_2 = 0.1425$	$R_1 = 0.0346,$ $wR_2 = 0.0738$
R indices (all data)	$R_1 = 0.1000, \\ wR_2 = 0.1532$	$R_1 = 0.0397,$ $wR_2 = 0.0758$
$\begin{array}{c} \Delta \rho_{\rm fin} \ ({\rm max/min}), \\ {\rm e} \ {\rm \AA}^{-3} \end{array}$	1.123/- 0.605	0.579/-0.337

<sup>a</sup>  $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$  and  $wR_2 = \{ \Sigma [w(F_o^2 - F_c^2)^2] / [w(F_o^2)^2] \}^{1/2}$ ,  $[F_o > 4\sigma(F_o)]$ 

to one Ni<sup>II</sup> ion adopting a monodentate mode and leaving an uncoordinated deprotonated carboxylate group, which is relatively uncommon [21]. For the bibp ligand, there are two coordination modes, i.e. monodentate terminal group and bidentate linker. Hereinto, one third of bibp takes bidentate mode to connect two metal-coordinated spheres into a binuclear molecule (Scheme 1)

The discrete binuclear motifs are cross-linked by hydrogen-bond interaction among coordinated water molecules, Hbtc<sup>2-</sup> oxygen atoms and bibp nitrogen atoms [O1W-H1B···O3, O2W-H2A···O4 and O1W-H1A···N4 for 2.751(3), 2.714(4) and 2.814(5) Å, respectively], thus leading the formation of 2D supramolecular network (Fig. 1b). Interestingly, adjacent 2D layers are further connected through hydrogen bonds O6-H6...O4 and O2W-H2B...O5 [2.592(4) and 2.880(4) Å] into a 3D supramolecular framework. The topological method was applied to explore the nature of this fascinating framework. The Hbtc<sup>2-</sup> ligand is three-connected by linking to three Ni<sup>II</sup> ions and could be simplified as a three-connected node. Except for three  $Hbtc^{2-}$  nodes, the Ni<sup>II</sup> center is also connected with two equivalent Ni<sup>II</sup> ions by bibp or doublebibp connectors; the Ni<sup>II</sup> ion is considered as a five-

Complex 1			
Ni1-01	2.055(3)	Ni1–O1W	2.057(3)
Ni1–N1	2.077(4)	Ni1–N5	2.078(4)
Ni1–O3W	2.101(3)	Ni1–O2W	2.096(3)
O1W-Ni1-N1	92.53(13)	O3W-Ni1-N5	174.16(14)
O1-Ni1-N1	95.24(13)	O1W-Ni1-O2W	87.46(12)
O1W-Ni1-O3W	92.06(12)	O1-Ni1-O2W	84.75(12)
O1-Ni1-O3W	87.37(12)	N1-Ni1-O2W	176.72(13)
N1–Ni1–O3W	90.52(13)	O3W-Ni1-O2W	86.19(12)
O1W-Ni1-N5	93.22(14)	N5-Ni1-O2W	91.56(14)
01-Ni1-N5	87.06(13)	N1-Ni1-N5	91.72(15)
Complex 2			
Ni101	2.0361(16)	Ni1–N1	2.052(2)
Ni1–N4A	2.086(2)	Ni1–O1W	2.1091(18)
Ni1–O3B	2.1255(16)	Ni1–O4B	2.1883(16)
O1-Ni1-N1	97.68(8)	O1-Ni1-N4A	89.06(7)
N1-Ni1-N4A	92.07(8)	O1-Ni1-O1W	85.86(7)
N1-Ni1-O1W	92.99(8)	N4A-Ni1-O1W	173.27(7)
O1-Ni1-O3B	158.10(7)	N1-Ni1-O3B	103.59(7)
N4A-Ni1-O3B	95.27(7)	O1W-Ni1-O3B	87.86(7)
O1-Ni1-O4B	97.76(6)	N1-Ni1-O4B	164.55(7)
N4A-Ni1-O4B	87.61(7)	O1W-Ni1-O4B	88.69(7)
O3B-Ni1-O4B	61.10(6)		

<sup>a</sup> Symmetry mode for **2**, A: x + 1, -y + 1/2, z + 1/2; B: x, y + 1, z

connected node. Therefore, the combination of nodes and connectors affords a binodal (3,5)-connected network with the Schäfli symbol of  $[4^2.6] \cdot [4^2.6^5.8^3]$  [22], which calculated by TOPOS 4.0 program [23] (Fig. 1c). Further topological analysis suggests that such two independent frameworks are interlocked with each other, and the most fascinating structural feature is that 1 represents an interpenetrating supramolecular network (Fig. 1d). Free water molecules are dispersed and further stabilize the 3D supramolecular architecture.

#### Crystal Structure of $[Ni(Hbtc)(bibp)(H_2O)]_{\infty}$ (2)

Similar to **1**, compound **2** also crystallizes in the monoclinic space group  $P2_1/c$ , containing four symmetry-related Ni<sup>II</sup> ions in each unit cell. As shown in Fig. 2a, the geometry of Ni<sup>II</sup> ion is surrounded by two nitrogen atoms from individual bibp molecules, three oxygen atoms from two partially deprotonated Hbtc<sup>2-</sup> ions and a water molecule, which gives a distortedly octahedral coordination environment. The Ni–N distances are 2.052(2) and 2.086(2) Å, and Ni–O bond lengths span a narrow range [2.0361(16)–2.1883(16) Å], which are in accord with above reported values of **1**. In **2**, the bibp ligand bridges adjacent Ni<sup>II</sup> nodes to form a W-type 1D chain, and the partially deprotonated Hbtc<sup>2-</sup> ligand also links Ni<sup>II</sup> ions to



Fig. 1 a View of the octahedral coordination environment in 1 (hydrogen atoms except carboxyl group omitted for clarity); b view of the 2D supramolecular layer based on a binuclear motif in 1; c view



Scheme 1 Structures of the ligands used in this work

form a linear chain with two carboxylate groups, which adopt monatomic and bidentate chelated modes, respectively. Thus the extended structure illustrates a 2D wave-like (4,4) grid (Fig. 2b).

Interestingly, two adjacent 2D grids are associated with each other through hydrogen bonds O5–H5A···O4 and O1W–H1A···O2 [2.635(2) and 2.778(2) Å], resulting in a 3D supramolecular framework. In this double-layer architecture, the Hbtc<sup>2–</sup> ligand bridges four Ni<sup>II</sup> ions and could be simplified as a four-connected node. Except for four Hbtc<sup>2–</sup> nodes, the Ni<sup>II</sup> center is also connected with two equivalent Ni<sup>II</sup> ions by bibp connectors; thus the Ni<sup>II</sup> ion is considered as a six-connected node. The topological approach with TOPOS 4.0 program [23] reveals a binodal (4,6)-connected supramolecular framework with the Schäfli symbol of [4<sup>4</sup>.5<sup>2</sup>]·[4<sup>4</sup>.5<sup>6</sup>.6<sup>4</sup>.7] [22] (Fig. 2c). Further topological analysis suggests that, along b axis, two adjacent double-layer architectures pack tightly in a staggered mode to form an interdigitating network via weak  $\pi$ – $\pi$ 

of the bimodal (3,5)-connected framework in 1; d view of the interpenetrating supramolecular network in 1

interactions with the centroid–centroid separation of ca. 3.7 and 4.2 Å (Fig. 2d) [19].

Structural Comparison of 1, 2 and 3

The reaction system of Ni<sup>II</sup>-H<sub>3</sub>btc-bibp has been previously studied by a pH-adjusting hydrothermal method, which only affords compound **3** with 3D (4, 4)-connected framework, and complexes **1–2** have not been observed [13]. Interestingly, in this paper, three compounds **1–3** have been synthesized from the identical system by one-pot solvothermal reaction, which provides an ideal example to study on the complexes. The great difference may be due to the pH value: in the preceding hydrothermal reaction, the additive NaOH causes a complete deprotonation of H<sub>3</sub>btc to give an exclusive btc<sup>3–</sup> ion, which further participates in the coordination assembly to afford **3**. However, in our solvothermal reaction, different deprotonated styles of H<sub>3</sub>btc are available, and thus various coordination polymers could be generated.

In this study, the compounds 1-3 are obtained under same conditions, displaying a diversity of discrete binuclear molecule, 2D (4,4) layer and 3D (4,4)-connected network structures. As described above, the bibp act as monodentate terminal group and bidentate linker, showing the similar coordination modes in the three compounds. As a comparison, it is easy to find that the complexities of the title compounds 1-3 strongly rely on the various bridging



Fig. 2 a View of the octahedral coordination environment in 2 (hydrogen atoms except carboxyl group omitted for clarity), symmetry transformations used to generate equivalent atoms: A = x + 1, –

modes of the 1,3,5-benzenetricarboxylic acid, resulting from completely or partially de-protonated sites. In compound 1, the partially deprotonated ligand  $Hbtc^{2-}$  coordinates to one Ni<sup>II</sup> ion adopting a monodentate mode,one third of bibp ligand takes bidentate mode to connect two metal-coordinated spheres into a binuclear molecule. Whereas in 2, the  $Hbtc^{2-}$  ligand links neighboring Ni<sup>II</sup> ions to form a linear chain with two carboxylate groups, which adopt monatomic and bidentate chelated modes, respectively. The bibp ligand further bridges adjacent Ni<sup>II</sup> nodes into 2D (4,4) network. In 3, the repeating basic secondary building unit (SBU) in this complex consists of three nickel ions, carboxylate oxygen atoms bonding to neighboring nickel ions. The fully deprotonated btc and bibp ligands link the trinuclear secondary building units to form a 3D (4,4)-connected network.

Interestingly, the number of coordination water molecules combined with each metal ion shows the selfassembly of coordination polymer. According to chemical formulas, each Ni<sup>II</sup> ion in 1-3 possesses three, one and 2/3 crystal coordination water molecules, respectively. From 1 to 3, the coordination crystal water molecule of complexes 1-3 is gradually squeezed by the organic ligand, and further replaced by the hetero-atom, which clearly shows the progress of self-assembly.

y + 0.5, z + 0.5; B = x, y + 1, z. **b** view of the 2D wave-like layer in **2**; **c** view of the binodal (4,6)-connected supramolecular framework in **2**; **d** view of the interdigitating network in **2** 

#### Conclusion

Two complexes **1** and **2** have been synthesized from a onepot solvethermal reaction, compounds **1** and **2** illustrate various valence-bonded architectures, i.e. discrete binuclear molecule, 2D (4,4) layer. Furthermore, hydrogen bonds in **1** and **2** have been investigated to afford an interpenetrating binodal (3,5)-connected supramolecular network with the Schäfli symbol of  $[4^2.6] \cdot [4^2.6^5.8^3]$  and interdigitating binodal (4,6)-connected supramolecular network with the Schäfli symbol of  $[4^4.5^2] \cdot [4^4.5^6.6^4.7]$ , respectively. The results demonstrate that the bridging modes of the 1,3,5-benzenetricarboxylic acid and hydrogen bonds interaction can exert significant influences on the topologies of final nickel(II) complexes.

#### **Supplementary Data**

Crystallographic data (excluding structure factors) for the structure in this paper have been deposited with the Cambridge Crystallographic Data Centre as the supplementary publication no. CCDC 868356–868357. This data can be obtained from the Cambridge Crystallographic Data Center, 12 Union Road, Cambridge CB2 1EZ, UK;

Fax: +44-1223-336033; E-mail: deposit@ccdc.cam.ac.uk or on the web http://www.ccdc.cam.ac.uk.

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