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2-Aminopyridinium isonicotinate 2-aminopyridine

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Key indicators

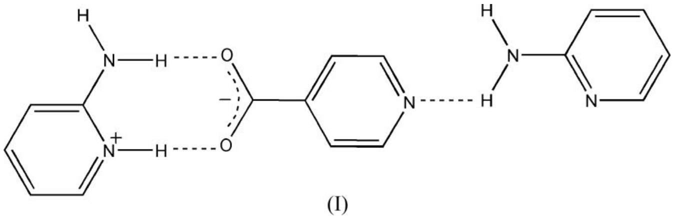
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.163
Data-to-parameter ratio = 16.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_5H_7N_2^+\cdot C_6H_4NO_2^-\cdot C_5H_6N_2$, the components are linked into a two-dimensional network through N—H···O and N—H···N hydrogen bonds. Adjacent layers are further linked by C—H···O hydrogen bonds, forming a three-dimensional framework.

Comment

2-Aminopyridine is one of the most frequently used synthons in supramolecular chemistry based on hydrogen bonds (Gellert & Hsu, 1988; Banerjee & Murugavel, 2004; Bis & Zaworotko, 2005; Bis *et al.*, 2006). In this paper, we report the crystal structure of the title compound, (I), which contains this molecule.



(I)

The asymmetric unit of (I) contains one 2-aminopyridinium cation, one isonicotinate anion and one neutral 2-aminopyridine molecule (Fig. 1). Due to the three hydrogen bonds (entries 1 to 3 in Table 1), the dihedral angles between the three aromatic pyridine rings are less than 30°: the angle between the planes N1/C1–C5 and N2/C7–C11 is 23.1 (1)°, that between the planes N1/C1–C5 and N4/C12–C16 is 29.2 (1)°, and that between the planes N2/C7–C11 and N4/C12–C16 is 10.1 (1)°.

The supramolecular structure of (I) contains both N—H···X (X = O or N) and C—H···O hydrogen bonds (Table 1). In detail, the amine group of the 2-aminopyridinium cation acts as hydrogen-bond donor, *via* two H atoms, to atoms O1

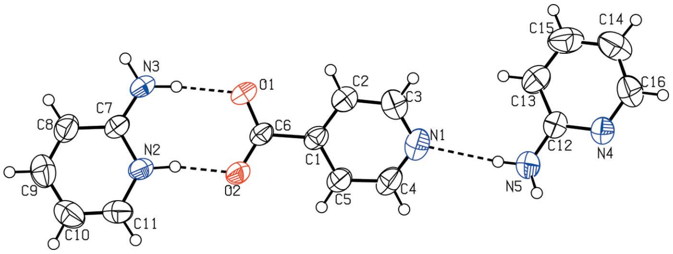


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds between the components are shown as dashed lines.

and O2^{i} (Table 1). These contacts produce chains including cations and anions, which run parallel to [101] (Fig. 2). In a similar way, the amine group of the neutral 2-aminopyridine molecule acts as a donor, *via* atom H5*A*, to atom N4^{ii}, thereby forming a centrosymmetric $R_2^2(8)$ ring (Batten & Robson, 1998). N5—H5*B*···N1 hydrogen bonds link these motifs into chains parallel to [101], giving a two-dimensional network (Fig. 2). Finally, the only direction-specific interaction between adjacent layers is the weak C11—H11···O1^{iii} hydrogen bond (Table 1, entry 6).

Experimental

Compound (I) was formed by dissolving 2-aminopyridine (0.188 g, 2 mmol) and isonicotinic acid (0.123 g, 1 mmol) in absolute ethanol (20 ml). The resulting solution was stirred at 323 K for 30 min and then slowly cooled to room temperature. Crystals of (I) suitable for X-ray crystallographic analysis were grown by slow evaporation of the solution at the bottom of the vessel.

Crystal data

$C_5H_7N_2^+ \cdot C_6H_4NO_2^- \cdot C_5H_6N_2$
$M_r = 311.35$
Monoclinic, $P2_1/n$
$a = 5.6204\ (11)$ Å
$b = 25.623\ (5)$ Å
$c = 11.256\ (2)$ Å
$\beta = 96.748\ (4)^\circ$
$V = 1609.8\ (5)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 298\ (2)$ K
0.23 × 0.20 × 0.15 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.980$, $T_{max} = 0.991$
9742 measured reflections
3733 independent reflections
2478 reflections with $I > 2/s(I)$
$R_{int} = 0.032$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.163$
$S = 1.07$
3733 reflections
223 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2	0.95 (2)	1.75 (2)	2.685 (2)	167.4 (17)
N3—H3*B*···O1	0.94 (2)	1.87 (2)	2.808 (2)	172.6 (19)
N5—H5*B*···N1	0.84 (3)	2.29 (3)	3.118 (3)	174 (2)
N3—H3*A*···O2^{i}	0.91 (2)	1.92 (2)	2.832 (2)	178 (2)
N5—H5*A*···N4^{ii}	0.92 (3)	2.26 (3)	3.168 (3)	169 (2)
C11—H11···O1^{iii}	0.93	2.32	3.130 (2)	146

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+4, -y, -z+2$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

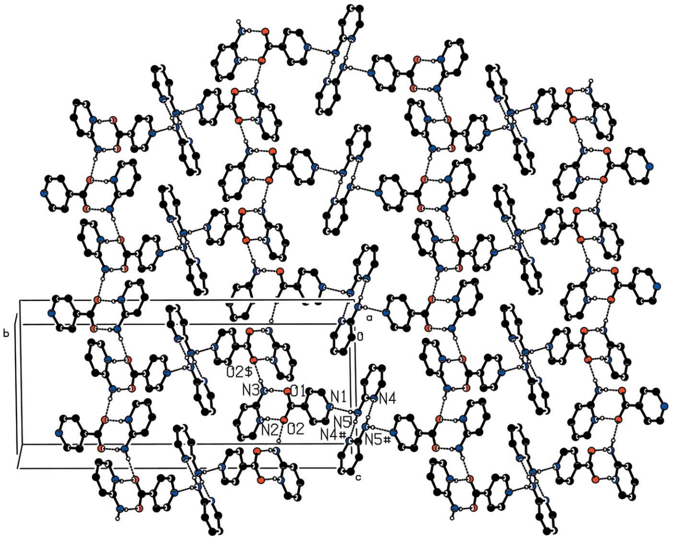


Figure 2
Part of the crystal structure of (I). Dashed lines indicate hydrogen bonds. For the sake of clarity, H atoms not involved in the motifs shown have been omitted. Atoms marked with a dollar ($) or a hash sign (#) are generated by the symmetry operators $(-\frac{1}{2}+x, \frac{1}{2}-y, -\frac{1}{2}+z)$ and $(4-x, -y, 2-z)$, respectively.

Aromatic H atoms were placed in idealized positions and refined with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms bonded to N atoms were located in a difference map and their coordinates were refined, with $U_{iso}(H) = 1.2U_{eq}(N)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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References

Banerjee, S. & Murugavel, R. (2004). *Cryst. Growth Des.* **4**, 545–552.
Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed.* **37**, 1460–1494.
Bis, J. A., McLaughlin, O. L., Vishweshwar, P. & Zaworotko, M. J. (2006). *Cryst. Growth Des.* **6**, 2648–2650.
Bis, J. A. & Zaworotko, M. A. (2005). *Cryst. Growth Des.* **5**, 1169–1179.
Bruker (2001). *SMART* (Version 5.628) and *SAINT-Plus* (Version 6.45). Bruker AXS Inc., Madison, Wisconsin, USA.
Gellert, R. W. & Hsu, I.-N. (1988). *Acta Cryst.* C**44**, 311–313.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SADABS*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.