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Journal of MOLECULAR STRUCTURE

Journal of Molecular Structure 879 (2008) 150-155

www.elsevier.com/locate/molstruc

# Synthesis, crystal structure and theoretical investigation of two infinite two-dimensional supra-molecular compounds

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> Received 23 June 2007; received in revised form 18 August 2007; accepted 22 August 2007 Available online 2 September 2007

## Abstract

Two supra-molecular compounds: (1,1'-biphenyl)-4,4'-diammonium bis(3,5-dinitrobenzoate) (1) and 4,4'-methylene bis(benzenammonium) bis(3,5-dinitrobenzoate) monohydrate (2) were synthesized and characterized by IR spectrum, UV spectrum and element analysis. The single crystal structure analysis indicates that these compositions in two compounds are linked through N–H···O and O–H···O hydrogen bonds into infinite two-dimensional structure. Moreover, theoretical investigation was performed by using RHF/6-31G(d) method, and their stabilities, frontier molecular orbital composition and Mulliken charge distribution were discussed. © 2007 Elsevier B.V. All rights reserved.

Keywords: 3,5-Dinitrobenzoate; Crystal structure; Hydrogen bonds; Theoretical investigation; Mulliken

## 1. Introduction

In recent years, there has been increasing interest in the use of hydrogen bonding for the design and synthesis of supra-molecular assemblies and molecular architectures because hydrogen bonding has long been considered to be of importance in biological systems and molecular recognition [1-6]. Moreover, lots of literatures in which quantum chemical methods were applied to analyze H-bonding systems [7–9] have been reported, such as electronic properties, interaction energy and vibrational spectra, and so on. It is well known that 3,5-dinitrobenzoic acid has two strongly electron-withdrawing groups so that its carboxylate group deprotonized easily. Moreover, carboxylate anion and two nitro groups can easily form hydrogen bonds as hydrogen bonds acceptor with other hydrogen bonds donors and further construct zero-, one- or higherdimensional structure. Herein we select (1,1'-biphenyl)-4,4'-diamine and longer 4,4'-methylene bis(benzenamine) ligand because both them have two -NH2 groups and

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can act as strong hydrogen bond acceptor. Besides, the changing length of hydrogen bond acceptor may affect the final structure of **1** and **2**. To best of our knowledge, some supra-molecular compounds relating to 3,5-dinitrobenzoic acid have been reported [10–19]. However, in those reported literatures theoretical investigation has not been seen. Herein we present synthesis, crystal structure and theoretical investigation of two infinite two-dimensional supra-molecular compounds.

# 2. Experimental

#### 2.1. Materials and physical measurements

All chemicals were of reagent grade as received from commercial sources and used without further purification. C, H, N elemental analysis was performed on Perkin-Elmer 240C elemental analyzer; Infrared spectrum was recorded as KBr pellets on a Nicolet 170SXFT-IR spectrometer in the range of 400–4000 cm<sup>-1</sup>. The UV spectrum was performed on a Shimzu UV-250 spectrometer in the 190–350 nm range. Quantum chemical calculation of two compounds was performed from the crystal data with

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<sup>0022-2860/\$ -</sup> see front matter @ 2007 Elsevier B.V. All rights reserved. doi:10.1016/j.molstruc.2007.08.025

# 2.2. Synthesis

# 2.2.1. Synthesis of 1

A 5 ml ethanol solution of (1,1'-biphenyl)-4,4'-diamine (0.25 mmol, 0.045 g) was added to an aqueous solution (25 ml) of 3,5-dinitrobenzoic acid (0.50 mmol, 0.10 g). The mixture was stirred for 10 min at 353 K. The solution was filtered, and the filtrate was allowed to stand at room temperature. After 10 days, colorless single crystals suitable for X-ray analysis were obtained. Anal. Calc. for C<sub>26</sub>H<sub>20</sub>N<sub>6</sub>O<sub>12</sub>: C, 51.32%; H, 3.31%; N, 13.81%. Found: C, 50.80%; H, 3.02%; N 13.40%. IR ( $v/cm^{-1}$ ): 3430.44(s), 1623.75(s), 1581.66(w), 1535.21(s), 1501.12(m), 1457.23(w), 1384.04(w), 1347.49(s), 1080.39(w), 814.77(w), 725.98(m), 715.89(m). UV ( $\lambda_{max}/nm$ ): 201, 242.

### 2.2.2. Synthesis of 2

4,4'-Methylene bis(benzenamine) (0.25 mmol, 0.05 g) was added to an aqueous solution (25 ml) of 3,5-dinitrobenzoic acid (0.50 mmol, 0.10 g). The mixture was stirred for 10 min at 353 K. The solution was filtered, and the filtrate was allowed to stand at room temperature. After a week, colorless single crystals suitable for X-ray analysis were obtained. Anal. Calc. for C<sub>27</sub>H<sub>24</sub>N<sub>6</sub>O<sub>13</sub>: C, 50.63%; H, 3.78%; N, 13.12%. Found: C, 50.11%; H, 3.47%; N, 12.83%. IR ( $v/\text{cm}^{-1}$ ): 3420.98(m), 3098.48(m), 1621.01(m), 1533.60(s), 1508.51(w), 1452.01(w), 1382.47(w), 1345.19(s), 1072.64(m), 723.95(m). UV ( $\lambda_{max}/\text{nm}$ ): 192, 202.

## 2.3. X-ray crystallography

Data collections were made on Bruker SMART APEX CCD area-detector diffractometer using graphite monochromated Mo-K $\alpha$  diffraction ( $\lambda = 0.71073$  Å) at 298(2) K. The intensities were corrected by Lorentz-polarization factors and empirical absorption. The structures were solved by direct methods and refined by a full-matrix least squares technique based on  $F^2$  using the SHELXTL-97[21] program. All non-hydrogen atoms were refined anisotropically. H atoms bound to N and C atoms were positioned geometrically and to water molecule were located from difference maps.

Crystallographic data for the title compounds are listed in Table 1. The selected bond lengths are given in Table 2. The hydrogen bonds data are presented in Table 3.

## 3. Results and discussion

### 3.1. Structure description

As shown in Fig. 1, the compound 1 consists of one (1,1'-biphenyl)-4,4'-diammonium cation and two

Table 1	
Crystal data for 1 and 2	

	1	2
Empirical formula	C <sub>26</sub> H <sub>20</sub> N <sub>6</sub> O <sub>12</sub>	C27H24N6O13
Formula weight	608.48	640.52
Crystal system	Monoclinic	Monoclinic
Space group	C2/c	P2/c
Unit cell dimensions		
a (Å)	27.069(15)	12.548(4)
<i>b</i> (Å)	4.709(3)	4.1444(12)
<i>c</i> (Å)	21.732(12)	27.736(8)
β(°)	107.450(8)	101.494(5)
$V(\text{\AA}^3)$	2643(3)	1413.5(7)
Ζ	4	2
$D_{\rm calcd}  ({\rm mg/m^3})$	1.529	1.505
$\mu (\mathrm{mm}^{-1})$	0.124	0.122
Reflections collected	6199	7169
Independent reflections	2366	2753
Goodness-of-fit on $F^2$	0.921	1.008
Final <i>R</i> indices $[I > 2.0\sigma(I)]$	$R_1 = 0.0544$	$R_1 = 0.0553$
	$wR_2 = 0.0959$	$wR_2 = 0.1292$
R indices (all data)	$R_1 = 0.1305$	$R_1 = 0.1101$
	$wR_2 = 0.1193$	$wR_2 = 0.1480$

 $\begin{aligned} R &= \sum ||F_o| - |F_c|| / \sum |F_o|, \ wR = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}, \ \mathbf{1}, \ w = 1 / [\sigma^2(F_o^2) + (0.0448P)^2], \ \mathbf{2}, \ w = 1 / [\sigma^2(F_o^2) + (0.0421P)^2], \ P = (F_o^2 + 2Fc^2) / 3. \end{aligned}$ 

Table 2						
Selected	bond	distances	(Å)	for 1	and <b>2</b>	

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	76(4) 79(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	76(4) 79(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	79(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	~ < 7
$\begin{array}{cccccccc} C(1)-C(2) & 1.387(4) & C(1)-C(7) & 1.513(4) & C(2)-C(3) & 1.3\\ C(3)-C(4) & 1.373(4) & C(4)-C(5) & 1.379(4) & C(5)-C(6) & 1.3\\ \textbf{2}\\ N(1)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4\\ N(2)-O(4) & 1.219(2) & N(2)-O(2) & 1.219(2) & N(2)-O(2) & 1.4\\ \end{array}$	35(4)
$\begin{array}{ccccccc} C(3)-C(4) & 1.373(4) & C(4)-C(5) & 1.379(4) & C(5)-C(6) & 1.3 \\ \textbf{2} \\ N(1)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(2)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-C(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-O(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-O(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-O(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(3) & 1.219(3) & N(1)-O(3) & 1.4 \\ N(3)-O(4) & 1.214(3) & N(1)-O(4) & 1.4 \\ N(4)-O(4) & 1.4 \\ N(4)-O(4)$	74(4)
<b>2</b> N(1)-O(4) 1.214(3) N(1)-O(3) 1.219(3) N(1)-C(3) 1.4	30(4)
N(1)-O(4) 1.214(3) N(1)-O(3) 1.219(3) N(1)-C(3) 1.4	
	75(4)
N(2)-O(6) 1.209(3) $N(2)-O(5)$ 1.212(3) $N(2)-C(5)$ 1.4	56(4)
O(1)-C(7) 1.253(3) O(2)-C(7) 1.235(3) C(1)-C(6) 1.3	77(3)
C(1)-C(2) 1.387(3) C(1)-C(7) 1.517(3) C(2)-C(3) 1.3	74(3)
C(3)-C(4) 1.363(4) $C(4)-C(5)$ 1.383(4) $C(5)-C(6)$ 1.3	3(3)

bis(3,5-dinitrobenzoate) anions. The cation herein occupies a special position on an inversion centre. The extensive hydrogen-bonding system, which involves all six symmetry independent 'active' H atoms from two protonized amine groups as hydrogen bonds donors and two oxygen atoms [O(1) and O(2)] from carboxylate group as hydrogen bonds acceptors, links the component ions into an infinite onedimensional chain along the [010] direction through N-H···O hydrogen bonds (Table 3). Adjacent chains are further organized into two-dimensional network by N-H···O hydrogen bonds parallel to the (001) plane (Fig. 2).

The compound **2** is composed of one 4,4'-methylene bis(benzenamine) cation, two bis(3,5-dinitrobenzoate) anions and two water molecules. Here, the cation and water molecule occupies a special position on an inversion centre (Fig. 3), similar to that of **1**. These ions and molecules build an infinite one-dimensional chain via N– $H \cdots O$  and  $O-H \cdots O$  hydrogen bonds along the [010] direction (Table 3). Moreover, adjacent chains result in

Table 3 Hydrogen bonds for 1 and 2

$D\!\!-\!\!H\!\!\cdot\!\cdot\!\cdot\!A^a$	$D \cdots H$ (Å)	$H \cdot \cdot \cdot A$ (Å)	$D{\cdots}A\;(\mathring{A})$	$D-H\cdots A$ (°)
1				
$N3-H3A\cdots O2$	0.89	1.89	2.762	168
$N3-H3B\cdots O1^{i}$	0.89	1.93	2.791	163
$N3\text{-}H3C\text{-}\cdot\text{-}O1^{ii}$	0.89	1.91	2.768	162
2				
N3–H3A···O1	0.89	2.39	2.981	124
$N3-H3B\cdots O7$	0.89	2.08	2.962	172
$N3-H3C\cdots O1^{iii}$	0.89	1.75	2.631	170
$O7-H7A \cdot \cdot \cdot O2$	0.84	2.01	2.734	144
$O7-H7B$ ··· $O2^{iv}$	0.83	1.94	2.734	160

<sup>a</sup> Symmetry codes: i = -x + 2, -y + 1, -z + 1; ii = -x + 2, -y + 2, -z + 1; iii = x, y - 1, z; iv = -x + 1, y, -z + 1/2.

an infinite two-dimensional network by N–H···O hydrogen bonds propagating in (001), as presented in Fig. 4.

Although 4,4'-methylene bis(benzenamine) has more a methylene group than that of (1,1'-biphenyl)-4,4'-diammonium cation, the structure of 2 is similar to that of 1, indicating the length changing of hydrogen bonding acceptor here has little influences on their structure. In addition, we can see from Table 2 that the different cation has little influences on the structure of bis(3,5-dinitrobenzoate) anions through hydrogen bonding and static electric interactions. During our investigation we found pH value has little influences on the information of 1 and 2. Whereas the mole ratio of 3.5-dinitrobenzoic acid and (1.1'-biphenyl)-4,4'-diamine (or 4,4'-methylene bis(benzenamine) play an important role in the products of 1 and 2. When the mole ratio was close to 2:1, the two compounds can be obtained easily. Unexpectedly, under similar reaction conditions, compound 2 combine one water molecule of crystallization. However, the appearance of water molecule takes an important role in the structure of 2, which acts a bridge via hydrogen bonds links these ions into a twodimensional network. If there are no water molecules, these ions only build a one-dimensional chain, as shown in Fig. 5.



Fig. 2. The crystal packing of **1**. Hydrogen bonds are indicated by dashed lines. For clarity, H atoms not involved in the hydrogen bonds have been omitted.

### 3.2. Theoretical calculation

#### 3.2.1. Stability

The total energy for two compounds is -2220.33 a.u. (1) and -2411.37 a.u. (2), respectively. Whereas the energy of HOMO is -0.35896 a.u. (1) and -0.16189 a.u. (2), and the energy of LUMO is -0.02798 a.u. (1) and 0.02958 a.u. (2)



Fig. 1. The crystal structure of 1, with the atomic numbering of the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labeled atoms by the symmetry code (3/2 - x, 3/2 - y, 1 - z).



Fig. 3. The crystal structure of **2**, with the atomic numbering of the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level. Unlabeled atoms are related to labeled atoms by the symmetry code (-x, y, 1/2 - z).



Fig. 4. The packing diagram of **2**. Hydrogen bonds are shown as dashed lines. For clarity, H atoms not involved in the hydrogen bonding have been omitted.

with the HOMO-LUMO gaps 0.38658 a.u. (1) and 0.19147 a.u. (2), respectively. These results mean two compounds have better stability.

#### 3.2.2. Frontier molecular orbital composition

In order to study their electronic structure, frontier molecular orbital populations have been analyzed. The atomic orbital composition for varies type of atoms in



Fig. 5. An infinite one-dimensional chain when water molecules have been omitted in  $\mathbf{2}$ .

the frontier molecular orbits were expressed as the atomic orbital coefficient square sum in the type of atomic orbits and corrected by normalizing the specific molecule orbital [22]. The stereographs of frontier molecular orbits of two compounds are shown in Figs. 6 and 7, respectively.

Orbital contribution investigation indicate: for 1, the composition of HOMO comes mainly from orbits of two carboxyl oxygen O(1#) and O(2#) (70.74%), six carbon



Fig. 6. The frontier molecular orbits (HOMO and LUMO) in 1.



Fig. 7. The frontier molecular orbits (HOMO and LUMO) in 2.

atoms of benzene ring from 3,5-dinitrobenzoate anion (24.62%) at the symmetry position (3/2 - x, 3/2 - y, 1 - z). In contrast, the components of LUMO come mainly from 10 carbon atoms of (1,1'-biphenyl)-4,4'-diammonium cation (85.48%), six hydrogen atoms bound to two protonated N(3) and N(3#) atoms (3.41%) (symmetry code #: 3/2 - x, 3/2 - y, 1 - z). The suggestions can be represented in Fig. 6. For **2**, the composition of HOMO comes mainly from orbits of water oxygen O(7) (39.23%) and O(7#) (14.32%) [symmetry code #: -x, y, 1/2 - z]. The components of LUMO come mainly from six carbon atoms (57.86%) of benzene ring, four nitro group oxygen (23.89%) and two N atoms of two nitro groups (16.43%)

Table 4				
Mulliken	charges	for 1	l and	2

at the (x, y, z) position. The suggestions can be reflected in Fig. 7. On the other hand, these results indicate that carboxyl group oxygen in 1 and water molecule in 2 are potentially active sites and can react with metal centers or hydrogen bonds donors [22,23].

### 3.2.3. Mulliken atomic charge distribution

The Mulliken atomic charge distribution of the labeled atoms for two compounds are listed in Table 4. In 1, the negative charges of 3,5-dinitrobenzoate anion are mainly populated on two carboxyl oxygen O(1) and O(2), which further suggests that these atoms are potentially active sites and can react with metal centers or hydrogen bonds donors [22,23], consistent with the above-mentioned conclusion. In contrast, positive charges of (1,1'-biphenyl)-4,4'-diammonium cation are not localized on the protonated nitrogen (N3 and N3#) [symmetry code #: 3/2 - x, 3/2 - y, 1 - z] atom but populated on six hydrogen atoms bound to them, suggesting that the positive charges in the cation are delocalized between the nitrogen and hydrogen atoms. The Mulliken atomic charge distribution of the atoms in 2 is similarly to that of 1, the negative charges of 3,5-dinitrobenzoate anion are populated on deprotonated O(1) and O(2) [O(1#), O(2#)] (symmetry code #: -x, y, 1/ 2 - z). Positive charges of 4,4'-methylene bis(benzenamine) cation are mainly populated on six hydrogen atoms bound to two protonated nitrogen atoms, too.

# 4. Supplementary material

Crystallographic data for the structural analysis of have been deposited with the Cambridge Crystallographic Data Center, CCDC number 651810 for complex **1** and CCDC number 651811 for complex **2**. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk or website: http:// www.ccdc.cam.ac.uk).

	8										
Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge	Atom	Charge
1											
N(1)	0.487485	N(2)	0.495149	N(3)	-0.758518	O(1)	-0.704482	O(2)	-0.79538	O(3)	-0.490975
O(4)	-0.451535	O(5)	-0.45515	O(6)	-0.450591	C(1)	-0.172651	C(2)	-0.086608	C(3)	0.129418
C(4)	-0.070615	C(5)	0.119151	C(6)	-0.05105	C(7)	0.818078	C(8)	0.04774	C(9)	-0.170266
C(10)	-0.156874	C(11)	0.047567	C(12)	-0.135241	C(13)	-0.165679	H(2)	0.228931	H(3A)	0.498334
H(3B)	0.429996	H(3C)	0.435024	H(4)	0.265148	H(6)	0.264485	H(9)	0.209942	H(10)	0.201857
H(12)	0.229767	H(13)	0.207433								
2											
N(1)	0.490219	N(2)	0.493068	N(3)	-0.74411	O(1)	-0.746	O(2)	-0.72151	O(3)	-0.45407
O(4)	-0.45061	O(5)	-0.45651	O(6)	-0.45554	O(7)	0.227747	C(1)	-0.21118	C(2)	-0.06712
C(3)	0.129777	C(4)	-0.06273	C(5)	0.1194	C(6)	-0.07404	C(7)	0.807865	C(8)	0.019988
C(9)	-0.18049	C(10)	-0.11901	C(11)	0.027393	C(12)	-0.14167	C(13)	-0.18727	C(14)	-0.32759
H(2)	0.255815	H(3A)	0.458746	H(3B)	0.425987	H(3C)	0.425478	H(4)	0.274286	H(6)	0.250226
H(7A)	0.274001	H(7B)	-0.452056	H(9)	0.201178	H(10)	0.188447	H(12)	0.214806	H(13)	0.201089
H(14A)	0.217582	H(14B)	0.217599								

#### Acknowledgements

This work was Support by Henan Provincial Natural Science Foundation of China (No. 0611011900) and Basic Research Foundation for Natural Science of Henan University (No. 04YBRW053).

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