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Color Variety of Organic Salt of *N,N'*-Bis(Glycinyl)Pyromellitic Diimide and *N*-Containing Base

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Color Variety of Organic Salt of *N*,*N*′-Bis(Glycinyl)Pyromellitic Diimide and *N*-Containing Base

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A series of organic salts obtained by mixing N,N′*-bis(glycinyl)pyromellitic diimide and* N*-containing bases has been synthesized. The composition of the above-mentioned organic salt is anionic* N,N′*-bis(glycinyl)pyromellitic diimide (*H_2***BPDI***) and cationic urotropine (***UTP***), 1,10-phenanthroline (***PHEN***), benzidine (***BZ***), and 4-(4′-methylpiperazin)methylquinolin-2(1H)-one (***MMQ***). Different connecting patterns of the network are dependent on the corresponding organic cation. In addition, crystalline* **2**(*H_2***BPDI**$\cdot$***HBPDI**$^-\cdot$***HPHEN**$^+$), **3**(*H_2***BPDI**$\cdot$***BPDI**$^{2-}\cdot$*H_2***BZ**$^{2+}$) *and* **4**(2***HBPDI**$^-\cdot$2***HMMQ**$^+\cdot$7H_2O) *exhibit* π-π *stacking interaction. The solid state of* **1**(***HBPDI**$^-\cdot$***HUTP**$^+$) *is colorless,* **2** *is light pink,* **3** *is red, and* **4** *is yellow.*

Keywords Benzidine; *N*,*N*′-bis(glycinyl)pyromellitic diimide; 4-(4′-methylpiperazin)-methylquinolin-2(1*H*)-one; 1,10-phenanthroline; urotropine

Introduction

Aromatic diimides have attracted great attention in recent years due to their potential applications in areas of supramolecular chemistry and materials [1]. Their peculiar features such as photophysical properties [2,3], which can be applied in the fields of conducting thin film [4] and molecular sensors [5,6], are worth investigating. Supramolecular assemblies such as hydrogen-bonded helical organic nanotubes [7] and supramolecular devices such as foldermer [8], switch [9], and ion channel [2] have also attracted much attention for their novel topologies and functions.

The family of diimides includes pyromellitic diimides, naphthalene diimide, perylene diimide, and their derivatives. The functionalization of diimide tetracarboxylic dianhydride with primary amine compound is an efficient route to introduce a large diversity of functional groups. Syntheses of symmetrical and unsymmetrical derivatives have been performed [10]. These derivatives feature aromatic diimide

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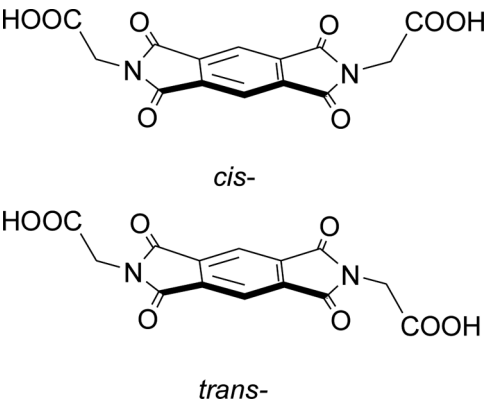
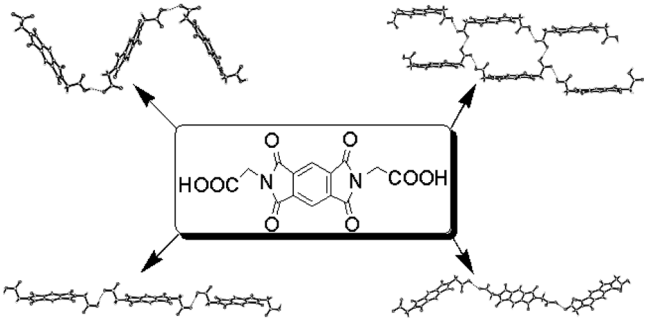


Scheme 1. Possible conformations of H_2BPDI.

cores, among which pyromellitic diimide is the simplest. *N*,*N*′-substituted pyromellitic diimide can be treated as a prototype in the research of aromatic diimides for its convenient synthesis process and structural characteristics. Bispyridyl-substituted pyromellitic diimide ligands have been used to generate metal-organic frameworks [11]. Diacid-substituted compounds were produced as intermediates of macromolecules [12]. However, studies of pyromellitic diimide derivatives have been limited. As a model, *N*,*N*′-bis(glycinyl)pyromellitic diimide (H_2**BPDI**) is semi-rigid compound with a rigid basal plane and two flexible acid groups. The molecule easily forms hydrogen bonds and also π-π stacking interaction, which offer a largely controlled use in crystal engineering. The inclusion of H_2**BPDI** with aromatic guests of anthracene, phenanthrene, and perylene, which mainly represent π-π stacking interaction, has been reported [13].

Herein, we wish to report the arrays of anionic *N*,*N*′-bis(glycinyl)pyromellitic diimide and cationic *N*-containing base based on hydrogen bond and π-π stacking interaction. Crystals of **1**–**4** (**1**, H**BPDI**$^-$·H**UTP**$^+$; **2**, H_2**BPDI** · H**BPDI**$^-$ · H**PHEN**$^+$; **3**, H_2**BPDI** · **BPDI**$^{2-}$ · H_2**BZ**$^{2+}$; **4**, 2H**BPDI**$^-$ · 2H**MMQ**$^+$ · 7H_2O) exhibit π-π stacking interaction. The solid state is grown by routine ways, wherein H_2**BPDI** has been found in neutral, anionic H**BPDI**$^-$ or **BPDI**$^{2-}$ forms and two steric possible conformations (Scheme 1 and Scheme 2), respectively. The color of the crystal is dependent on corresponding base: **1**, colorless; **2**, light pink; **3**, red; **4**, yellow.



Scheme 2. Conformations of H_2BPDI in different crystals.

Experimental

Materials and Methods

N,*N*′-bis(glycinyl)pyromellitic diimide (H_2**BPDI**) was synthesized according to the literature [13]. Reagents of analytical grade (which were purchased from Sinopharm Chemical Reagent Co., Ltd.) were used without further purification. Elemental analyses were obtained on an Elementar Vario EL analyzer. The infrared (IR) spectra were recorded with a Perkin Elmer Fourier transform infrared (FTIR) spectrometer with KBr pellets in the range 4,000–500 cm^{-1}. ^{1}H nuclear magnetic resonance (NMR) spectra were recorded on a Varian/Mercury-Plus 300 instrument. The fluorescence spectra were taken at room temperature on a Varian Cary Eclipse spectrofluorometer.

Syntheses and Characterization

Synthesis of N,N′-dis(glycinyl)pyromellitic diimide (H2BPDI). The compound was prepared by a literature method and characterized by ^{1}H NMR. Pyromellitic dianhydride (6.54 g, 30 mmol) was dissolved in glacial acetic acid (180 mL), which was warmed to 40°C. Powdered glycine (4.5 g, 60 mmol) was added to this solution and refluxed for 4 h. After cooling, the deposit was filtered and washed with water, and then dried to give the title compound (7.07 g, 70.9%). ^{1}H NMR (CD_3OD): δ 8.39 (s, 2**H**, ArH), 4.52 (s, 4H, C$\mathbf{H}_2$).

Synthesis of 1. A solution of H_2**BPDI** (0.1 mmol) in 25 mL MeOH was mixed with a solution of urotropine (0.1 mmol) in 5 mL MeOH with stirring. The solution was filtered and the filtrate was allowed to evaporate at room temperature for 12 h to give rise to a large amount of colorless block crystals (yield: 76%). Anal Calc. for $C_{20}H_{20}N_6O_8$: C, 50.85; H, 4.27; N, 17.78. Found: C, 50.81; H, 4.55; N, 17.95.

*Synthesis of **2**.* A solution of H_2**BPDI** (0.2 mmol) in 30 mL MeOH was mixed with a solution of 1,10-phenanthroline (0.2 mmol) in 10 mL MeOH. The resulting mixture was left to stand undisturbed. Block single crystals suitable for X-ray analysis were obtained after 1 day. Crystal of **2**, light pink, yield 52%. Anal Calc. for $C_{40}H_{24}N_6O_{16}$: C, 56.88; H, 2.86; N, 9.95. Found: C, 56.53; H, 2.99; N, 9.61.

*Synthesis of **3**.* A methanol solution of benzidine (0.4 mmol) was layered on top of a methanol solution of H_2**BPDI** in a tube (diameter 18 mm). After 1 day, red crystals were found at the interface (yield: 81%). Anal Calc. for $C_{52}H_{40}N_8O_{16}$: C, 60.47; H, 3.90; N, 10.85. Found: C, 60.88; H, 4.21; N, 10.69.

*Synthesis of **4**.* X-ray quality single crystals of **4** were grown by slow evaporation the MeOH solution of H_2**BPDI** and 4-(4′-methylpiperazin)methylquinolin-2(1*H*)-one. Crystal of **4**, yellow, yield 81%. Anal Calc. for $C_{58}H_{68}N_{10}O_{25}$: C, 53.37; H, 5.25; N, 10.73. Found: C, 53.81; H, 5.64; N, 11.11.

X-Ray Crystallography

Diffraction data were measured on a Bruker SMART CCD diffractometer using graphite monochromated MoKa radiation ($\lambda = 0.71073$ Å). The collected data were reduced with the program SAINT and empirical absorption correction was done with the SADABS program (Version 2.03, Bruker AXS Inc., Madison, WI, USA).

All structures were solved by the direct method and refined by the full-matrix least-squares method on F^2 with anisotropic thermal parameters for all nonhydrogen atoms. Crystallographic details of **1, 2, 3,** and **4** are listed in Table 1.

Results and Discussion

The crystal structure determination of **1** revealed the binding of H**BPDI**$^-$ anions forming a one-dimensional infinite zigzag-like chain via O−H···O hydrogen bond (O8···O2 [symmetry code: x, $3/2-y$, $1/2+z$)] 2.471(4) Å, O8−H8···O2 151°, Fig. 1). All H**BPDI**$^-$ anions adopt the *cis*-conformation where the included angle of the chain is 62.0°. Cationic urotropine is intercalated into the enclosed space by N−H···O hydrogen bond (N3···O2 [symmetry code: x, $-1+y$, z] 2.641(4) Å, N3−H2···O2 166°). There are no π-π interactions existing in crystalline **1**. Intricate C−H···O, C−H···N, C−H···π interactions (Table 2) further link these components to form a three-dimensional network.

The crystal structure determination of **2** reveals an unexpected structural motif. The self-assembly of *cis*-H_2**BPDI** and *cis*-H**BPDI**$^-$ building blocks by O−H···O hydrogen bonds (O8···O1 [symmetry code: $1+x$, $-1+y$, z] 2.597(6) Å, O8-H8···O1 158°; O9···O16 [symmetry code: $-1+x$, $1+y$, z] 2.685(6) Å, O9-H9···O16 147°; O15···O2 [symmetry code: $1+x$, $-1+y$, z] 2.503(6) Å, O15-H15···O2 167°) resulted in a 1D molecular ladder with a remarkably large [(*cis*-H_2**BPDI**)(μ-COO^-)(*cis*-H**BPDI**$^-$)(μ-COOH)] parallelogram ring having estimated ledges of 9.624 Å × 10.053 Å as shown in Fig. 2. Independent ladders are stacked by face-to-face π-π interaction with centroid-to-centroid distance of 3.86 Å (Fig. 3a). Thus, the two-dimesional network with open channels is represented in which one cationic phen is held in the spacious cavity in one corner by hydrogen bond (N5···O16 [symmetry code: $-1+x$, $1+y$, z] 2.766(8) Å, N5-H5A···O16 142°) and π-π interactions (the distance between centroids of ring confined by N5-C41-C42-C43-C44-C45 and ring confined by C5-C6-C7-C8-C9-C10 is 3.72 Å). This arrangement still leaves a cavity in the opposite corner that is occupied by phen ion stretching from adjacent chain (Fig. 3b). The latter phen ion is involved in π-π interaction with centroid-to-centroid distance of 3.67 Å (between the ring confined by N6-C46-C49-C50-C51-C52 and the ring confined by C19-C2-C21-C22-C23-C24). The phen plane has a dihedral angle of 9.0° with the aromatic plane of H**BPDI**$^-$. Many weak C-H···O hydrogen bonds (Table 3) have also been observed in the crystal.

In the structure of **3**, alternating *trans*-H_2**BPDI** and *trans*-**BPDI**$^-$ are linked by O-H···O hydrogen bond (O1···O6 2.549(3) Å, O1-H1···O6 176°) to extend a linear chain (Fig. 4). The dihedral angle between rigid planes is 1.6° and centers are arrayed in a straight line. Cationic benzidines are also linked to form a 1D chain by N-H···N hydrogen bonds (N3···N4 [symmetry code: x, $1+y$, z] 2.922(3) Å, N3-H3B···N4 166°). Chains of hosts and guests are arranged in a crossover fashion (Fig. 5). The nodes are fixed by multiple N-H···O hydrogen bonds (N3···O3 [symmetry code: $1-x$, $1-y$, $-z$] 2.951(3) Å, N3-H3A···O3 109°; N3···O6 [symmetry code: $-1+x$, y, z] 2.828(3) Å, N3-H3A···O6 166°; N3···O5 [symmetry code: $1-x$, $1-y$, $1-z$] 2.797(3) Å, N3-H3C···O5 176°; N4···O8 [symmetry code: $1-x$, $-y$, $1-z$] 3.018(3) Å, N4-H4A···O8 145°; N4···O1 [symmetry code: x, $-1+y$, z] 3.218(3) Å, N4-H4A···O1 131°; N4···O2 [symmetry code: $1-x$, $-y$, $-z$] 3.114(3) Å, N4-H4A···O1 155°). Viewing along the b axis, different layers are arranged without interaction between the same kind of chains. Only one C-H···O

Table 1. Crystallographic data for **1**–**4**

Compound	**1**	**2**	**3**	**4**
Empirical formula	$C_{20}H_{20}N_6O_8$	$C_{40}H_{24}N_6O_{16}$	$C_{52}H_{40}N_8O_{16}$	$C_{58}H_{68}N_{10}O_{25}$
Formula weight	472.42	844.65	1,032.92	1,305.22
Temperature (K)	293(2)	296(2)	293(2)	298(2)
Crystal system space group	Orthorhombic Pbca	Triclinic P1	Triclinic P-1	Monoclinic P21/c
Unit cell dimensions	$a = 18.492(4)$ Å $b = 10.702(4)$ Å $c = 20.247(3)$ Å	$a = 7.439(3)$ Å $b = 11.076(4)$ Å $c = 12.688(4)$ Å $\alpha = 106.418(6)^\circ$ $\beta = 98.413(6)^\circ$ $\gamma = 102.298(6)^\circ$	$a = 9.834(2)$ Å $b = 11.266(2)$ Å $c = 11.743(2)$ Å $\alpha = 64.23(3)^\circ$ $\beta = 78.54(3)^\circ$ $\gamma = 77.89(3)^\circ$	$a = 7.3874(15)$ Å $b = 14.408(3)$ Å $c = 28.289(6)$ Å $\beta = 91.78(3)^\circ$
Volume (Å^3)	4,006.8(19)	955.7(6)	1,137.0(4)	3,009.6(11)
Z	8	1	1	2
Calculated density (Mg m^{-3})	1.566	1.468	1.508	1.440
Absorption coefficient (mm^{-1})	0.124	0.116	0.114	0.114
F(000)	1,968	434	536	1,372
Theta range for data collection°	2.01–26.00	1.99–25.00	1.94–28.34	3.07–25.00
Limiting indices	$-1 \le h \le 22$ $-1 \le k \le 13$ $-1 \le l \le 22$	$-8 \le h \le 8$ $-10 \le k \le 13$ $-14 \le l \le 15$	$-13 \le h \le 13$ $-14 \le k \le 14$ $-15 \le l \le 10$	$-7 \le h \le 8$ $-17 \le k \le 17$ $-33 \le l \le 33$
Reflections collected (unique)	4,826 (3,882) (R(int) = 0.0482)	4,950 (4,031) (R(int) = 0.0151)	7,507 (5,299) (R(int) = 0.0263)	22,291 (5,264) (R(int) = 0.0682)
Data/restraints/parameters	3,882/0/312	4,031/4/567	5,299/0/351	5,264/12/431
Goodness-of-fit on F^2	1.005	1.040	1.003	1.079
Final R indices ($I > 2\sigma$ (I))	$R^1 = 0.0623$ $wR^2 = 0.1208$	$R^1 = 0.0531$ $wR^2 = 0.1455$	$R^1 = 0.0562$ $wR^2 = 0.1123$	$R^1 = 0.0758$ $wR^2 = 0.2066$
R indices (all data)	$R^1 = 0.1456$ $wR^2 = 0.1532$	$R^1 = 0.0675$ $wR^2 = 0.1594$	$R^1 = 0.1221$ $wR^2 = 0.1380$	$R^1 = 0.1126$ $wR^2 = 0.2455$
Largest diff. Peak and hole (e Å^{-3})	0.238 and −0.278	0.997 and −0.182	0.201 and −0.243	0.595 and −0.358

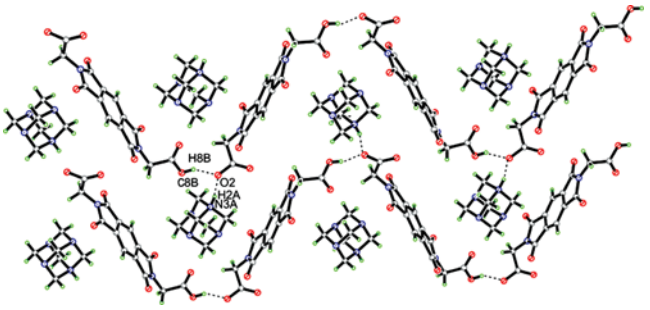


Figure 1. Self-assembled 1D chain structure in **1**.

Table 2. C–H···N(O) and C–H···π interactions in **1**

D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	∠D-H···A(°)	Symmetry operator
C2-H2A···N5	0.97	2.57	3.426(5)	148	$-x, 1/2+y, 1/2-z$
C2-H2B···O7	0.97	2.36	3.275(5)	157	$x, 3/2-y, -1/2+z$
C6-H6···O1	0.93	2.49	3.381(5)	159	$1/2-x, -1/2+y, z$
C9-H9···O1	0.93	2.47	3.369(5)	162	$-x, 2-y, 1-z$
C15-H15A···O5	0.97	2.43	3.339(5)	156	$-x, 1-y, 1-z$
C15-H15B···O4	0.97	2.47	3.311(5)	145	$1/2-x, -1/2+y, z$
C19-H19B···O7	0.97	2.52	3.437(5)	158	$x, 3/2-y, -1/2+z$
C15-H15A···Cg1[a]	0.97	2.89	3.315(4)	108	
C15-H15B···Cg2[a]	0.97	2.99	3.315(4)	101	
C18-H18A···Cg3[a]	0.97	2.96	3.867(4)	156	$x, 3/2-y, -1/2+z$

[a]Cg1 and Cg2 are the centers of gravity of the C5-C6-C7-C8-C9-C10 ring and N2-C11-C8-C7-C12 ring, respectively.

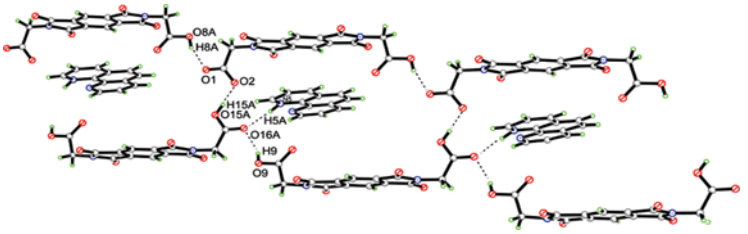


Figure 2. 1D ladder-like assembly of **2** showing the enclathration of cationic **PHEN**.

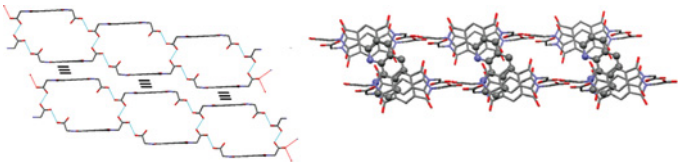


Figure 3. For **2**: (a) π-π interaction between ladders and (b) **PHEN** ions are trapped in the adjacent chains.

Table 3. C-H···O interactions in **2**

D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	∠D-H···A (°)	Symmetry operator
C2-H2B···O5	0.97	2.51	3.389(8)	151	$x,1+y,z$
C7-H7···O12	0.93	2.46	3.344(7)	159	$x,y,-1+z$
C13-H13A···O9	0.97	2.58	3.465(7)	151	$x,-1+y,-1+z$
C13-H13B···O3	0.97	2.60	3.408(8)	141	$x,-1+y,z$
C16-H16A···O14	0.97	2.53	3.378(8)	146	$x,1+y,z$
C21-H21···O6	0.93	2.44	3.330(7)	161	$x,y,1+z$
C27-H27A···O11	0.97	2.55	3.358(8)	141	$x,-1+y,z$
C42-H42···O4	0.93	2.53	3.108(10)	120	$2+x,y,z$
C43-H43···O4	0.93	2.51	3.093(8)	121	$1+x,y,z$
C52-H52···O10	0.93	2.56	3.483(13)	173	$-1+x,y,z$

hydrogen bond (C25···O7 [symmetry code: $1-x$, $1-y$, $-z$] 3.246(3) Å, C25-H25···O7 132°) has been found.

The difference between **1, 2** and **3, 4** has a torsion chain consisting of *trans*-H**BPDI**$^-$ by a hydrogen bond (O1···O8 [symmetry code: x, $1/2-y$, $1/2+z$] 2.543 Å, O1-H1··O8 172°, Fig. 6). Different parts are held together by water molecules (3.5 per unit) through hydrogen bonds (N3···O9 [symmetry code: $-x$, $1-y$, $1-z$] 3.041 Å, N3-H3··O9 121°; N5···O10 [symmetry code: $1-x$, $-1/2+y$, $3/2-z$] 2.772 Å, N5-H5··O10 171°; O10···O8 [symmetry code: $1+x$, $1/2-y$, $1/2+z$] 2.726 Å, O10-H10C··O8 165°; O10···O12 [symmetry code: $1+x$, y, z] 2.715 Å, O10-H10D···O12 159°; O11···O10 2.861 Å, O11-H11C··O10 124°; O11···O13 [symmetry code: $1-x$, $-1/2+y$, $3/2-z$] 2.922 Å, O11-H11D···O13

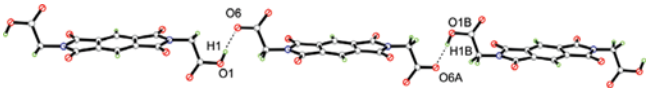


Figure 4. The hydrogen-bonded 1D linear chain in **3**.

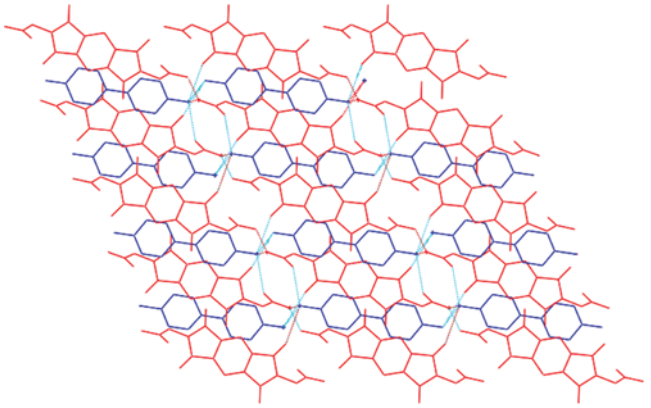


Figure 5. View of the arrangement of chains in **3** along the *b* direction.

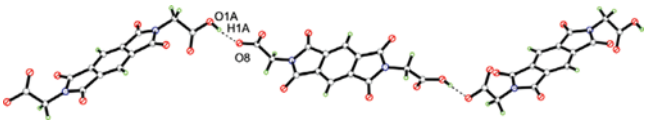


Figure 6. View of the 1 D chains in **4**.

105°; O11···O7 [symmetry code: x, $1/2-y$, $1/2+z$] 2.797 Å, O11-H11D···O7 131°; O12···O9 2.733 Å, O12-H12C···O9 167°; O12···O5 [symmetry code: $-x$, $1-y$, $1-z$] 2.875 Å, O12-H12D···O5 154°). Cationic 4-(4′-methylpiperazin)methylquinolin-2(1*H*)-one-(**MMQ**) is a multifunctional species that can be both an acceptor and a donor for hydrogen bonding involved in the hydrogen-bonded framework. The aromatic ring of the **MMQ** ion insert between rigid planes of H**BPDI**$^-$ with π-π separation of 3.69 Å forms an -A-B-A-B- infinite column (Fig. 7). C-H···O interactions (Table 4) also stabilize the network.

The photoluminescent (PL) property of **2**–**4** has also been investigated in the solid state at room temperature (Fig. 8). Emission peaks were present at about 407 ($\lambda_{ex}=365$ nm) for **2**, 404 nm for **3** ($\lambda_{ex}=254$ nm), and 468 nm for **4** ($\lambda_{ex}=254$ nm). The photoluminescence can be attributed to the π^*-π transitions from the organic salts. There is no π-π interaction in **1**, and **2, 3, 4** exhibit π-π interactions to hold the stacking structures. Patterns of π-π interaction led to varied color, which was due to the electronic interactions between ions. Without π-π interaction, **1** is colorless. In **2**, 1,10-phenanthroline (**PHEN**) a is nitrogen-containing heterocycle, and in **3**, benzidine (**BZ**) has amido groups. The excited state of **2, 3** is generated by exciting the *n*-electron of nitrogen atom to the π^* bonding orbit. The lone pair electrons are contribution to the conjugated π bond of the fluorescent molecule, which results in the increase of fluorescence intensity. In **4**, the oxygen atom of 4-(4′-methylpiperazin)

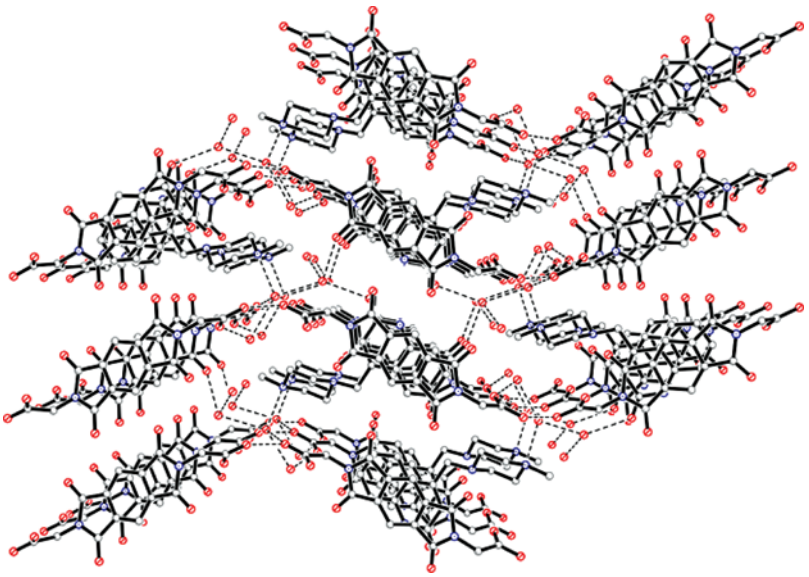


Figure 7. 3D packing of **4**, showing the hydrogen bond and π-π interaction.

Table 4. C-H···O interactions in **4**

D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	∠D-H···A (°)	Symmetry operator
C7-H7···O6	0.93	2.51	3.4221	168	$1-x, -y, 1-z$
C16-H16···O7	0.93	2.44	3.2723	149	$-1+x, y, z$
C25-H25B···O3	0.97	2.44	3.2582	142	$-1+x, y, z$
C26-H26A···O2	0.97	2.34	3.2469	156	
C26-H26B···O11	0.97	2.57	3.4062	145	$-1+x, y, z$
C27-H27B···O3	0.97	2.45	3.2105	135	
C29-H29A···O5	0.96	2.33	3.2162	153	$x, 1/2-y, 1/2+z$
C29-H29C···O13	0.96	2.52	3.2687	135	$1-x, -1/2+y, 3/2-z$
C29-H29C···O1	0.96	2.59	3.4072	144	$1-x, -1/2+y, 3/2-z$

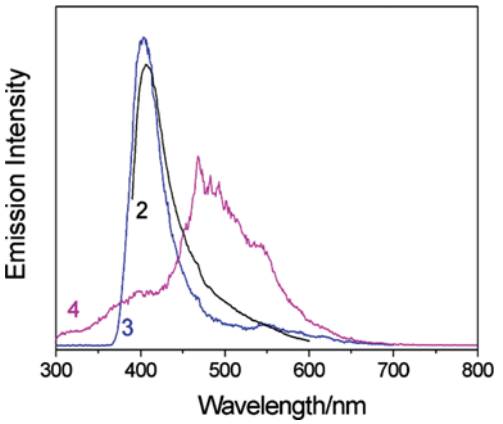


Figure 8. Emission spectra of **2**–**4** in the solid state at room temperature excited at 365 nm for **2** and 254 nm for **3**–**4**.

methylquinolin-2(1*H*)-one (**MMQ**) can be considered as an electron withdrawing group, which may decrease the fluorescence intensity and wavelength red shift. So different modes of closely packed components in the solid state with fixed conformation will lead to different emission behaviors. These results can provide information on the design of crystals with interesting color.

Conclusion

In this article, four organic salts based on *N*,*N*′-bis(glycinyl)-pyromellitic diimide have been investigated. Hydrogen bonding and π-π stacking are key factors in stacking structures. Varied organic bases led to varied assemblies and colors. It is not difficult to relate face-to-face π-π stacking with the varied color of these compounds.

Supplementary Materials

The detail crystallographic data of **1**–**4** have been deposited at the Cambridge Crystallographic Data Center as supplementary publication CCDC No. 742413–742416.

Copies of the data may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge, CB2 1EZ, UK (fax: +441223 336033; deposit@ccdc.cam.ac.uk or http://www.ccdc.cam.ac.uk).

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