Table 2. *Bond angles* (°) ($\sigma = 0.2°$ *for* C—C—C, $1.2–1.6°$ *for* C—C—H, H—C—H)

C(8)—C(9)—C(10)	127·1	C(9)—C(8)—C(7)	127·6
C(9)—C(10)—C(1)	123·1	C(8)—C(7)—C(6)	122·6
C(10)—C(1)—C(2)	126·8	C(7)—C(6)—C(5)	126·2
C(10)—C(1)—C(11)	116·5	C(7)—C(6)—C(11)	116·6
C(2)—C(1)—C(11)	116·3	C(5)—C(6)—C(11)	116·8
C(1)—C(2)—C(3)	122·8	C(6)—C(5)—C(4)	122·7
C(2)—C(3)—C(4)	127·3	C(5)—C(4)—C(3)	126·8
C(1)—C(11)—C(6)	97·6		
C(8)—C(9)—H(9)	114·8	C(9)—C(8)—H(8)	113·9
C(10)—C(9)—H(9)	116·8	C(7)—C(8)—H(8)	117·2
C(9)—C(10)—H(10)	117·7	C(8)—C(7)—H(7)	119·8
C(1)—C(10)—H(10)	118·8	C(6)—C(7)—H(7)	117·5
C(1)—C(11)—H(11*A*)	112·2	C(6)—C(11)—H(11*A*)	112·8
C(1)—C(11)—H(11*B*)	112·6	C(6)—C(11)—H(11*B*)	110·6
C(1)—C(2)—H(2)	119·6	C(6)—C(5)—H(5)	117·5
C(3)—C(2)—H(2)	117·2	C(4)—C(5)—H(5)	119·4
C(2)—C(3)—H(3)	116·8	C(5)—C(4)—H(4)	118·2
C(4)—C(3)—H(3)	114·2	C(3)—C(4)—H(4)	113·2
H(11*A*)—C(11)—H(11*B*)	110·6		

alternation is correlated to the deviation from planarity of the perimeter ring (Fig. 1*b*). The strain introduced by the methano bridge leads to bond-angle distortions (Table 2). The maximum absolute value of the torsion

angles τ along the ring is 35·6 (3)° (if $|\tau| > 90°$, it is replaced by $180 − |\tau|$).

The intramolecular distance C(1)···C(6) is 2·235 (3) Å, slightly shorter than the corresponding 2·269 (5) Å found in DIF. The three shortest intermolecular contacts, ranging from 2·82 (3) to 2·89 (2) Å, are between C and H atoms. The remaining intermolecular distances are consistent with normal van der Waals packing radii.

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Isopropylammoniomethanesulfonate

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Abstract. $C_4H_{11}NO_3S$, monoclinic, $P2_1/n$, $a = 10.458$ (6), $b = 5.698$ (3), $c = 12.794$ (6) Å, $\beta = 112.44$ (4)°, $M_r = 153.20$, $Z = 4$, $D_m = 1.43$ (flotation), $D_x = 1.444$ Mg m^{-3}, $\mu(Mo K\alpha) = 0.39$ mm^{-1}. The structure was solved by direct methods and refined by full-matrix least-squares calculations. The final R was 0·056 for 1039 measured reflections. The ammonium group of one molecule is hydrogen-bonded to O(1) and O(3) belonging to the sulfonate groups of molecules related to it by the twofold screw axis.

Introduction. Crystals of (I) were kindly provided by Professor R. A. M. C. De Groote of the Chemistry and Molecular Physics Department, Institute of Physics and Chemistry of São Carlos.

$$\begin{array}{c} CH_3 \\ \diagdown \\ \diagup \\ CH_3 \end{array} CH-\overset{+}{N}H_2-CH_2-SO_3^-$$

(I)
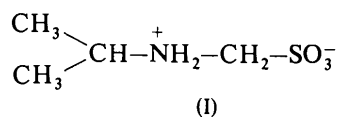
This structure determination has been undertaken to study the hydrogen-bonding scheme in this zwitterion

which was obtained during an investigation of aminomethanesulfonate derivatives of aliphatic compounds.

A crystal of approximate dimensions 0·4 × 0·5 × 0·6 mm was used for the data collection on a CAD-4 diffractometer. The cell parameters were refined from the setting angles for 25 reflections. Three-dimensional intensities were collected using graphite-monochromated Mo $K\alpha$ radiation up to $2\theta = 60°$. The ω–2θ scanning mode with varying interval was used. Of the 1267 recorded independent reflections, 1039 were observed above background [$I > 2\sigma(I)$, where $\sigma(I)$ was based on counting statistics]. The data were reduced to structure factors without absorption correction.

The structure was solved by application of *MULTAN* (Germain, Main & Woolfson, 1971) to the 162 reflections with $E > 1.50$. All the non-hydrogen atoms appeared clearly on the E map based on the set of phases giving the highest combined figure of merit. All the H atoms were placed at their calculated positions.

Refinement was carried out by full-matrix least-

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *with their estimated standard deviations in parentheses*

The B_{eq} values are the equivalent isotropic temperature factors (Hamilton, 1959).

	x	y	z	B_{eq} (Å^2)
S	2090 (1)	2923 (2)	5924 (2)	1·8 (2)
O(1)	3364 (2)	2294 (5)	6873 (4)	2·6 (2)
O(2)	1920 (2)	1819 (5)	4866 (4)	3·3 (2)
O(3)	1897 (2)	5469 (5)	5871 (4)	2·4 (2)
N	814 (2)	2623 (5)	7400 (4)	1·8 (2)
C(1)	−434 (3)	2038 (7)	7686 (6)	2·1 (2)
C(2)	−84 (4)	2722 (10)	8913 (8)	4·2 (3)
C(3)	−1702 (4)	3295 (10)	6876 (7)	3·9 (3)
C(4)	701 (3)	1783 (7)	6268 (6)	2·0 (2)

squares calculations with anisotropic thermal parameters for the non-hydrogen atoms and isotropic thermal parameters equal to 6·0 Å^2 for the H atoms. The function minimized was $\sum w_i(k|F_o| - |F_c|)^2$ where $w_i = [\sigma(F_o)^2 + (0.05F_o)^2]^{-1}$ for the observed and $w_i = 0$ for the unobserved reflections. The atomic scattering factors used were those of Cromer & Waber (1974) and the dispersion-correction coefficients were those of Cromer & Ibers (1974).

The final refinement cycle gave $R = 0.072$ for all reflections and $R = 0.056$ for the observed reflections only.

The final atomic parameters are given in Table 1.*

Discussion. Bond lengths and angles are given in Fig. 1, which also includes the atomic numbering.

The atoms S, O(2), N, C(1) and C(4) are approximately in a plane whose equation referred to conventional orthogonalized coordinates is $-0.383X + 0.807Y - 0.449Z = -1.587$, the distances of the atoms to this plane being respectively 0·060 (1), −0·015 (3), −0·076 (3), 0·057 (4) and −0·026 (4) Å. The atoms O(1), O(3), C(2) and C(3) not included in the calculation of the mean plane deviate from it by −1·065 (3), 1·327 (2), −0·192 (5) and −1·421 (5) Å. The mean plane does not bisect the C(2)—C(1)—C(3) angle, the torsion angles C(4)—N—C(1)—C(2) and C(4)—N—C(1)—C(3) being respectively equal to +172·8 and −64·0°.

Although there are short intramolecular contacts between N and O(1), 2·996 (3) Å, and O(3), 3·072 (3) Å, the hydrogen-bonding scheme is entirely intermolecular. It consists of an infinite spiral extending around the twofold screw axis and is depicted in Fig. 1. The corresponding distances and angles are given in Table 2.

The distance between S and O(2), not involved in

* Lists of structure factors, anisotropic thermal parameters, hydrogen-atom parameters and tables of bond lengths have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35512 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
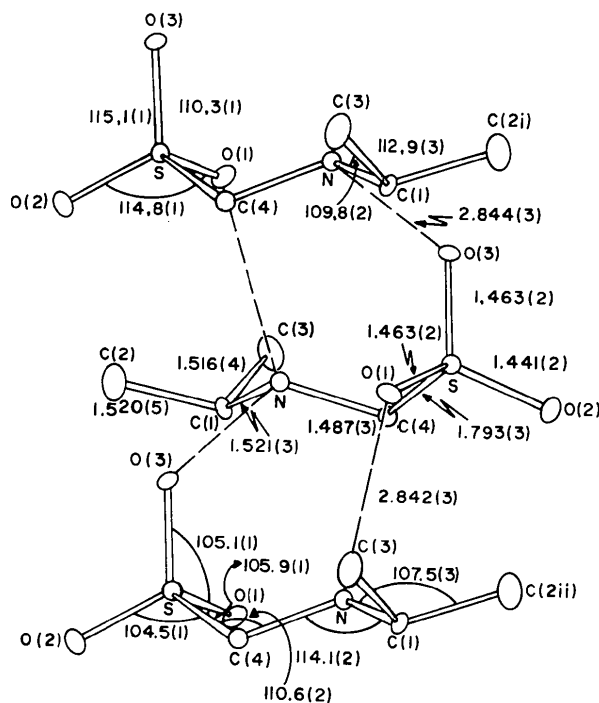

Fig. 1. Representation of the hydrogen-bonding scheme giving the bond lengths (Å), and angles (°) and the atomic numbering. (See Table 2 for symmetry code.)

Table 2. *Hydrogen-bonding distances* (Å) *and angles* (°) *with their estimated standard deviations in parentheses*

i	j	k	D_{ij}	D_{jk}	D_{ik}	$\angle ijk$
N	H(10)	O(1i)	0·93 (5)	2·05 (5)	2·842 (3)	168 (5)
N	H(11)	O(3ii)	1·02 (4)	1·93 (5)	2·844 (3)	171 (4)

Symmetry code: (i) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$; (ii) $\frac{1}{2} - x, -\frac{1}{2} + y, \frac{3}{2} - z$.

hydrogen bonding, is significantly shorter than the other two S—O bond distances and the O(1)—S—O(3) angle is 4·7 (1)° smaller than the average [115·0 (1)°] of the other two O—S—O angles.

All calculations were performed in this Institute on a PDP 11/45, using the Nonius SDP crystallographic programs.

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