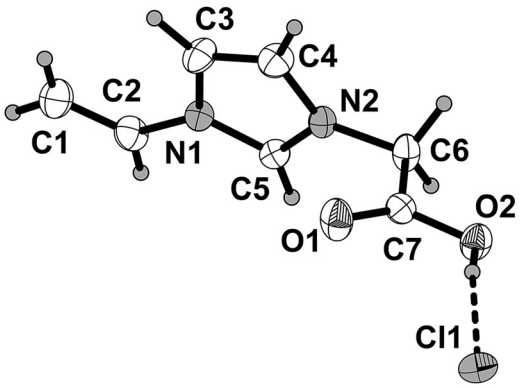
Wenqi Song, Miaoxiu Yang, Liwei Qian and Zongcheng Miao*

The crystal structure of 3-(carboxymethyl)-1-ethenyl-1*H*-imidazol-3-ium chloride, $C_7H_9N_2O_2Cl$



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Abstract

$C_7H_9N_2O_2Cl$, orthorhombic, $P2_12_12_1$ (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, $R_{gt}(F)$ = 0.0257, $wR_{ref}(F^2)$ = 0.0653, T = 193 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.

Table 1: Data collection and handling.

Crystal:	White block
Size:	0.12 × 0.10 × 0.10 mm
Wavelength:	Ga *K*α radiation (1.34139 Å)
μ:	2.40 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	53.9°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	6914, 1569, 0.058
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1512
$N(param)_{refined}$:	109
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

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

***Corresponding author: Zongcheng Miao**, Xi'an Key Laboratory of Advanced Photo-Electronics Materials and Energy Conversion Device, School of Science, Xijing University, Xi'an, Shaanxi 710123, China, E-mail: miaozongcheng@xijing.edu.cn
Wenqi Song, Xi'an Key Laboratory of Advanced Photo-Electronics Materials and Energy Conversion Device, School of Science, Xijing University, Xi'an, Shaanxi 710123, China, E-mail: songwenqi0123@163.com. https://orcid.org/0000-0003-1491-050X
Miaoxiu Yang, Newspaper Office, China National Pulp and Paper Research Institute, Beijing 100102, China
Liwei Qian, College of Bioresources Chemical and Materials Engineering, Shaanxi University of Science and Technology, Xi'an, Shaanxi 710021, China

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	0.6449 (4)	0.4346 (2)	0.49308 (6)	0.0396 (5)
O2	0.9993 (4)	0.6084 (2)	0.46099 (6)	0.0332 (4)
H2	0.910999	0.597840	0.431534	0.050*
N1	0.5574 (4)	0.4078 (2)	0.66066 (7)	0.0245 (4)
N2	0.8576 (4)	0.4460 (3)	0.59509 (7)	0.0245 (4)
C1	0.2174 (7)	0.3258 (4)	0.72964 (10)	0.0433 (7)
H1A	0.239099	0.203952	0.720253	0.052*
H1B	0.090119	0.359102	0.757977	0.052*
C2	0.3623 (6)	0.4473 (4)	0.70364 (9)	0.0326 (6)
H2A	0.336768	0.568259	0.713804	0.039*
C3	0.6405 (6)	0.2402 (3)	0.64289 (10)	0.0319 (6)
H3	0.578565	0.129104	0.657098	0.038*
C4	0.8244 (6)	0.2649 (3)	0.60195 (9)	0.0324 (6)
H4	0.915635	0.174327	0.581345	0.039*
C5	0.6947 (5)	0.5292 (3)	0.63113 (8)	0.0249 (5)
H5	0.678708	0.654526	0.635200	0.030*
C6	1.0204 (6)	0.5321 (4)	0.55221 (9)	0.0304 (6)
H6A	1.212609	0.475470	0.549014	0.036*
H6B	1.049405	0.659126	0.561296	0.036*
C7	0.8625 (5)	0.5175 (3)	0.49881 (8)	0.0256 (5)
Cl1	0.69956 (13)	0.62937 (7)	0.35499 (2)	0.02952 (17)

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 crystalizes in $P2_12_12_1$. 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.

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