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The crystal structure of 3-(1-ethenyl-1*H*-imidazol-3-ium-3-yl)propane-1-sulfonate, C₈H₁₂N₂O₃S

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Abstract

C₈H₁₂N₂O₃S, monolonic, $P2_1/n$ (no. 14), $a = 6.0324(5)$ Å, $b = 7.1692(6)$ Å, $c = 21.6655(17)$ Å, $\beta = 97.022(3)^\circ$, $V = 929.95(13)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0409$, $wR_{\text{ref}}(F^2) = 0.1201$, $T = 193$ K.

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The molecular 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.

Source of material

Synthesis of the title compound was carried out by alkylation reaction [5]. In brief, 1-vinylimidazole (1.88 g, 0.02 mol) was dissolved in 10 mL acetonitrile at 50 °C. Under vigorous magnetic stirring 1,3-propane sultone (3.66 g, 0.03 mol) was dropped slowly into the reactor using constant pressure funnel. The mixture was stirred at 50 °C for 24 h to afford

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.12 × 0.10 × 0.10 mm
Wavelength:	Ga K α radiation (1.34139 Å)
μ :	1.96 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	61.0°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	8208, 2162, 0.060
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1924
$N(\text{param})_{\text{refined}}$:	127
Programs:	Bruker [1], SHELX [2, 3], Olex2 [4]

4.53 g of a white precipitate, which was further purified by washing with small amounts of acetone and dried by lyophilization. The colorless crystals were obtained by solvent diffusion method at room temperature.

Experimental details

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

Comment

Polymers composed of zwitterions have the properties of anti-protein pollution, anti-bacterial adhesion and anti-coagulation due to the introduction of hydrophilic groups such as hydroxyl, carboxyl and sulfonic acid groups into the chain. One of the most commonly used polymerizable zwitterionic monomer is 3-(1-ethenyl-1*H*-imidazol-3-ium-3-yl)propane-1-sulfonate, which is an effective antifouling material monomer for resistance against protein adsorption and cell adhesion [5–8]. The characteristics of the crystal structures are very important for the application of the materials. However, so far there is no report of the crystal structure of the 3-(1-ethenyl-1*H*-imidazol-3-ium-3-yl)propane-1-sulfonate.

The title compound crystallizes in $P2_1/n$. The asymmetric unit of the title structure (see the Figure) comprises one zwitterionic title sulfonate molecule [9]. Bond lengths and angles in crystal structure of the title structure are within normal ranges [9, 10].

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
C1	−0.1832 (3)	0.8089 (3)	0.44002 (9)	0.0334 (4)
H1A	−0.071672	0.747458	0.420182	0.040*
H1B	−0.310286	0.860773	0.415804	0.040*
C2	−0.1620 (3)	0.8221 (2)	0.50060 (8)	0.0280 (4)
H2	−0.275371	0.884069	0.519546	0.034*
C3	0.2302 (3)	0.6909 (2)	0.52317 (8)	0.0281 (4)
H3	0.275751	0.693560	0.482733	0.034*
C4	0.3527 (3)	0.6317 (3)	0.57617 (7)	0.0273 (3)
H4	0.500866	0.584430	0.579773	0.033*
C5	0.0275 (3)	0.7227 (2)	0.60061 (7)	0.0239 (3)
H5	−0.092048	0.751148	0.623774	0.029*
C6	0.2796 (2)	0.5898 (2)	0.68834 (6)	0.0238 (3)
H6A	0.308454	0.453824	0.688505	0.029*
H6B	0.150001	0.611918	0.711326	0.029*
C7	0.4836 (3)	0.6887 (2)	0.72204 (7)	0.0230 (3)
H7A	0.613117	0.675402	0.698386	0.028*
H7B	0.452268	0.823219	0.726681	0.028*
C8	0.5324 (2)	0.5966 (2)	0.78562 (7)	0.0231 (3)
H8A	0.554832	0.461412	0.779409	0.028*
H8B	0.399467	0.610960	0.807842	0.028*
N1	0.0254 (2)	0.7468 (2)	0.53955 (6)	0.0238 (3)
N2	0.2233 (2)	0.65252 (19)	0.62376 (6)	0.0222 (3)
O1	0.95343 (19)	0.68680 (17)	0.79675 (6)	0.0297 (3)
O2	0.80235 (19)	0.55323 (19)	0.88556 (5)	0.0333 (3)
O3	0.7116 (2)	0.87061 (18)	0.85457 (6)	0.0325 (3)
S1	0.76925 (6)	0.68519 (5)	0.83398 (2)	0.02176 (17)

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