Yan Zeng* and Chao-Jun Du

The crystal structure of 2-amino-5-carboxypyridin-1-ium iodide monohydrate, C₆H₉IN₂O₃

Abstract

C₆H₉IN₂O₃, monoclinic, P2₁/c (no. 14), a = 9.3654(2) Å, b = 8.0312(2) Å, c = 12.7668(3) Å, β = 107.825(1), V = 914.16(4) Å³, Z = 4, R_p(F) = 0.0156, wR_p(F²) = 0.0354, T = 150(2) K.

CCDC no.: 2069955

The asymmetric unit of the title crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

*Corresponding author: Yan Zeng, College of Chemistry and Chemical Engineering, Xinxing University, Xinxing, Henan, 453003, P. R. China, E-mail: zengyaner@126.com. https://orcid.org/0000-0001-7694-7434

Chao-Jun Du, School of Biochemical and Chemical Engineering, Nanyang Institute of Technology, Nanyang, Henan, 473000, P. R. China. https://orcid.org/0000-0002-4767-7057

Source of materials

All the raw materials were used as received without further purification. An amount of 1.38 g (10 mmol) 6-aminonicotinic acid was mixed with 10 mL 40% hydroiodic acid at room temperature. Then the mixture was
filtered and stood after stirring for 30 min. One week later, colorless block crystals of the title compound suitable for single crystal X-ray diffraction measurement were obtained, yield 84% (based on 6-aminonicotinic acid).

**Experimental details**

The structure was solved by direct methods with the SHLXS-2018 program. All H-atoms from C and N atoms were positioned with idealized geometry and refined isotropically (Uiso(H) = 1.2Ueq(C) and Uiso(H) = 1.2Ueq(N)) using a riding model with C–H = 0.95 Å and N–H = 0.88 Å. The hydrogen atoms at oxygen atoms were refined with the distance of O2–H2A = 0.84 Å, O1W–H1WA = 0.87 Å and O1W–H1WB = 0.87 Å, respectively (Uiso(H) = 1.5Ueq(O)).

**Comment**

The 6-amino-nicotinic acid was used as a bifunctional ligand for Zn(II), Mn(II) and Co(II), Cd(II), and Ca(II) and Sr(II) to construct coordination polymers and metal-organic frameworks [5–9]. There also have been some salts of it such as its chloride, bromide, nitrate and dihydrogen phosphate [10–12] which are based on the monoprotonated cation of 6-amino-nicotinic acid. However, the crystal structure of it’s iodide has not been reported.

The title compound, 2-aminoo-5-carboxypyridin-1-ium iodide monohydrate, with the formula of C6H5IN2O3, crystallizes monoclinically, P21/c (no. 14). The asymmetric unit is made of one N-protonated 2-aminoo-5-carboxypyridin-1-ium cation, one iodine anion, and one water molecule. All the bond lengths of the title compound are in the normal ranges [13]. The N atom of the pyridine is protonated to give the 2-aminoo-5-carboxypyridin-1-ium cation to balance the iodine anion. All the atoms of the 2-aminoo-5-carboxypyridin-1-ium cation are nearly co-planar. There is a one dimensional chain generated by hydrogen bond N1–H1B···O1.

**Author contributions:** All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

**Research funding:** Key Science and Technology Projects in Henan Province (182102311076 and 182102210276), the Project of State key Laboratory of Motor Vehicle Biofuel Technology (KFKT2021001), the Nanyang Institute of Technology Cross-Science Research Project (NITC2021007) and the Rare earth industry fund project of Institute of Green Process Manufacturing Innovation in Chinese Academy of Sciences (IAGM2020DB10).

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

**References**