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2-Aminopyridinium benzoate

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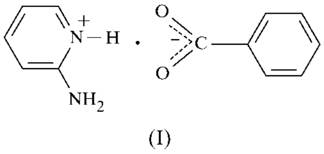
Cyclic eight-membered hydrogen-bonded rings exist in the title compound, $C_5H_7N_2^+ \cdot C_7H_5O_2^-$, involving the 2-aminopyridinium and benzoate ions. Each benzoate ion has two intramolecular hydrogen bonds. 2-Aminopyridinium benzoate ion pairs are linked by N—H···O hydrogen bonds, with an N···O distance of 2.8619 (14) Å.

Comment

The present work is part of a structural study of complexes of 2-aminopyridinium systems with hydrogen-bond donors, and we report here the structure of 2-aminopyridinium benzoate, (I). A series of similar complexes formed from 2-aminopyridine and carboxylates has been reported previously (Büyükgüngör & Odabaşoğlu, 2002; Odabaşoğlu *et al.*, 2003). Hydrogen bonding plays a key role in molecular recognition (Goswami & Ghosh, 1997) and crystal-engineering research (Goswami *et al.*, 1998). The design of highly specific solid-state structures is of considerable significance in organic chemistry, due to their important applications in the development of new optical, magnetic and electronic systems (Ballardini *et al.*, 1994, Lehn, 1992).



(I)

A view of the hydrogen-bonded structure of (I) and its numbering scheme are shown in Fig. 1. The complex owes its formation to hydrogen bonds between atoms O1 and O2 of the benzoate ion and atoms H13 and H14 of the 2-aminopyridinium ion, respectively. There is an eight-membered ring in the structure, formed as a result of the O1···H13 and O2···H14 hydrogen bonds. In addition to these hydrogen bonds, there is an intermolecular N—H···O hydrogen bond connecting units of (I) (Fig. 2). The hydrogen-bond distances in (I) are shorter than in 2-aminopyridinium salicylate [O1···N1 = 2.699 (4) Å and O2···N2 = 2.868 (16) Å; Gellert & Hsu, 1988].

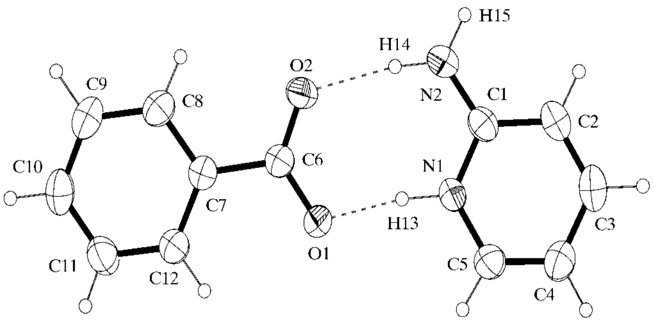


Figure 1
A view of the two ionic moieties of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii and hydrogen bonds are indicated by dashed lines.

2-Aminopyridine is protonated in acidic solutions. The bonding of the H atom to the ring N atom of 2-aminopyridine, but not to the amino N atom, gives an ion for which an additional resonance structure can be written (Acheson, 1967). The present investigation, like our previous work (Büyükgüngör & Odabaşoğlu, 2002; Odabaşoğlu *et al.*, 2003), clearly shows that the positive charge in the 2-aminopyridinium ion of (I) is on the amino group.

The phenyl and pyridine rings of (I) display an almost coplanar configuration, with a dihedral angle of 8.4 (2)°. The C1—N2 bond is 1.3332 (15) Å, and is approximately equal to a C═N double-bond length (Shanmuga Sundara Raj, Fun, Lu *et al.*, 2000), indicating that atom N2 of the amino group must also be *sp*^{2} hybridized. This is also supported by the C1—N2—H14 angle of 120.3 (9)°, and by the fact that atoms C1, N2, H14

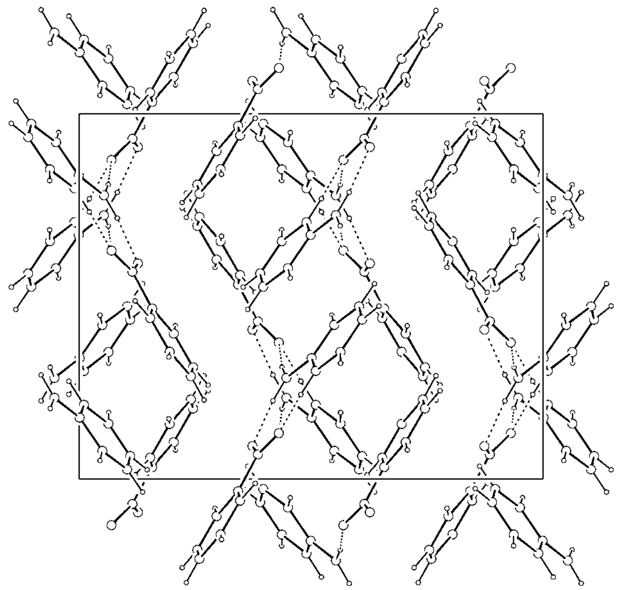


Figure 2
A packing diagram for (I), viewed along the *b* axis. The *a* axis is to the right and the *c* axis is upwards.

and H15 lie almost in the pyridine plane, with a maximum deviation of 0.09 (1) Å for atom H15. Similar bond distances and angles have been observed in 2-aminopyridinium succinate–succinic acid (Büyükgüngör & Odabaşoğlu, 2002) and 2-aminopyridinium adipate monoadipic acid dihydrate (Odabaşoğlu *et al.*, 2003), and in some 2-aminopyridine-containing molecules (Yang *et al.*, 1995; Grobelny *et al.*, 1995; Shanmuga Sundara Raj, Fun, Zhao *et al.*, 2000).

Experimental

The title compound was prepared by mixing 2-aminopyridine and benzoic acid in a 1:1 molar ratio in ethanol (95%) at 353 K. Crystals of (I) were obtained by slow evaporation of the solvent.

Crystal data

$C_5H_7N_2^+ \cdot C_7H_5O_2^-$
$M_r = 216.24$
Orthorhombic, *Pbca*
$a = 12.2129$ (17) Å
$b = 11.5137$ (16) Å
$c = 15.456$ (2) Å
$V = 2173.4$ (5) Å^3
$Z = 8$
$D_x = 1.322$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 986 reflections
$\theta = 2.8$–26.6°
$\mu = 0.09$ mm^{-1}
$T = 208$ (2) K
Prism, colourless
0.40 × 0.30 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
$T_{\min} = 0.964$, $T_{\max} = 0.986$
13 050 measured reflections
2650 independent reflections
1664 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.065$
$\theta_{\max} = 28.8°$
$h = -16 \rightarrow 16$
$k = -14 \rightarrow 14$
$l = -12 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.088$
$S = 0.89$
2650 reflections
194 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2]$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.0145 (12)

Table 1
Selected geometric parameters (Å, °).

O1—C6	1.2740 (13)	N1—C5	1.3570 (15)
O2—C6	1.2466 (13)	N2—C1	1.3332 (15)
N1—C1	1.3505 (14)		
C1—N1—C5	121.74 (10)	O2—C6—C7	118.09 (10)
O2—C6—O1	124.02 (10)	O1—C6—C7	117.88 (10)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H13···O1	0.985 (14)	1.678 (14)	2.6552 (12)	170.9 (12)
N2—H14···O2	0.940 (15)	1.868 (16)	2.7996 (14)	170.6 (13)
N2—H15···O1$^{\rm i}$	0.924 (16)	1.942 (16)	2.8619 (14)	173.9 (13)

Symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} + y, z$.

Refined C—H distances are in the range 0.950 (13)–0.997 (13) Å, and $U_{\rm iso}$ values for H atoms are in the range 0.041 (3)–0.066 (5) Å^2.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1997).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1405). Services for accessing these data are described at the back of the journal.

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