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3-(1-Methylpiperidinio)-1-propanesulfonate

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Key indicators

Single-crystal X-ray study
T = 106 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.085
Data-to-parameter ratio = 10.5

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

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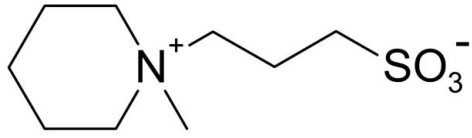
The title sulfobetaine (NDSB-221), $C_9H_{19}NO_3S$, is used for protein solubilization and stabilization. The piperidine ring has a chair conformation, with the sulfopropyl group in an equatorial position. The trimethylene spacer adopts a fully extended conformation.

Comment

3-(1-Methylpiperidinio)-1-propanesulfonate (NDSB-221), (I), belongs to a group of non-detergent sulfobetaines (NDSBs) used as solubilization and renaturation agents in protein purification (Vuillard *et al.*, 1995; Goldberg *et al.*, 1995). Other compounds from this group are used in isoelectric focusing, differential scanning calorimetry (Collins *et al.*, 2006) and protein crystallization (Vuillard *et al.*, 1994; Vuillard *et al.*, 1996).



(I)

The most important interactions for the structural stability of (I) are between charged quaternary ammonium and sulfonate groups. There are several short contacts (Table 1) in which H and O atom distances are at least 0.3 Å shorter than the sum of the van der Waals radii.

It has been suggested (Vuillard *et al.*, 1995) that the conformation of the sulfopropyl group in NDSBs may be important for interactions with proteins during the solubilization process. In the crystal structure of (I) reported in this paper, the torsion angles S1—C1—C2—C3 and C1—C2—C3—N1 have values of 174.22 (11) and 179.28 (13)°, respectively, and thus the three-methylene linker has an extended conformation, which is similar to what was observed in the cases of trimethylammoniopropane sulfonate (Yokoyama *et al.*, 2003) and 3-(ethyldimethylammonio)propane sulfonate (Koclega *et al.*, 2006). The piperidine ring of (I) has a chair conformation, with the sulfopropyl group in an equatorial position.

Experimental

NDSB-221, (I), was purchased from Anatrace. Crystallization was performed at room temperature and the crystal used for the X-ray diffraction experiment was obtained by slow evaporation of a propan-2-ol solution.

Crystal data

$C_9H_{19}NO_3S$
M_r = 221.31
Monoclinic, $P2_1/c$
a = 8.300 (1) Å
b = 9.485 (1) Å
c = 13.993 (1) Å
β = 96.396 (4)°
V = 1094.75 (19) Å^3
Z = 4
D_x = 1.343 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 2.51 mm^{-1}
T = 106 (2) K
Plate, colourless
0.52 × 0.13 × 0.05 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scan with χ offset
Absorption correction: multi-scan (Otwinowski *et al.*, 2003)
T_{min} = 0.69, T_{max} = 0.88
4068 measured reflections
2140 independent reflections
2063 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 72.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.085
S = 1.10
2140 reflections
204 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2 + 0.6719P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0034 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O1^{i}	0.973 (19)	2.329 (19)	3.2409 (19)	155.7 (15)
C4—H4C···O2^{ii}	0.973 (18)	2.414 (18)	3.364 (2)	165.0 (15)
C4—H4B···O3^{iii}	0.95 (2)	2.46 (2)	3.3753 (19)	161.3 (15)
C8—H8A···O3^{iii}	0.99 (2)	2.40 (2)	3.390 (2)	173.9 (16)
C3—H3B···O2^{iv}	0.977 (19)	2.494 (19)	3.3949 (19)	153.2 (15)
C9—H9B···O2^{iv}	0.966 (18)	2.342 (19)	3.285 (2)	165.1 (14)

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

All H atoms were located in electron-density difference maps and their positional and displacement parameters were refined freely [C—H = 0.95 (2)–1.013 (19) Å].

Data collection: *HKL-2000* (Otwinowski & Minor, 1997); cell refinement: *HKL-2000*; data reduction: *HKL-2000*; program(s) used to solve structure: *HKL-3000SM* (Minor *et al.*, 2006) and *SHELXS97* (Sheldrick, 1997); 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*.

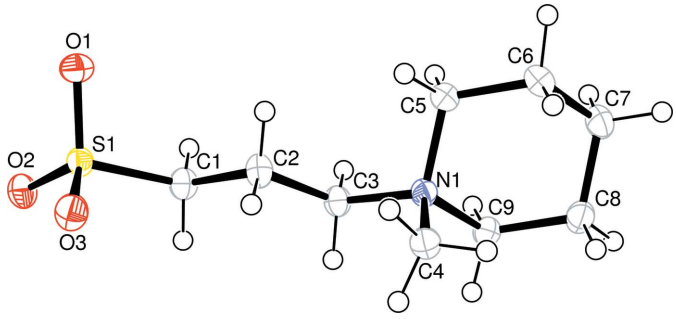


Figure 1
The molecular structure of NDSB-221, (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

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