The crystal structure of 3-(carboxymethyl)-1-ethenyl-1H-imidazol-3-ium chloride, C$_7$H$_9$N$_2$O$_2$Cl

Abstract
C$_7$H$_9$N$_2$O$_2$Cl, orthorhombic, P2$_1$2$_1$2$_1$ (no. 19), $a = 4.6321(3)$ Å, $b = 7.5132(4)$ Å, $c = 24.7605(14)$ Å, $V = 861.71(9)$ Å$^3$, $Z = 4$, $R_{	ext{gt}}(F) = 0.0257$, $wR_{	ext{ref}}(F^2) = 0.0653$, $T = 193$ K.

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

Source of material
Synthesis of the title compound was carried out according to the literature [5]. In brief, chloroacetic acid (4.22 g) was dissolved in 100 mL ethyl acetate in a 250 mL three-necked flask which was equipped with a magnetic stirrer (410 rpm) and a thermometer. Then 1-vinylimidazole (3.5 g) was added. The structure was kept at 50 °C for 24 h until the reaction was completed. After filtering and washing with 200 mL ethyl acetate three times, a white solid of 1-vinyl-3-carboxymethylimidazolium chloride was obtained, and then dried in a vacuum at 35 °C for 48 h.

Experimental details
All the H atoms on the benzene rings were placed geometrically and refined without any constraints or restraints.

Comment
An ionic liquid is an organic salt with an organic cation and suitable anion combination, which have been widely studied in catalysis, chemical industry, electrochemistry, biomass conversion, extraction, and many other areas [6]. In recent years, carboxyl functionalized ionic liquids have been designed and received much attention. One of the most commonly used carboxyl functionalized polymerizable ionic liquid monomer was 1-vinyl-3-carboxymethylimidazolium chloride, which could be used for preparing smart responsive hydrogel [7], catalyst [8], nanocomposite electrode [9], molecularly imprinted
composite [10], et al. Although some directly related structure can be found [11–13], there is no report on a crystal structure of the title compound.

So here we report the crystal structure of the title compound. The title compound crystallizes in P2₁2₁2₁. The asymmetric unit of the title compound (see the Figure) comprises a vinylimidazolium cation, a carboxymethyl, and a chloride anion. Organic cations and chloride anions are connected by one classical hydrogen bond O–H⋯Cl and several weak C–H⋯Cl bonds. Bond lengths and angles in the crystal structure are within normal ranges.

**Acknowledgment:** This work was supported by the Youth Innovation Team of Shaanxi Universities.

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

**Research funding:** This project was funded the Science Research Foundation of Xijishu University (XJ18T03).

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

### References

1. Bruker. APEX-2, SAINT+ (version 6.02) [Includes XPREP and SADABS]; Bruker AXS Inc.: Madison, WI, USA, 2016.