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ORIGINAL PAPER

Crystal and Molecular Structure of the 1:2 Adduct Formed Between *N*,*N*′-Butylenebis(imidazole) and Carboxylic Acid Derivatives

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Abstract Two imidazolyl derived complexes [*N*,*N*′-butylenebis(imidazole): (fumaric acid)$_2$ (**1**), and *N*,*N*′-butylenebis(imidazole): (2,4,6-trinitrophenol)$_2$ (**2**)] were prepared and structurally characterized by X-ray crystallography. Compound **1** crystallizes in the triclinic, space group P−1, with $a = 5.9990(12)$ Å, $b = 8.1772(16)$ Å, $c = 10.419(2)$ Å, $\alpha = 86.88(2)°$, $\beta = 84.73(3)°$, $\gamma = 77.03(4)°$, $V = 495.67(17)$ Å^3, $Z = 1$. For **1**, two dimensional network structure is formed through imidazolium moieties forming hydrogen bonds to di-ionic carboxylate groups of fumarate chains. In the same network layers and adjacent layers, C–H···O contact also accompanies the N^+–H···O^- hydrogen bonds, all these lead the extended architecture to show a three-dimensional lamellar structure. Compound **2** crystallizes in the triclinic, space group $P-1$, with $a = 7.0236(14)$ Å, $b = 8.2831(17)$ Å, $c = 12.053(2)$ Å, $\alpha = 106.05(4)°$, $\beta = 99.13(2)°$, $\gamma = 98.84(3)°$, $V = 650.8(2)$ Å^3, $Z = 1$. In **2**, two parallel imidazolium cations and two antiparallel 2,4,6-trinitrophenolate anions formed 32-membered rings through hydrogen bonding interaction, these rings extended along the *c* axis direction to form one dimensional railway structure. Adjacent parallel railways connect further through C–H···O hydrogen bonds between the 2-CH of the imidazole ring and the NO_2 group O atoms. These weak interactions combined, the complex showed 3D layer structure.

Keywords Crystal structure · *N*,*N*′-Butylenebis(imidazole) · Hydrogen bonds

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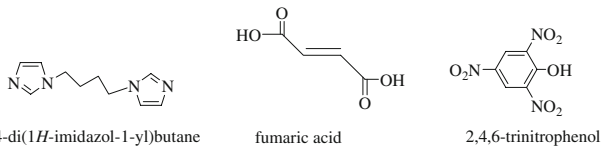
Introduction

Nowadays, hydrogen bonding has been widely developed in the area of crystal engineering, supramolecular chemistry, material science, and biological recognition [1–7]. The application of intermolecular hydrogen bonds is a well known and efficient tool to regulate the molecular arrangement in a crystal structure [6, 7]. Through hydrogen bond we can form co-crystals and organic salts. In pharmaceuticals, salt formation is often used in order to modify the properties of the compounds [8]. Salt formation can be used to increase or decrease solubility, to improve stability and to reduce hygroscopicity of a drug product. Assemble through hydrogen bond, there have been reported many topology structures such as an infinite 1-D chain structure [9], and 3-D layer structure [10].

The carboxylic acid group is an important hydrogen bonding functional group in crystal engineering [11]. Carboxylic acids aggregate in the solid state as dimer, catemer, and bridged motifs [12–14]. Thus, it is interesting to carry out premeditated crystal design not only with carboxylic acids [14], but, as recent trends indicate, by exploiting the robust and directionary recognition of carboxylic acids with *N*-heterocyclic moieties [15–17]. In this context, 4,4′-bipyridine [9, 18, 19], phenazine [20–22], 2-pyridone



Scheme 1 Hydrogen bond synthons discussed in this paper

[23–25], and imidazole derivatives [26, 27] have emerged as important complementary ligands for the crystal engineering of carboxylic acids. When carboxylic acids interact with Im(imidazoles) and Bzim(benzimidazoles) the solid-state outcome is often an organic salt, not a co-crystal, as a result of proton transfer [28–33]. Aakeröy [34] reported direct assemble of ditopic imidazoles/benzimidazoles and dicarboxylic acids into co-crystals via selective O–H···N hydrogen bonds. For we are interested in the crystal engineering assembling through weak interaction [35, 36], here in we report the crystal structure of two complexes assembled through hydrogen bonding interactions.

In this study, we get two organic complexes composed of carboxylic acids and symmetric ditopic bis-imidazol-1-yl compounds (Scheme 1), namely *N*,*N*′-butylenebis(imidazole): (fumaric acid)$_2$ (**1**), and *N*,*N*′-butylenebis(imidazole): (2,4,6-trinitrophenol)$_2$ (**2**).

Experimental Section

Materials and Methods

All reagents were commercially available and used as received. *N*,*N*′-butylenebis(imidazole) was prepared as described previously [37]. The C, H, and N microanalysis were carried out with a Carlo Erba 1106 elemental analyzer. The FT-IR spectra were recorded from KBr pellets in range 4,000–400 cm^{-1} on a Mattson Alpha-Centauri spectrometer. Melting points of new compounds were recorded on an XT-4 thermal apparatus without correction.

Preparation of the Complexes

*N,N′-Butylenebis(imidazole): (Fumaric Acid)$_2$ (**1**)*

N,*N*′-Butylenebis(imidazole) (0.019 g, 0.1 mmol) was dissolved in 1 mL of ethanol. To this solution was added fumaric acid (0.024 g, 0.2 mmol) in 3 mL ethanol. Colorless prisms were afforded after 1 week of slow evaporation of the solvent, yield 24 mg, 55.8%. mp 209–210 °C. Elemental analysis performed on crystals exposed to the atmosphere: Calc. for $C_{18}H_{22}N_4O_8$: C 51.14, H 5.21, N 13.26. Found: C 51.07, H 5.16, N 13.22. Infrared spectrum (KBr disc, cm^{-1}): 3427s, 3131s, 1642s, 1621s, 1455 m, 1373s, 1284m, 1167m, 1090m, 983m, 842m, 759m, 648m, 513m.

*N,N′-Butylenebis(imidazole): (2,4,6-Trinitrophenol)$_2$ (**2**)*

N,*N*′-butylenebis(imidazole) (0.019 g, 0.1 mmol) was dissolved in 1 mL of methanol. To this solution was added 2,4,6-trinitrophenol (0.046 g, 0.2 mmol) in 10 mL methanol. Pale yellow block crystals were afforded after several hours, yield 39 mg, 60%. mp 258–260 °C. Elemental analysis performed on crystals exposed to the atmosphere: Calc. for $C_{22}H_{20}N_{10}O_{14}$: C 40.71, H 3.08, N 21.59. Found: C 40.68, H 3.07, N 21.55. Infrared spectrum (KBr disc, cm^{-1}): 3446m, 3146m, 3060m, 2957m, 2848m, 1614s, 1561s, 1546s, 1526s, 1484s, 1435m, 1364s, 1316s, 1274s, 1165m, 1076m, 914m, 786m, 767m, 747m, 706m, 625m, 539m.

X-Ray Crystallography

Suitable crystals were mounted on a glass fiber on a Bruker SMART 1000 CCD diffractometer operating at 50 kv and 40 mA using Mo Kα radiation (0.71073 Å). Data collection and reduction were performed using the SMART and SAINT software [38]. The structures were solved by direct methods, and the non-hydrogen atoms were subjected to anisotropic refinement by full-matrix least squares on F^2 using SHELXTL package [39].

Hydrogen atom positions for all of the structures were located in a difference map and refined independently. Further details of the structural analysis are summarized in Table 1. Selected bond lengths and angles for complexes **1** and **2** are listed in Table 2, the relevant hydrogen bond parameters are provided in Table 3.

Results and Discussion

Preparation and General Characterization

N,*N*′-butylenebis(imidazole) has good solubility in common organic solvents, such as CH_3OH, C_2H_5OH, CH_3CN, $CHCl_3$, and CH_2Cl_2. The crystals were grown by slow evaporation of the corresponding solution at room temperature. Crystallization of *N*,*N*′-butylenebis(imidazole) with fumaric acid or picric acid were carried out in a 1:2 ratio. The two complexes are not hygroscopicity, and they all crystallized with no solvent molecules accompanied. The molecular structures and their atom labelling schemes for the two structures are illustrated in Figs. 1, 3.

In the preparation of **1**, and **2**, the acids were mixed directly with the base in methanol and/or ethanol solution, which was allowed to evaporate at ambient conditions to

Table 1 Summary of X-ray crystallographic data for complexes **1**–**2**

	1	**2**
Formula	$C_{10}H_{16}N_4,C_4H_4O_4,C_4H_2O_4$	$C_{10}H_{16}N_4,2(C_6H_2N_3O_7)$
Fw	422.40	648.48
T (K)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Triclinic	Triclinic
Space group	$P-1$	$P-1$
a (Å)	5.9990(12)	7.0236(14)
b (Å)	8.1772(16)	8.2831(17)
c (Å)	10.419(2)	12.053(2)
α (°)	86.88(2)	106.05(4)
β (°)	84.73(3)	99.13(2)
γ (°)	77.03(4)	98.84(3)
V (Å^3)	495.67(17)	650.8(2)
Z	1	1
D_{calcd} (Mg/m^3)	1.415	1.655
Absorption coefficient (mm^{-1})	0.113	0.141
F(000)	222	334
Crystal size (mm^3)	0.50 × 0.36 × 0.16	0.36 × 0.24 × 0.07
θ range (°)	3.17–27.52	3.00–26.00
Limiting indices	$-7 \le h \le 7$ $-10 \le k \le 10$ $-13 \le l \le 13$	$-8 \le h \le 8$ $-10 \le k \le 10$ $-13 \le l \le 14$
Reflections collected	4,927	5,709
Reflections independent (R_{int})	2,257 (0.0151)	2,554 (0.0263)
Goodness-of-fit on F^2	1.058	1.064
R indices [$I > 2\sigma(I)$]	0.0405, 0.1248	0.0442, 0.1061
R indices (all data)	0.0512, 0.1312	0.0667, 0.1184
Largest diff. peak and hole (e Å^{-3})	0.195, −0.285	0.183, −0.238

give the final crystalline products. The elemental analysis data for the compounds are in good agreement with their compositions. The infrared spectra of **1** and **2** are consistent with their chemical formulas determined by elemental analysis and further confirmed by X-ray diffraction analysis. The very strong and broad features at approximately 3,400–3,200 cm^{-1} in the spectra of the two compounds arise from O–H or N–H stretching frequencies. Aromatic and imidazolyl ring stretching and bending are attributed to the medium intensity bands in the regions of 1,500–1,630 cm^{-1} and 600–750 cm^{-1}, respectively. The intense peak at 1,642 cm^{-1} was derived from the existence of the C=O stretches, and the band at 1,284 cm^{-1} exhibited the presence of the C–O stretches of the fumarate. The absence of bands at ca. 2,500 cm^{-1} and 1,900 cm^{-1} in compound **1**, and **2**, was interpreted as a lack of co-crystal formation [40].

IR spectroscopy has also proven to be useful for the recognition of proton transfer compounds [41, 42]. The most distinct feature in the IR spectrum of proton transfer compounds is the presence of strong asymmetrical and symmetrical stretching frequencies at 1,550–1,610 cm^{-1} and 1,300–1,420 cm^{-1} in compound **2**, respectively [43].

X-Ray Structure of *N*,*N*′-Butylenebis(imidazole): (Fumaric Acid)$_2$ **1**

The asymmetric unit of **1** consists of half a molecule of *N*,*N*′-butylenebis(imidazole), one half of fumaric acid and one half of a fumarate ion, which is shown in Fig. 1. Only one N atom of 1-(4-(1H-imidazol-1-yl)-butyl)-1H-imidazole is protonated by fumaric acid. In the compound, there are two pairs of ion pair with no included solvent molecules, which is well agreement with the micro-analysis results.

The N(1)–O(4)#4(Symmetry code 4: $x + 1$, y, z) distance in these contacts is 2.626 (2) Å, which is considerably less than the sum of the van der Waals radii for N and O (3.07 Å) [44], so in the solid state, there is consistently ionic hydrogen bonds formed between the imidazolium NH$^+$ and the fumarate ions, which is to be expected [45].

Table 2 Selected bond lengths [Å] and angles [°] for **1–2**

1				
	N(2)–C(1)	1.3244(17)	N(2)–C(3)	1.3749(18)
	N(2)–C(4)	1.4718(16)	N(1)–C(1)	1.3181(18)
	N(1)–C(2)	1.3616(19)	O(1)–C(6)	1.2041(18)
	O(2)–C(6)	1.3025(17)	O(3)–C(8)	1.2624(17)
	O(4)–C(8)	1.2471(17)	C(1)–N(2)–C(3)	108.39(12)
	C(1)–N(2)–C(4)	125.04(12)	C(3)–N(2)–C(4)	126.55(12)
	C(1)–N(1)–C(2)	108.93(12)	N(1)–C(1)–N(2)	108.75(12)
2				
	N(1)–C(1)	1.319(3)	N(1)–C(2)	1.365(3)
	N(2)–C(1)	1.329(3)	N(2)–C(3)	1.370(3)
	N(2)–C(4)	1.476(3)	N(3)–O(3)	1.212(2)
	N(3)–O(2)	1.222(2)	N(3)–C(10)	1.459(2)
	N(4)–O(4)	1.224(2)	N(4)–O(5)	1.228(2)
	N(4)–C(8)	1.446(3)	N(5)–O(6)	1.216(2)
	N(5)–O(7)	1.228(2)	N(5)–C(6)	1.453(3)
	O(1)–C(11)	1.254(2)	C(1)–N(1)–C(2)	108.65(19)
	C(1)–N(2)–C(3)	108.50(17)	C(1)–N(2)–C(4)	129.06(17)
	C(3)–N(2)–C(4)	122.43(17)	O(3)–N(3)–O(2)	124.03(18)
	O(3)–N(3)–C(10)	117.89(17)	O(2)–N(3)–C(10)	118.07(17)
	O(4)–N(4)–O(5)	122.23(18)		

Table 3 Hydrogen bond distances and angles in studied structures **1–2**

D–H···A	*d*(D–H) [Å]	*d*(H···A) [Å]	*d*(D···A) [Å]	<(DHA) [°]
1				
N(1)–H(2)···O(4)#4	0.86(2)	1.77(2)	2.626(2)	170.9(2)
O(2)–H(10)···O(3)#4	0.99(2)	1.52(2)	2.504(2)	173(2)
2				
N(1)–H(10)···O(7)#2	0.88(3)	2.39(3)	2.988(3)	126(2)
N(1)–H(10)···O(1)#2	0.88(3)	1.88(3)	2.699(3)	155(2)

Symmetry transformations used to generate equivalent atoms for **1**: #4 $x + 1, y, z$

Symmetry transformations used to generate equivalent atoms for **2**: #2 $x, y - 1, z$

Each imidazolium NH^+ forms one hydrogen bond with one oxygen atom of the fumarate ions. It was found that protonation of the imidazole ring nitrogen atoms causes no significant change in conformation of (1-(4-(1H-imidazol-1-yl)butyl)-1H-imidazole) in 1 in comparison to the corresponding neutral molecule (1-(4-(1H-imidazol-1-yl)butyl)-1H-imidazole) [46]. The imidazole rings in 1 have *trans*-(ap) position in respect to C5–C5a bond (angle C4–C5–C5a–C4a, 180°), which is different from the corresponding 1,1′-(1, 4-butanediyl)bis(imidazolium) dihydrochloride [46]. It is clear that the difference in bond lengths of C–O within the

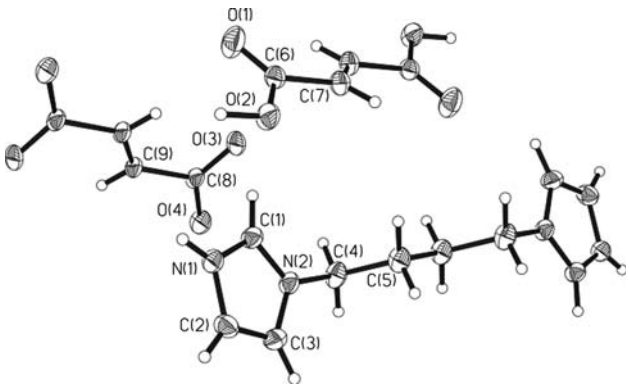


Fig. 1 The structure of **1**, showing the molecular components and atom numbering scheme. Displacement *ellipsoids* are drawn at the 30% probability level

carboxylic acid group (0.098 Å) is much greater than the one found in the fumarate anions (0.0153 Å). Also the average distances for C–O(1.2548 Å) in fumarate is less than the single bond C–O(1.3025 Å) and greater than the double bond C=O(1.2041 Å) in carboxylic acid group of fumaric acid. This supports our assignment of the fumarate anions. C–O distances (O(4)–C(8), 1.2471(17) Å) clearly indicate that the acid moieties in the compound are dianions when it formed hydrogen bonds with the imidazoliun nitrogen atoms. So the negative charge in CO_2^- group is localized on O(4) atom. Whereas the corresponding distances for CO_2^-···HOOC (O(2)–C(6), 1.3025(17) Å) support the existence of non-ionic acid moieties indicating co-crystal formation. The significant difference in O–C bond distances of the compound is mainly because of the fact that O(2) is involved in stronger hydrogen bonding with O(3) of fumarate compared to O(4) which is involved with hydrogen bonding of N^+–H···O^- of the imidazole moiety. In the structure, there are chains of fumarate moieties linked via CO_2^-···HOOC hydrogen bonds in which the two carboxylate O(C=O) atoms form two hydrogen bonds in bis-monodentate fashion with the neutral fumaric acid. The fumarate also gives strong electrostatic interactions between both charged units, the other two fumarate O(C–O) atoms also form two hydrogen bonds in bis-monodentate mode with the two imidazole N atoms. While the fumaric acid only acts as double donor(OH) to the di-ionic fumarate. Two dimensional network structure is formed through imidazolium moieties forming hydrogen bonds to di-ionic carboxylate groups of fumarate chains, which is shown in Fig. 2. In the same network layers, C–H···O contact also accompanies the N^+–H···O^- hydrogen bond, which utilizes H3, H2A on imidazole ring and O3, and O4 on the CO_2^- carbonyl oxygen atom (C3···O3, 3.379 Å; C2···O4, 3.478 Å). Adjacent layers are also connected by C–H···O (C1–H1···O3, C1···O3, 3.244 Å) contact, all these lead the extended architecture to show a three-dimensional lamellar structure.

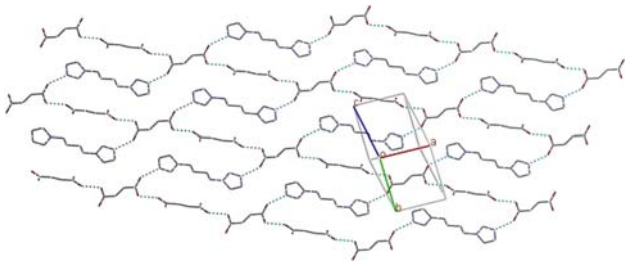


Fig. 2 Infinite two-dimensional network structure of **1**

X-Ray Structure of *N*,*N*′-Butylenebis(imidazole): (2,4,6-Trinitrophenol)$_2$ (**2**)

Complex **2** was prepared by reaction of a methanol solution of 2,4,6-trinitrophenol and *N*,*N*′-butylenebis(imidazole) in 2:1 ratio, which crystallizes as triclinic pale yellow crystals in the centrosymmetric space group P−1. The structure of **2** with the atom-numbering scheme is shown in Fig. 3. The OH groups of 2,4,6-trinitrophenol are ionized by proton transfer to one of the imidazole moieties of *N*,*N*′-butylenebis(imidazole). Both of the terminal N atoms of bis-imidazol-1-yl are protonated. In the whole molecule there existed an inversion center locating in the middle point of C5 and C5A. The dihedral angles between the imidazole ring and the benzene ring is 78.45°.

In the solid state, there is consistently hydrogen bonds formed between the imidazolium NH^+, and the 2,4,6-trinitrophenolate ions. Each imidazolium NH^+ forms two hydrogen bonds with two oxygen atoms of the 2,4,6-trinitrophenolate ions, one is the oxygen atom of the 2,4,6-trinitrophenolate ions, the other oxygen atom comes from the NO_2 group.

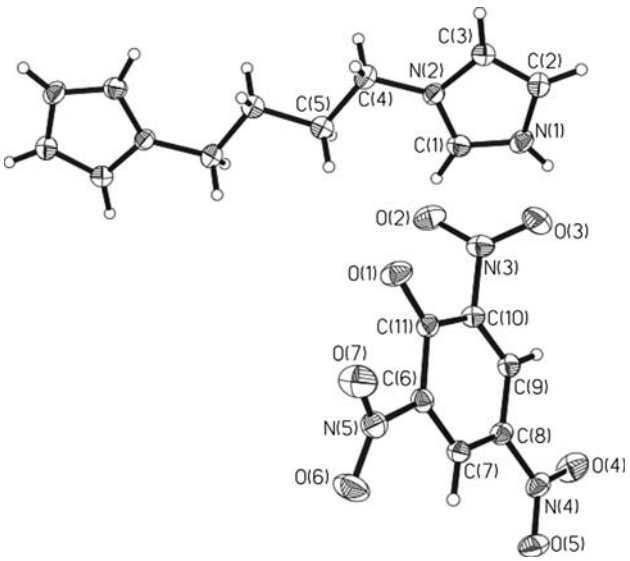


Fig. 3 The structure of **2**, showing the atom-numbering scheme. Displacement *ellipsoids* are drawn at the 30% probability level

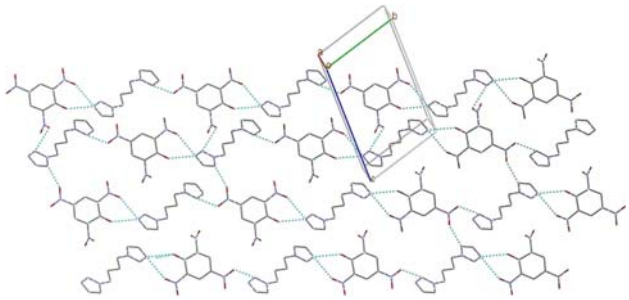


Fig. 4 2D network structure of **2** viewed from the *a* axis

Imidazolium cations and 2,4,6-trinitrophenolate anions self-assembled via N^+–H···O^- hydrogen bonds to form bis-2,4,6-trinitrophenolate terminated compound, and the two terminated 2,4,6-trinitrophenolates exist in *trans* conformation. The N···O and H···O bond lengths ranged from 2.699(3) to 2.988(3) Å, and from 1.88(3) to 2.39(3) Å, respectively. The N^+–H···O^- bond angles ranged from 126(2) to 155(2)°. These values are consistent with values reported from a statistical analysis of N–H···O hydrogen bonds involving imidazolium residues in forming crystal structures [47] and from a study of N^+–H···O^- hydrogen bonding in salts of imidazole with monocarboxylic acids [48].

Two parallel imidazolium cations and two antiparallel 2,4,6-trinitrophenolate anions formed 32-membered rings through hydrogen bonding interaction, these rings extended along the *c* axis direction to form one dimensional railway structure. Adjacent parallel railways connect further through C–H···O hydrogen bonds between the 2-CH of the imidazole ring and the NO_2 group O atoms (C–O distance is 3.024 Å) to form 2D network structure, which is shown in Fig. 4. The 2D network further stacks into 3D layer structure.

Supporting Information Available

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic data center, CCDC Nos. 673178 for **1**, and 674979 for **2**. Copies of this information may be obtained free of charge from the +44(1223)336-033 or Email: deposit@ccdc.cam.ac.uk or www: http://www.ccdc.cam.ac.uk.

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