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3-(Morpholinium-1-yl)propanesulfonate

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Key indicators

Single-crystal X-ray study
T = 103 K
Mean σ(C–C) = 0.001 Å
R factor = 0.026
wR factor = 0.075
Data-to-parameter ratio = 18.5

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

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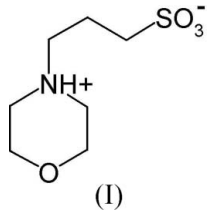
The crystal structure of the title compound, $C_7H_{15}NO_4S$, was determined at 103 K. There are two molecules in the asymmetric unit with different conformations of the aliphatic chains. In the solid state, the title molecule is a zwitterion.

Comment

The introduction of sulfonic compounds as zwitterionic buffers, *e.g.* MES [2-(*N*-morpholino)ethanesulfonic acid], MOPS [3-(*N*-morpholino)propanesulfonic acid] and HEPES {[4-(2-hydroxyethyl)-1-piperazine]ethanesulfonic acid}, has allowed better study of many biological processes (Good *et al.*, 1966; Good & Izawa, 1972; Ferguson *et al.*, 1980). The crystal structures of MES, its sodium salt (Christensen *et al.*, 1993; Deschamps *et al.* 2002) and HEPES (Wouters *et al.*, 1996) have already been reported. In this paper, the crystal structure of MOPS, (I), is presented. Different conformations of the propanesulfonate chain in the two molecules of the asymmetric unit are illustrated by their torsion angles (Table 1).



(I)

The title compound is zwitterionic in the crystal structure, as is also observed in the structures of MES monohydrate and of HEPES. The N atoms are protonated, as confirmed by location of the H atoms in a difference Fourier map. Both N atoms are proton donors in N—H···O intermolecular hydrogen bonds (Table 2). Hydrogen bonds occur only between molecules with different conformations of the aliphatic chains. There are also short contacts between O atoms of the sulfonic groups (O2*a*, O2*b* and O3*a*) and C atoms (C3*a*, C4*a*, C7*a* and C7*b*), with O···C distances ranging from 3.139 to 3.401 Å and O···H—C angles greater than 150°. Both morpholine rings have chair conformations.

Experimental

3-(*N*-Morpholino)propanesulfonic acid was purchased from FLUKA. The crystal of (I) for data collection was obtained at room temperature by slow evaporation of 1 *M* MOPS solution in water.

Crystal data

$C_7H_{15}NO_4S$
M_r = 209.26
Monoclinic, $P2_1/c$
a = 6.149 (1) Å
b = 11.255 (1) Å
c = 27.402 (1) Å
β = 90.431 (1)°
V = 1896.4 (4) Å^3
Z = 8
D_x = 1.466 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12720 reflections
θ = 2.3–32.0°
μ = 0.33 mm^{-1}
T = 103 (2) K
Plate, colourless
0.10 × 0.10 × 0.02 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans with χ offset
Absorption correction: multi-scan (Otwinowski *et al.*, 2003)
T_{min} = 0.958, T_{max} = 0.994
12720 measured reflections
6578 independent reflections
5857 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
θ_{max} = 32.0°
$h = -9 \rightarrow 9$
$k = -16 \rightarrow 16$
$l = -40 \rightarrow 40$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.075
S = 1.06
6578 reflections
355 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2 + 0.5917P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

Table 1
Selected torsion angles (°).

N1*b*—C3*b*—C2*b*—C1*b*	−177.97 (7)	C3*a*—C2*a*—C1*a*—S1*a*	−173.62 (6)
N1*a*—C3*a*—C2*a*—C1*a*	−60.82 (10)	C4*a*—N1*a*—C3*a*—C2*a*	−176.19 (7)
C3*b*—C2*b*—C1*b*—S1*b*	−175.84 (6)	C4*b*—N1*b*—C3*b*—C2*b*	177.91 (7)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*a*—H0*a*···O4*b*	0.89 (1)	1.84 (1)	2.7227 (10)	174 (1)
N1*b*—H0*b*···O3*a*^{i}	0.88 (1)	1.92 (1)	2.7871 (10)	171 (1)

Symmetry code: (i) $x-1, y, z$.

Data collection: *HKL2000* (Otwinowski & Minor, 1997); cell refinement: *HKL2000*; data reduction: *HKL2000*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990) and *HKL2000*; program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997) and *HKL2000*; molecular graphics: *HKL2000*, *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP3* (Farrugia, 1997) and O (Jones *et al.*, 1991); software used to prepare material for publication: *HKL2000* and *SHELXL97*.

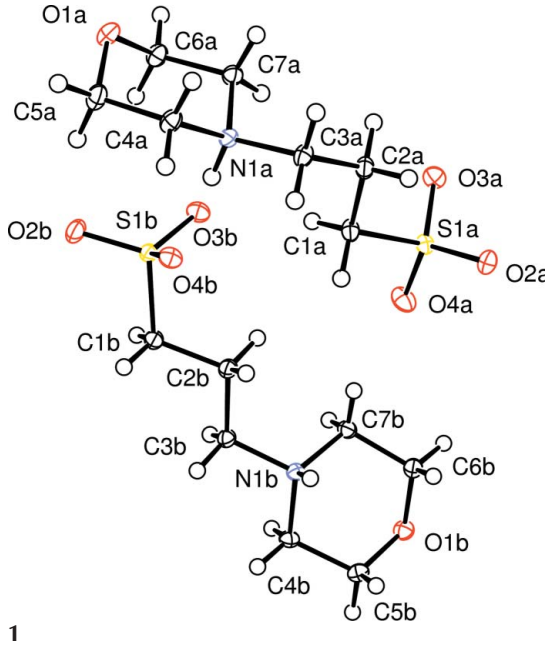


Figure 1
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii.

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