

Tian-Tian Pan, Jia-Geng Liu and
Duan-Jun Xu*Department of Chemistry, Zhejiang University,
People's Republic of China

Correspondence e-mail: xudj@mail.hz.zj.cn

Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.048
 wR factor = 0.146
Data-to-parameter ratio = 15.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

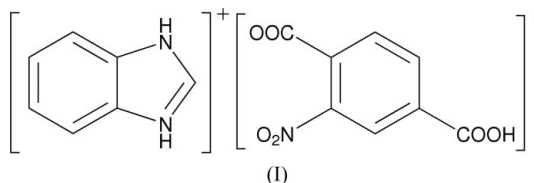
Benzimidazolium hydrogen nitroterephthalate

In the title compound, $\text{C}_7\text{H}_7\text{N}_2^+ \cdot \text{C}_8\text{H}_4\text{NO}_6^-$, the partially overlapped arrangement and the shorter face-to-face distance of 3.457 (4) Å indicate π - π stacking between parallel benzimidazolium cations, whereas the longer face-to-face distance of 3.649 (6) Å suggests normal van der Waals contacts between parallel benzene rings of neighbouring nitroterephthalate anions.

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Comment

Structure determinations have revealed that π - π stacking interactions commonly occur in metal complexes incorporating aromatic heterocyclic ligands, such as imidazole and benzimidazole (Pan & Xu, 2004), but are rarely found for other aromatic ligands, such as benzoate and its derivatives. As part of our ongoing investigations of the nature of π - π stacking, the title compound, (I), containing both benzimidazolium cations and nitroterephthalate anions, has been prepared, and its X-ray crystal structure is presented here.



The molecular structure of (I) is shown in Fig. 1. The crystal structure of (I) consists of benzimidazolium (bzim) cations and nitroterephthalate (ntph) anions; they link to each other *via* $\text{N}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonding (Table 1).

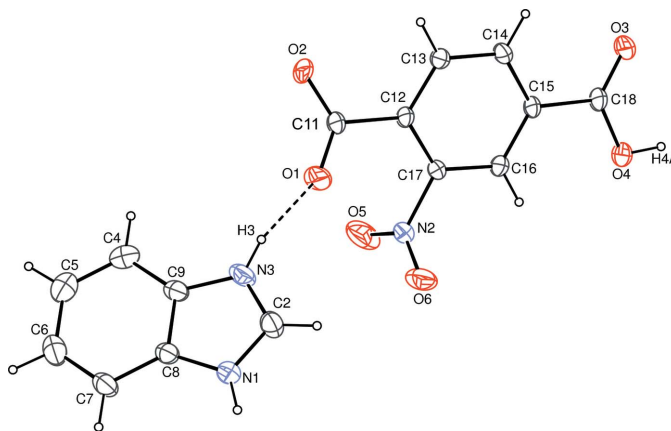


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). The dashed line indicates a hydrogen bond.

The two carboxylate groups of ntp are twisted out of the plane of the benzene ring by 8.31 (11)° for C18 (carboxylic acid) and 23.80 (11)° for C11 (carboxylate). This favours the formation of hydrogen bonds between bzim and ntp. The difference of 0.108 (3) Å in C–O bond distances for C18 suggests this is a neutral carboxylic acid group, which agrees with the peak in a difference Fourier map.

A partially overlapped arrangement between parallel bzim cations and between parallel benzene rings of neighbouring ntp anions is observed in the crystal structure of (I) (Fig. 2). The face-to-face distance of 3.457 (4) Å indicates the existence of π – π stacking between bzim cations, whereas the face-to-face distance of 3.649 (6) Å suggests normal van der Waals contacts between the benzene rings of neighbouring ntp anions.

Experimental

Na₂CO₃ (0.21 g, 2 mmol) and nitroterephthalic acid (0.42 g, 2 mmol) were dissolved in a hot water–ethanol solution (20 ml, 1:3 v/v). Benzimidazole (0.24 g, 2 mmol) was then added to this solution. The mixture was refluxed for 4 h and filtered after cooling to room temperature. Colourless single crystals of (I) were obtained after three weeks.

Crystal data

C ₇ H ₇ N ₂ ⁺ ·C ₈ H ₄ NO ₆ [−]	Z = 2
M _r = 329.27	D _x = 1.493 Mg m ^{−3}
Triclinic, P1̄	Mo K α radiation
a = 8.445 (6) Å	Cell parameters from 6302 reflections
b = 9.076 (4) Å	θ = 2.8–25.0°
c = 9.755 (4) Å	μ = 0.12 mm ^{−1}
α = 98.051 (2)°	T = 295 (2) K
β = 91.905 (2)°	Block, colourless
γ = 97.891 (2)°	0.36 × 0.30 × 0.24 mm
V = 732.3 (7) Å ³	

Data collection

Rigaku R-AXIS RAPID diffractometer	2593 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.022$
Absorption correction: none	$\theta_{\text{max}} = 27.5^\circ$
7282 measured reflections	$h = -10 \rightarrow 10$
3323 independent reflections	$k = -11 \rightarrow 11$
	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0827P)^2 + 0.1449P]$
$R[F^2 > 2\sigma(F^2)] = 0.048$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.146$	$(\Delta/\sigma)_{\text{max}} < 0.001$
S = 1.06	$\Delta\rho_{\text{max}} = 0.31 \text{ e } \text{Å}^{-3}$
3323 reflections	$\Delta\rho_{\text{min}} = -0.29 \text{ e } \text{Å}^{-3}$
217 parameters	
H-atom parameters constrained	

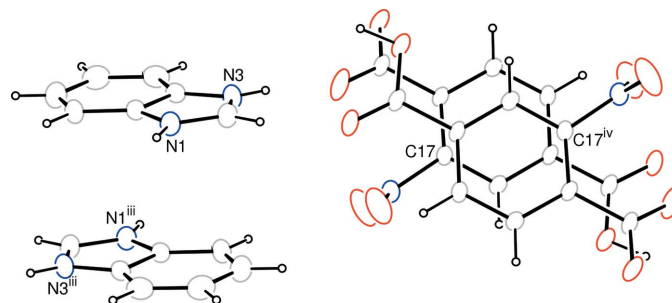


Figure 2

The partially overlapped arrangement of neighbouring aromatic rings [symmetry codes: (iii) $-x, -y, 1 - z$; (iv) $1 - x, 1 - y, -z$].

Table 1

Hydrogen-bond geometry (Å, °).

D–H...A	D–H	H...A	D...A	D–H...A
N1–H1...O2 ⁱ	0.91	1.82	2.724 (3)	170
N3–H3...O1	0.84	1.78	2.619 (3)	171
O4–H4A...O2 ⁱⁱ	0.97	1.65	2.619 (2)	173

Symmetry codes: (i) $x, y - 1, z$; (ii) $x, y, z - 1$.

H atoms on the carboxylic O atom and bzim N atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{carrier})$. Other H atoms were placed in calculated positions, with C–H = 0.93 Å and included in the final cycles of refinement in the riding mode, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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