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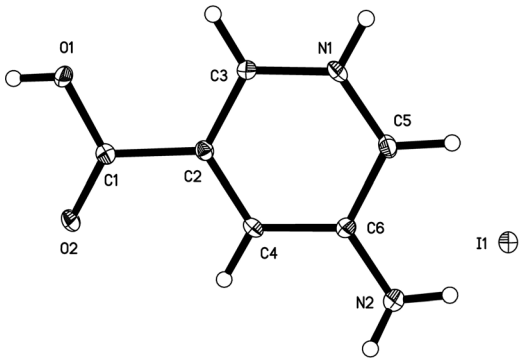
The crystal structure of 3-amino-5-carboxypyridin-1-ium iodide, $C_6H_7IN_2O_2$



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Abstract

$C_6H_7BrN_2O_2$, triclinic, $P\bar{1}$ (no. 2), a = 7.4522(4) Å, b = 7.4741(5) Å, c = 8.3144(5) Å, α = 90.036(3)°, β = 99.808(3)°, γ = 117.724(2)°, V = 402.25(4) Å^3, Z = 2, $R_{gt}(F)$ = 0.0156, w$R_{ref}(F^2)$ = 0.0367, T = 150.0 K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

An amount of 1.38 g 5-aminonicotinic acid was added to 15 mL 30% hydroiodic acid solution and stirred for 10 min at room temperature; then filtered. The filtrate was allowed to evaporate in open air. Yellow crystals were obtained after five days, yield 69% (based on 5-aminonicotinic acid).

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Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.20 × 0.15 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	3.93 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	26.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	8304, 1656, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1583
$N(param)_{refined}$:	102
Programs:	Bruker [1], Olex2 [2], SHELX [3, 4]

Experimental details

The structure was solved by direct methods with the SHELXS program. All H-atoms from C and N atoms were positioned with idealized geometry (U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.2U_{eq}(N)) using a riding model with C–H = 0.95 Å and N–H = 0.88 to 0.885 Å. Also the H atom at O1 was included using a riding model with the O–H distance of 0.84 Å(U_{iso}(H) = 1.5U_{eq}(O)).

Comment

Aminonicotinic acid and its derivatives can act as organic ammonium cations with inorganic anions to make organic ammonium salts, such as 2-amino-3-carboxypyridin-1-ium salts [5–7] and 3-amino-5-carboxypyridin-1-ium salts [8–16]. To the best of our knowledge, except some 3-aminonicotinic acid containing metal complexes [17–22], only one example of a 3-aminonicotinic acid based salt, the 3-amino-5-carboxypyridin-1-ium perchlorate monohydrate, has been reported [22]. Thus, we report the crystal structure of 3-amino-5-carboxypyridin-1-ium iodide.

The asymmetric unit of the title structure is made of one 3-amino-5-carboxypyridin-1-ium cation and one iodide anion. The N atom from the pyridine ring is protonated, while the NH_2 group keeps as it is. The organic cations are linked by hydrogen bonds N1–H1A···O2 to generate one-dimensional chains, further forming two-dimensional double planes by the hydrogen bond N2–H2B···O1 and C3–H3···O1, and finally building a three-dimensional

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8119 (4)	0.7150 (4)	0.2517 (3)	0.0161 (5)
C2	0.6551 (3)	0.7259 (3)	0.3367 (3)	0.0140 (4)
C3	0.4644 (4)	0.6912 (4)	0.2493 (3)	0.0169 (5)
H3	0.428817	0.659204	0.133927	0.020*
C4	0.7037 (3)	0.7709 (4)	0.5048 (3)	0.0154 (5)
H4	0.834881	0.794433	0.563597	0.019*
C5	0.3704 (4)	0.7457 (4)	0.4957 (3)	0.0179 (5)
H5	0.268128	0.750234	0.547437	0.021*
C6	0.5610 (4)	0.7820 (4)	0.5894 (3)	0.0155 (5)
I1	0.12489 (2)	0.78034 (2)	0.87556 (2)	0.01748 (6)
N1	0.3326 (3)	0.7044 (3)	0.3329 (3)	0.0188 (4)
H1	0.212402	0.684639	0.277168	0.023*
N2	0.6044 (3)	0.8273 (4)	0.7538 (3)	0.0256 (5)
H2A	0.489634	0.795466	0.790863	0.031*
H2B	0.662993	0.756820	0.801785	0.031*
O1	0.7437 (3)	0.6601 (3)	0.0936 (2)	0.0197 (4)
H1A	0.843744	0.685455	0.047467	0.030*
O2	0.9831 (3)	0.7531 (3)	0.3249 (2)	0.0241 (4)

supramolecular structure by weak $\pi\cdots\pi$ and H$\cdots$I interactions. The iodide anion is regulated by weak interactions O1–H1$\cdots$I1, N2–H2A$\cdots$I1, C5–H5$\cdots$I1, and C7–H7$\cdots$I1. All bondlengths are normal and comparable with the reported results [15, 22].

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Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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