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3-(Ethyldimethylammonio)propanesulfonate

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Key indicators

Single-crystal X-ray study
T = 106 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.092
Data-to-parameter ratio = 16.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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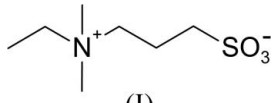
In the title sulfobetaine (NDSB-195), $C_7H_{17}NO_3S$, the three-methylene spacer between the ammonium and sulfonate groups is in a fully extended conformation. Interactions between the charged ammonium and sulfonate groups are the most important for the crystal packing.

Comment

Ethyldimethylammoniopropane sulfonate (NDSB-195) belongs to a family of compounds that are used as additives in protein purification (Expert-Bezançon *et al.*, 2003) and crystallization (Vuillard *et al.*, 1994). This non-detergent sulfobetaine (NDSB) has good solubilization properties, can be easily synthesized, is stable in a wide range of pH and does not absorb significantly near-UV light (Vuillard *et al.* 1995). NDSB-195 is a V-type activator of the recombinant catalytic subunit of casein kinase II (Benetti *et al.*, 1998). The activity of the enzyme treated with NDSB-195 after 24 h is higher than that of the control and remains so for weeks, even when the enzyme is stored at room temperature. NDSB-195 can be used to solubilize proteins during isoelectric focusing under non-denaturing conditions and enhance extraction yields for microsomal proteins and nuclear proteins (Goldberg *et al.*, 1995; Vuillard *et al.*, 1996).



(I)

The molecular structure of NDSB-195, (I), is shown in Fig. 1. Results obtained in membrane-protein extraction experiments (Vuillard *et al.*, 1995) show that sulfopropyl NDSBs with a three-methylene bridge between N and S are more efficient than sulfobutyl NDSBs with a four-methylene bridge between N and S. It was proposed (Vuillard *et al.*, 1995) that in solution, the sulfopropyl NDSBs might adopt a cyclic conformation and form an ionic link between N^+ and SO_3^-. This hydrocarbon cluster might screen some hydrophobic protein–protein interactions and slow down protein aggregation. In the crystal structure of NDSB-195, this cyclic conformation is not observed, and torsion angles S1—C1—C2—C3 and C1—C2—C3—N1 have values 179.97 (11) and −174.78 (13)°, respectively. The conformation of the sulfopropyl group in NDSB-195 is very similar to the conformation observed in the crystal structure of zwitterionic trimethylammoniopropane sulfonate (Yokoyama *et al.*, 2003). The most important feature for packing in the crystal structure of NDSB-195 is interactions between the charged ammonium and sulfonate groups. The

ammonium N atom is surrounded by four O atoms from four sulfonate groups (Fig. 2). These O atoms form a strongly distorted tetrahedron around atom N1 with O···N1 distances in the range 3.633 (2)–3.992 (2) Å. There are also weak C—H···O interactions; those for which the interaction distance is 0.3 Å shorter than the sum of the atomic van der Waals radii are shown in Table 1.

Experimental

NDSB-195 was purchased from ANATRACE. Crystallization was performed at room temperature and the crystals used for X-ray diffraction experiments were obtained by slow evaporation of a 10% propionic acid solution.

Crystal data

$C_7H_{17}NO_3S$
M_r = 195.28
Orthorhombic, *Pbca*
a = 12.369 (1) Å
b = 11.964 (1) Å
c = 12.844 (1) Å
V = 1900.7 (3) Å^3
Z = 8
D_x = 1.365 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 2.82 mm^{-1}
T = 106 (2) K
Block, colorless
0.23 × 0.16 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scan with χ offset
Absorption correction: multi-scan (Otwinowski *et al.*, 2003)
T_{min} = 0.61, T_{max} = 0.80
3381 measured reflections
1839 independent reflections
1695 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 72.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.092
S = 1.03
1839 reflections
110 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2 + 1.4076P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.00085 (14)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O3^{i}	0.97	2.36	3.302 (2)	164
C4—H4B···O1^{ii}	0.97	2.42	3.250 (2)	143
C7—H7C···O3^{iii}	0.96	2.44	3.318 (2)	152
C7—H7B···O1^{iv}	0.96	2.48	3.347 (2)	150

Symmetry codes: (i) $x-\frac{1}{2}, y, -z+\frac{1}{2}$; (ii) $-x, -y, -z+1$; (iii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

H atoms were positioned geometrically and treated as riding, with C—H = 0.96 and 0.97 Å for CH_3 and CH_2, respectively, and U_{iso}(H) = xU_{eq}(C) (x = 1.5 and 1.2).

Data collection: *HKL-2000* (Otwinowski & Minor, 1997); cell refinement: *HKL-2000*; data reduction: *HKL2000*; program(s) used to solve structure: *HKL-3000SM* (Minor *et al.*, 2006) and *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *HKL-3000SM* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *HKL-3000SM*, *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *HKL-3000SM*.

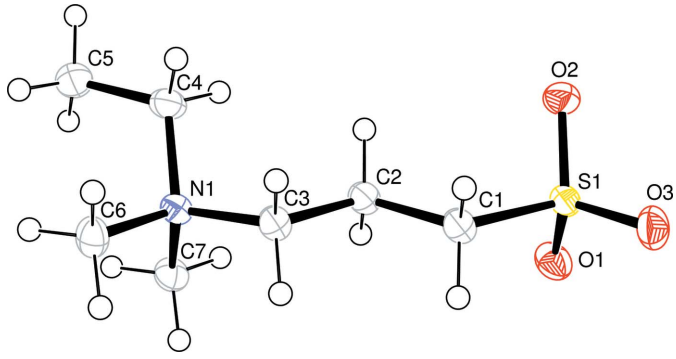


Figure 1
The molecular structure and atom-labeling scheme for (I), with displacement ellipsoids drawn at the 50% probability level and H atoms drawn as spheres of arbitrary radii.

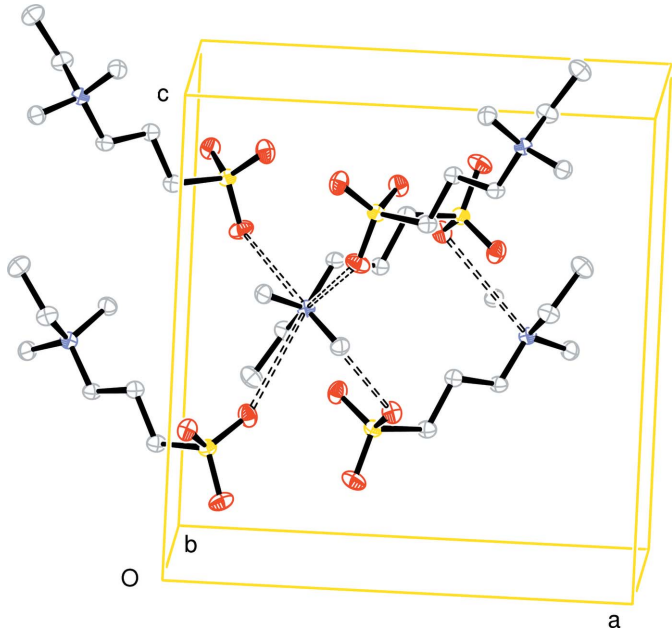


Figure 2
The crystal packing of NDSB-195. Contacts between the ammonium N atom and four closest O atoms are marked by dashed lines. H atoms have been omitted.

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