

## 4-(4-Pyridylamino)pyridinium isophthalate

Jarrod J. M. Amoore and  
Cameron J. Kepert\*School of Chemistry, F11, University of Sydney,  
NSW 2006, AustraliaCorrespondence e-mail:  
c.kepert@chem.usyd.edu.au

## Key indicators

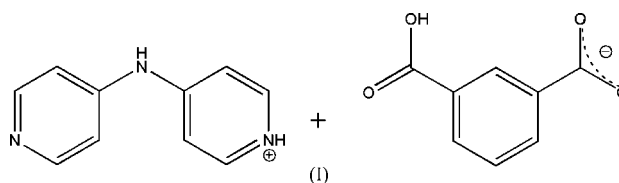
Single-crystal X-ray study  
 $T = 150$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.037  
 $wR$  factor = 0.101  
Data-to-parameter ratio = 16.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title salt,  $\text{C}_{10}\text{H}_{10}\text{N}_3^+\cdot\text{C}_8\text{H}_5\text{O}_4^-$ , the protonated 4,4'-dipyridylamine and deprotonated isophthalic acid molecules are bound together in the crystal structure through  $\pi$ - $\pi$  stacking,  $\text{O}\cdots\text{H}-\text{N}$ ,  $\text{O}\cdots\text{H}-\text{C}$  and  $\text{N}\cdots\text{H}-\text{O}$  interactions.

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## Comment

The title compound, (I), involved the co-crystallization of two different organic molecules. Co-crystallization of two or more molecules, one often being a carboxylic acid and the other a proton acceptor, has received increased interest in recent years (Aakeroy *et al.*, 2003; Bhogala & Nangia, 2003; Reddy *et al.*, 2004; Du *et al.*, 2005). Here, the asymmetric unit of the crystal structure comprises one protonated 4,4'-dipyridylamine molecule and one singly deprotonated isophthalic acid molecule (Fig. 1). The pyridine rings of the 4-(4-pyridylamino)pyridinium cation do not lie in the same plane, but are instead twisted with respect to one another, the C7–C8–C3–C4 torsion angle being  $32.47(11)^\circ$ . The unprotonated pyridine rings of the cations are involved in  $\pi$ - $\pi$  stacking interactions [centroid-to-centroid distance =  $3.7440(5)$  Å] with the isophthalate anions and with other unprotonated pyridine rings of adjacent cations [centroid-to-centroid distances =  $4.1992(6)$  Å; Janiak, 2000]. Three  $\text{O}\cdots\text{H}-\text{N}$  and  $\text{N}\cdots\text{H}-\text{O}$  hydrogen-bonding interactions (Desiraju, 2002) link the molecules into a three-dimensional network (Figs. 2 and 3). There are no solvent molecules present in the crystal structure.



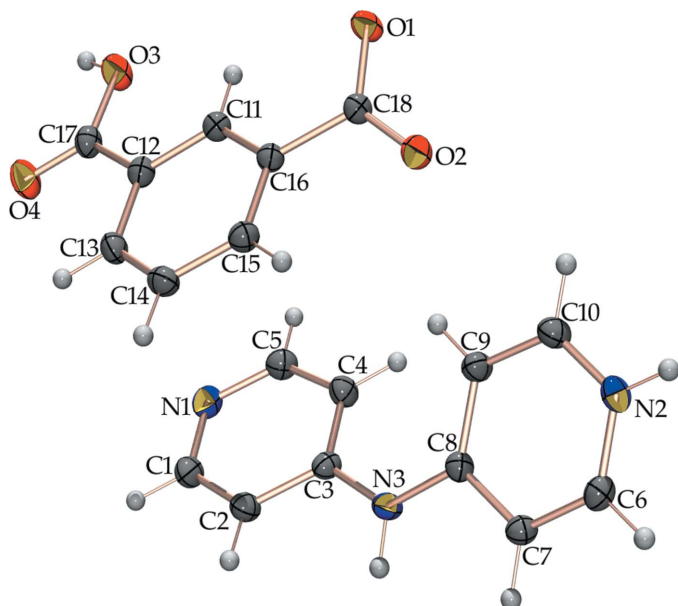
## Experimental

Isophthalic acid was purchased commercially and 4,4'-dipyridylamine was synthesized according to literature methods (Zapf *et al.*, 1998). Single crystals of the title salt suitable for X-ray crystallography were grown from a solution of 4,4'-dipyridylamine and isophthalic acid in deuterated methanol.

## Crystal data

$\text{C}_{10}\text{N}_3\text{H}_{10}^+\cdot\text{C}_8\text{H}_5\text{O}_4^-$   
 $M_r = 337.33$   
Monoclinic,  $P2_1/n$   
 $a = 9.3246(18)$  Å  
 $b = 15.134(3)$  Å  
 $c = 11.655(2)$  Å  
 $\beta = 107.787(3)^\circ$   
 $V = 1566.1(5)$  Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.431$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 936 reflections  
 $\theta = 2.7$ – $27.9^\circ$   
 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 150(2)$  K  
Irregular polyhedron, light yellow  
 $0.34 \times 0.31 \times 0.25$  mm



**Figure 1**  
View of the asymmetric unit of (I), with displacement ellipsoids drawn at the 50% probability level.

**Data collection**

Bruker SMART 1000 CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick 1996)  
 $T_{\min} = 0.900$ ,  $T_{\max} = 0.98$   
 15761 measured reflections

3742 independent reflections  
 3246 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.023$   
 $\theta_{\text{max}} = 28.0^\circ$   
 $h = -12 \rightarrow 12$   
 $k = -19 \rightarrow 19$   
 $l = -15 \rightarrow 15$

**Refinement**

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.101$   
 $S = 1.03$   
 3742 reflections  
 227 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.7162P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.41 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$

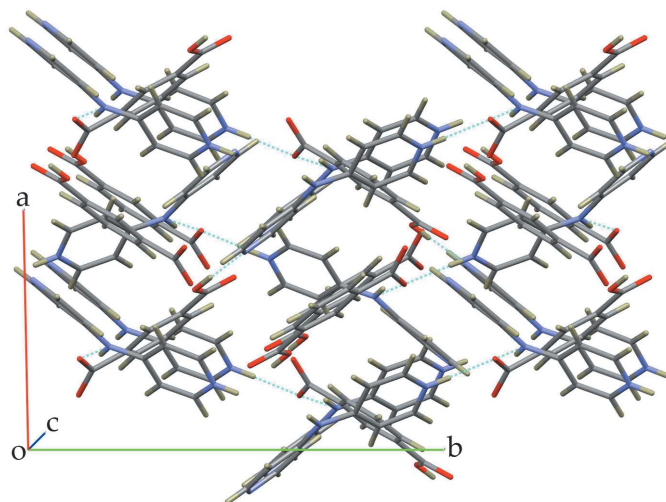
**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2A\cdots O1^i$	0.88	1.84	2.7134 (14)	174
$O3-H3A\cdots N1^{ii}$	0.84	1.83	2.6720 (14)	178
$N3-H3B\cdots O1^{iii}$	0.88	1.94	2.7987 (13)	166

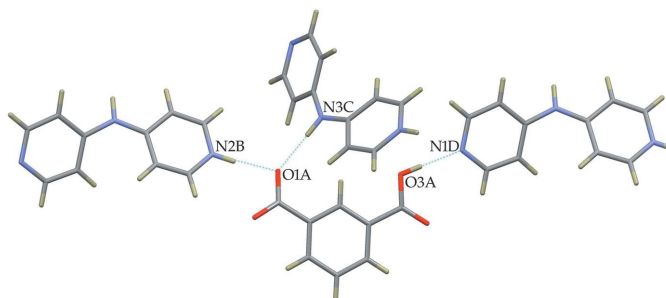
Symmetry codes: (i)  $-x, -y, -z + 1$ ; (ii)  $-x + 1, -y + 1, -z + 1$ ; (iii)  $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$

All H atoms were positioned geometrically ( $O-H = 0.84$ ,  $N-H = 0.88$  and  $C-H = 0.95 \text{ \AA}$ ) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$ .

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SAINT-Plus (Bruker, 1997); program(s) used to solve structure: SHELXS86 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics:



**Figure 2**  
View of the crystal structure of (I), showing the cations and anions bound together by a combination of  $\pi$ - $\pi$  stacking and hydrogen-bonding interactions. Hydrogen bonds are drawn as dashed lines.



**Figure 3**  
View of the hydrogen-bonding interactions in the crystal structure of (I). Hydrogen bonds are drawn as dashed lines.

ORTEP3 (Farrugia, 1997) and MERCURY (Version 1.4; Bruno *et al.*, 2002); software used to prepare material for publication: XCIF (Bruker, 2001).

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