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2-Aminopyridinium 5-formylsalicylate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.069
Data-to-parameter ratio = 14.4

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

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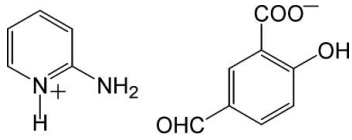
In the crystal structure of the title compound, $(2APH)^+$-$(5FSAH)^-$ (2AP is 2-aminopyridine and $5FSAH_2$ is 5-formylsalicylic acid) or $C_5H_7N_2^+\cdot C_8H_5O_4^-$, $(2APH)^+$ cations and $(5FSAH)^-$ anions are connected through hydrogen bonds, forming a one-dimenstional chain structure.

Comment

Weak interactions, such as hydrogen bonding and π–π stacking, have attracted much interest as a result of their significance in chemistry and biology, especially in the field of crystal engineering (Moghimi, *et al.*, 2002; Aghabozorg, *et al.*, 2005). Carboxylic acids are important in crystal engineering due to their strong and directional O—H···O and N—H···O bonds; this is the main hydrogen-bonding motif often encountered in carboxylic acid–amine complexes (Banerjee & Murugavel, 2004; Lautié & Belabbes, 1996). In this paper, we present the preparation and crystal structure of the title compound (I).



(I)

The title compound (I) is composed of $(2APH)^+$ cations and $(5FSAH)^-$ anions (Fig.1). The bond distances and angles show normal values (Table 1). There are complex hydrogen-bonding interactions in the crystal structrue of (I). As shown in Fig. 2, there is an O—H···O interaction between the OH and one carboxylate O atom for each $(5FSAH)^-$ anion. In addition, two carboxylate O atoms of the $(5FSAH)^-$ anion are hydrogen bonded to the amino N or pyridine N atom from one $(2APH)^+$ cation, respectively, resulting in a $(2APH)^+$-$(5FSAH)^-$ unit. These units are connected through a hydrogen bond between the formyl O atom of one unit and the amino N atom of the adjacent unit. For the hydrogen-bonding interactions in (I), hydroxyl O atom and N atoms play a role as donors, and the carboxylate O atom and formyl O atom as acceptors. The data for the hydrogen bonds are listed in Table 2.

Experimental

A mixture of 2-aminopyridine(0.094 g, 1 mmol) and 5-formylsalicylic acid (0.166 g, 1 mmol) in water (10 ml) was stirred for 30 min in air. The mixture was then transferred to and sealed in an 18 ml Teflon-lined autoclave, which was heated at 393 K for 89 h. After the mixture

had been allowed to cool slowly to room temperature, colourless crystals of the title compound (I) were filtered off, washed with distilled water, and dried at ambient temperature.

Crystal data

$C_5H_7N_2^+\cdot C_8H_5O_4^-$
$M_r = 260.25$
Monoclinic, $P2_1/c$
$a = 12.358\ (5)$ Å
$b = 7.191\ (5)$ Å
$c = 14.000\ (5)$ Å
$\beta = 104.382\ (5)^\circ$
$V = 1205.1\ (11)$ Å^3
$Z = 4$
$D_x = 1.434$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7362 reflections
$\theta = 1.7$–28.3°
$\mu = 0.11$ mm^{-1}
$T = 293$ K
Block, colourless
0.43 × 0.25 × 0.23 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.866$, $T_{max} = 0.976$
7481 measured reflections
2842 independent reflections
1387 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 28.3^\circ$
$h = -15 \rightarrow 14$
$k = -9 \rightarrow 9$
$l = -16 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.069$
$S = 0.96$
2842 reflections
198 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0181P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O3—C7	1.2322 (16)	N1—C9	1.3514 (18)
O2—C7	1.2808 (16)	N2—C10	1.3288 (19)
O1—C1	1.3467 (16)	O4—C8	1.2140 (18)
N1—C10	1.3370 (18)		
C10—N1—C9	122.80 (14)	O3—C7—C6	119.84 (14)
N2—C10—N1	118.17 (15)	O2—C7—C6	115.68 (13)
N2—C10—C11	123.49 (15)	O4—C8—C4	125.08 (17)
O3—C7—O2	124.47 (14)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H8···O2^{i}	0.918 (9)	1.786 (9)	2.7019 (18)	175.4 (14)
N2—H7···O3^{i}	0.916 (9)	1.947 (9)	2.862 (2)	176.5 (15)
O1—H1···O2	0.912 (9)	1.639 (11)	2.4970 (18)	155.2 (17)
N2—H6···O4^{ii}	0.894 (9)	2.110 (10)	2.987 (2)	166.7 (16)

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

All H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. Other H atoms were located in a difference map and refined isotropically.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

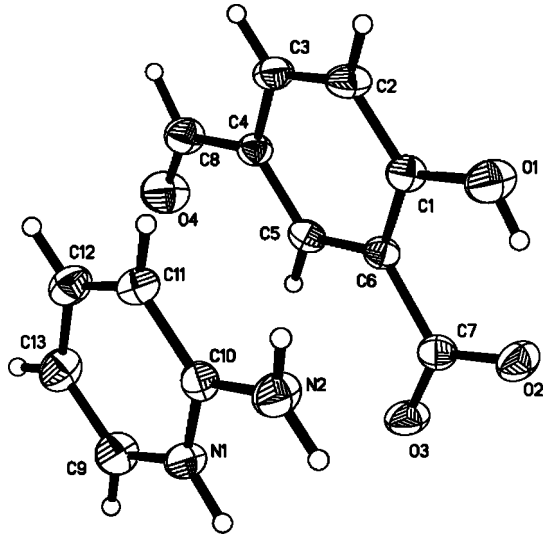


Figure 1
View of the structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

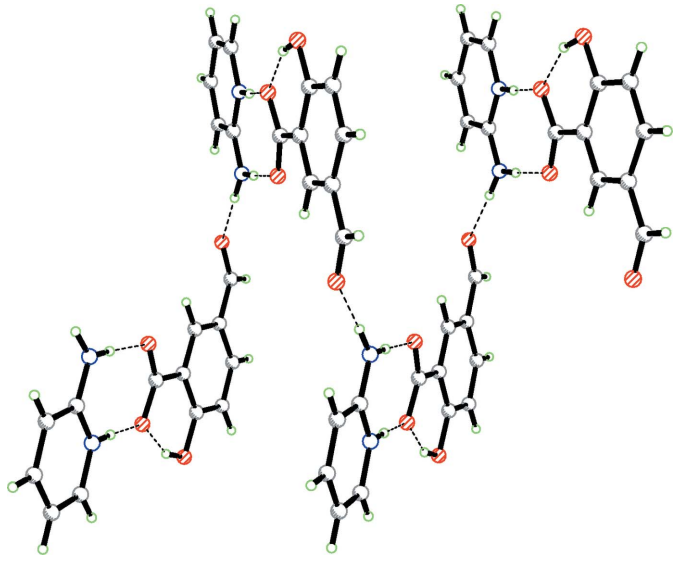


Figure 2
One-dimensional chain of (I), formed through hydrogen-bonding (dashed lines) interactions.

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