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Key indicators

Single-crystal X-ray study
T = 295 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.031
wR factor = 0.085
Data-to-parameter ratio = 11.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

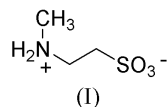
Zwitterionic 2-(methylamino)ethanesulfonic acid

The title compound, *N*-methyltaurine, $\text{C}_3\text{H}_9\text{NO}_3\text{S}$, was isolated from the marine sponge *Xestospongia pacifica* from Swain Reefs, Queensland. The crystal structure displays extensive $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonding interactions between the amine H atoms and sulfonate O atoms in the zwitterionic molecule.

Comment

In a recent study, *N*-methyltaurine is reported to be a major osmolyte in a specimen of the tubeworm *Lamellibrachia* sp. (Yin *et al.*, 2000). Osmolytes are small organic molecules that regulate cell volume by countering osmotic pressure exerted by sea water and it seems reasonable to assume that *N*-methyltaurine performs a similar role in *Xestospongia pacifica*.

Molecules of 2-(methylamino)ethanesulfonic acid, (I), crystallize in the zwitterionic form with the sulfonic acid H atom transferred to the N atom (Fig. 1 and Table 1). The bond lengths and angles are in accord with conventional values (Allen *et al.*, 1987) and related structures (Görbitz *et al.*, 2000).



In the crystal structure, the molecules are linked *via* a number of $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds to form a three-dimensional network (Table 2).

Experimental

Compound (I) was isolated from a methanol extract of the marine sponge *Xestospongia pacifica* from Swain Reefs, Queensland. The extract was subjected to repeated gel-permeation chromatography on Sephadex LH-20 in methanol. Crystals of (I) were obtained on slow evaporation of the methanol from the parent fraction; m.p. 520 K (with decomposition). δ_{H} (400 MHz, $\text{DMSO}-d_6$, p.p.m.): 4.1 (2H, brs, NH_2), 3.16 (3H, s, $\text{N}-\text{CH}_3$), 3.14 (2H, t, $J_{2,1} = 6.4 \text{ Hz}$, H2), 2.77 (2H, t, $J_{1,2} = 6.4 \text{ Hz}$, H1), (ESMS+): 161.8 (MNa^+), (ESMS-) 137.8 ($M-\text{H}$).

Crystal data

$\text{C}_3\text{H}_9\text{NO}_3\text{S}$
 $M_r = 139.18$
Orthorhombic, $P2_12_12_1$
 $a = 9.061 (3) \text{ \AA}$
 $b = 11.931 (3) \text{ \AA}$
 $c = 5.4924 (15) \text{ \AA}$
 $V = 593.8 (3) \text{ \AA}^3$
 $Z = 4$
 $D_x = 1.557 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
Cell parameters from 25 reflections
 $\theta = 12.9\text{--}17.3^\circ$
 $\mu = 0.46 \text{ mm}^{-1}$
 $T = 295 \text{ K}$
Prism, colorless
 $0.40 \times 0.40 \times 0.15 \text{ mm}$

Data collection

Rigaku AFC-7R diffractometer
 ω - 2θ scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.836$, $T_{\max} = 0.934$
 1011 measured reflections
 820 independent reflections
 793 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -11 \rightarrow 5$
 $k = 0 \rightarrow 15$
 $l = -3 \rightarrow 7$
 3 standard reflections
 every 150 reflections
 intensity decay: 0.3%

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.085$
 $S = 1.06$
 820 reflections
 74 parameters
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.18P]$
 where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.27 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.24 \text{ e } \text{\AA}^{-3}$
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.154 (12)
 Absolute structure: Flack (1983)
 Flack parameter = -0.09 (13)

Table 1

Selected geometric parameters (\AA , $^\circ$).

S1—O1	1.4564 (18)	S1—C1	1.779 (3)
S1—O2	1.4654 (18)	N1—C2	1.485 (3)
S1—O3	1.452 (2)	N1—C3	1.480 (3)
O1—S1—O2	111.33 (10)	O3—S1—C1	105.15 (11)
O1—S1—O3	113.89 (11)	C2—N1—C3	114.10 (19)
O1—S1—C1	106.29 (11)	S1—C1—C2	111.59 (15)
O2—S1—O3	113.15 (12)	N1—C2—C1	110.44 (18)
O2—S1—C1	106.28 (11)		

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H5 \cdots O1 ⁱ	0.85	2.13	2.862 (3)	144
N1—H5 \cdots O3 ⁱⁱ	0.85	2.52	2.945 (3)	112
N1—H6 \cdots O2 ⁱⁱⁱ	0.85	2.02	2.798 (3)	152

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

H atoms were constrained as riding atoms, with C—H distances of 0.95 \AA and N—H distances of 0.85 \AA . $U_{\text{iso}}(\text{H})$ values were set to $1.2U_{\text{eq}}$ for the parent atom.

Data collection: *MSC/AFC-7 Diffractometer Control Software* (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC-7 Diffractometer Control Software*; data reduction: *TEXSAN*

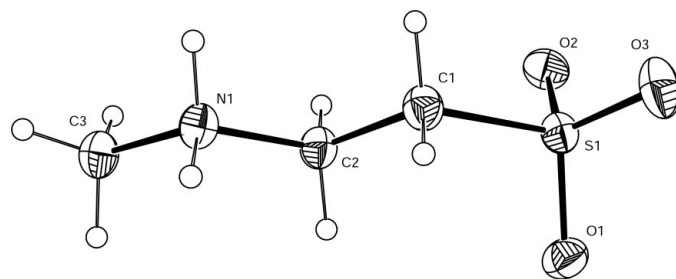


Figure 1

ORTEP-3 (Farrugia, 1997) plot, showing the atomic numbering scheme for the molecule of (I). Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

(Molecular Structure Corporation, 1997–2001); program(s) used to solve structure: *TEXSAN*; program(s) used to refine structure: *TEXSAN* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1980–2001) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *TEXSAN* and *PLATON*.

The marine sponge *Xestospongia pacifica* Kelly-Borges & Bergquist, 1998 (phylum Porifera, class Demospongiae, order Haplosclerida, family Petrosiidae) was collected by hand using SCUBA from Swain Reefs, Queensland, Australia, at a depth of 28 m by Dr John Hooper and co-workers from the Sessile Marine Invertebrate section, Queensland Museum. A voucher sample (G305705) is lodged at the Queensland Museum, Brisbane, Australia.

References

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supporting information

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S1. Comment

Molecules of 2-(methylamino)ethanesulfonic acid, (I), crystallize in the zwitterionic form with the carboxyl proton transferred to the N atom (Fig. 1 and Table 1). The bond lengths and angles of the molecules are in accord with conventional values (Allan *et al.*, 1987) and related structures (Görbitz *et al.*, 2000).

In the crystal structure, the molecules are linked *via* a number of N–H \cdots O hydrogen bonds to form a three-dimensional network (Table 2).

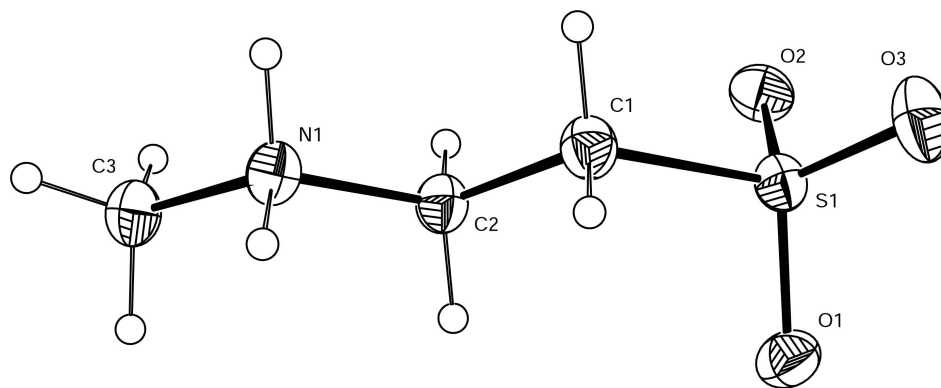
In a recent study, *N*-methyltaurine is reported to be a major osmolyte in a specimen of the tubeworm *Lamellibrachia sp.* (Yin *et al.*, 2000). Osmolytes are small organic molecules that regulate cell volume by countering osmotic pressure exerted by sea water and it seems reasonable to assume that *N*-methyltaurine performs a similar role in *Xestospongia pacifica*.

S2. Experimental

Compound (I) was isolated from the methanol extract of the marine sponge *Xestospongia pacifica* from Swain Reefs, Queensland. The extract was subjected to repeated gel-permeation chromatography on Sephadex LH-20 in methanol. Crystals of (I) were obtained on slow evaporation of the methanol from the parent fraction; m.p. 520 K (with decomposition). δ_{H} (400 MHz, DMSO- d_6 , p.p.m.): 4.1 (2H, brs, NH₂), 3.16 (3H, s, N–CH₃), 3.14 (2H, t, $J_{2,1} = 6.4$ Hz, H₂), 2.77 (2H, t, $J_{1,2} = 6.4$ Hz, H₁), (ESMS+): 161.8 (MNa⁺), (ESMS–) 137.8 (M–H).

S3. Refinement

H atoms were constrained as riding atoms, fixed to their parent C atoms at a C–H distance of 0.95 Å. $U_{\text{iso}}(\text{H})$ values were set to $1.2U_{\text{eq}}$ for the parent atom.

**Figure 1**

ORTEP-3 (Farrugia, 1997) plot showing the atomic numbering scheme for the molecule in the asymmetric unit of (I). Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

2-(methylamino)ethanesulfonic acid

Crystal data

$C_3H_9NO_3S$

$M_r = 139.18$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 9.061(3) \text{ \AA}$

$b = 11.931(3) \text{ \AA}$

$c = 5.4924(15) \text{ \AA}$

$V = 593.8(3) \text{ \AA}^3$

$Z = 4$

$F(000) = 296$

$D_x = 1.557 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.7107 \text{ \AA}$

Cell parameters from 25 reflections

$\theta = 12.9\text{--}17.3^\circ$

$\mu = 0.46 \text{ mm}^{-1}$

$T = 295 \text{ K}$

Prismatic, colorless

$0.40 \times 0.40 \times 0.15 \text{ mm}$

Data collection

Rigaku AFC-7R

diffractometer

Radiation source: Rigaku rotating anode

Graphite monochromator

ω - 2θ scans

Absorption correction: ψ scan

(North et al., 1968)

$T_{\min} = 0.836$, $T_{\max} = 0.934$

1011 measured reflections

820 independent reflections

793 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.8^\circ$

$h = -11 \rightarrow 5$

$k = 0 \rightarrow 15$

$l = -3 \rightarrow 7$

3 standard reflections every 150 reflections

intensity decay: 0.3%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.085$

$S = 1.06$

820 reflections

74 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.18P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.27 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.24 \text{ e \AA}^{-3}$

Extinction correction: *SHELXL97*,

$FC^* = KFC[1 + 0.001XFC^2\Lambda^3/\text{SIN}(2\Theta)]^{-1/4}$

Extinction coefficient: 0.154 (12)

Absolute structure: Flack (1983)

Absolute structure parameter: $-0.09(13)$

Special details

Experimental. The scan width was $(1.79 + 0.30 \tan \theta)^\circ$ with an ω scan speed of 16° per minute (up to 4 scans to achieve $I/\sigma(I) > 10$). Stationary background counts were recorded at each end of the scan, and the scan time:background time ratio was 2:1.

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All e.s.d.'s are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.43693 (6)	0.14685 (4)	0.65892 (11)	0.0246 (2)
O1	0.4695 (2)	0.02903 (14)	0.7028 (3)	0.0352 (5)
O2	0.4186 (2)	0.16966 (15)	0.3985 (3)	0.0345 (5)
O3	0.5385 (2)	0.22346 (18)	0.7776 (4)	0.0434 (6)
N1	-0.0013 (2)	0.12425 (16)	0.8055 (4)	0.0283 (6)
C1	0.2625 (3)	0.17323 (19)	0.7963 (4)	0.0280 (6)
C2	0.1429 (2)	0.10053 (18)	0.6876 (4)	0.0254 (6)
C3	-0.1270 (3)	0.0623 (2)	0.6983 (5)	0.0370 (8)
H1	0.26920	0.15830	0.96600	0.0340*
H2	0.23730	0.24990	0.77280	0.0340*
H3	0.16740	0.02380	0.71070	0.0310*
H4	0.13530	0.11560	0.51780	0.0310*
H5	0.00520	0.10670	0.95570	0.0340*
H6	-0.01880	0.19410	0.79380	0.0340*
H7	-0.21470	0.07870	0.78630	0.0450*
H8	-0.13910	0.08380	0.53300	0.0450*
H9	-0.10800	-0.01610	0.70630	0.0450*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0246 (3)	0.0251 (3)	0.0241 (3)	-0.0024 (2)	0.0023 (2)	-0.0027 (2)
O1	0.0403 (10)	0.0305 (8)	0.0347 (10)	0.0088 (7)	0.0035 (8)	0.0033 (7)
O2	0.0455 (11)	0.0326 (8)	0.0253 (8)	-0.0011 (8)	0.0048 (8)	0.0053 (7)
O3	0.0315 (9)	0.0519 (11)	0.0469 (11)	-0.0144 (9)	0.0029 (9)	-0.0189 (10)
N1	0.0245 (9)	0.0322 (10)	0.0283 (11)	0.0004 (8)	0.0018 (9)	-0.0025 (9)
C1	0.0254 (10)	0.0283 (10)	0.0302 (11)	0.0007 (9)	0.0052 (9)	-0.0081 (9)
C2	0.0242 (9)	0.0264 (9)	0.0256 (11)	-0.0001 (8)	0.0023 (10)	-0.0030 (9)
C3	0.0262 (11)	0.0404 (13)	0.0444 (16)	-0.0051 (10)	-0.0047 (12)	0.0019 (13)

Geometric parameters (\AA , $^\circ$)

S1—O1	1.4564 (18)	C1—C2	1.511 (3)
S1—O2	1.4654 (18)	C1—H1	0.9509

S1—O3	1.452 (2)	C1—H2	0.9516
S1—C1	1.779 (3)	C2—H3	0.9505
N1—C2	1.485 (3)	C2—H4	0.9523
N1—C3	1.480 (3)	C3—H7	0.9505
N1—H5	0.8532	C3—H8	0.9498
N1—H6	0.8508	C3—H9	0.9521
S1...H6 ⁱ	3.1535	C2...O1 ⁱⁱⁱ	3.243 (3)
O1...C2 ⁱⁱ	3.243 (3)	C2...O1 ⁱⁱ	3.381 (3)
O1...N1 ⁱⁱⁱ	2.862 (3)	C3...O1 ⁱⁱⁱ	3.260 (3)
O1...C2 ⁱⁱⁱ	3.381 (3)	C3...O1 ⁱⁱ	3.302 (3)
O1...C3 ⁱⁱⁱ	3.302 (3)	C3...O2 ^{vii}	3.268 (3)
O1...C3 ⁱⁱ	3.260 (3)	H1...O2 ^{ix}	2.7375
O2...C3 ⁱ	3.268 (3)	H1...H5	2.4707
O2...N1 ⁱ	2.798 (3)	H1...O3 ^{viii}	2.8884
O3...N1 ^{iv}	2.945 (3)	H2...H6	2.4169
O3...C1 ^{iv}	3.334 (3)	H3...O1	2.7384
O1...H3	2.7384	H3...H9	2.5405
O1...H8 ⁱⁱ	2.7318	H3...O2 ⁱⁱ	2.6455
O1...H4 ⁱⁱ	2.6216	H4...O2	2.7267
O1...H5 ⁱⁱⁱ	2.1253	H4...H8	2.5165
O2...H1 ^v	2.7375	H4...O1 ⁱⁱⁱ	2.6216
O2...H9 ⁱⁱⁱ	2.7233	H4...O3 ^{vii}	2.6625
O2...H6 ⁱ	2.0198	H5...H1	2.4707
O2...H4	2.7267	H5...O1 ⁱⁱ	2.1253
O2...H3 ⁱⁱⁱ	2.6455	H5...O3 ^{viii}	2.5185
O3...H7 ^{vi}	2.8260	H6...H2	2.4169
O3...H1 ^{iv}	2.8884	H6...S1 ^{vii}	3.1535
O3...H4 ⁱ	2.6625	H6...O2 ^{vii}	2.0198
O3...H5 ^{iv}	2.5185	H6...O3 ^{viii}	2.6036
O3...H6 ^{iv}	2.6036	H7...O3 ^x	2.8260
N1...O1 ⁱⁱ	2.862 (3)	H8...H4	2.5165
N1...O2 ^{vii}	2.798 (3)	H8...O1 ⁱⁱⁱ	2.7318
N1...O3 ^{viii}	2.945 (3)	H9...H3	2.5405
C1...O3 ^{viii}	3.334 (3)	H9...O2 ⁱⁱ	2.7233
O1—S1—O2	111.33 (10)	S1—C1—H2	109.00
O1—S1—O3	113.89 (11)	C2—C1—H1	109.00
O1—S1—C1	106.29 (11)	C2—C1—H2	109.03
O2—S1—O3	113.15 (12)	H1—C1—H2	109.17
O2—S1—C1	106.28 (11)	N1—C2—H3	109.31
O3—S1—C1	105.15 (11)	N1—C2—H4	109.11
C2—N1—C3	114.10 (19)	C1—C2—H3	109.43
C2—N1—H6	108.52	C1—C2—H4	109.29
C3—N1—H5	108.38	H3—C2—H4	109.24
C2—N1—H5	108.30	N1—C3—H7	109.77
H5—N1—H6	109.05	N1—C3—H8	109.53
C3—N1—H6	108.41	N1—C3—H9	109.46

S1—C1—C2	111.59 (15)	H7—C3—H8	109.51
N1—C2—C1	110.44 (18)	H7—C3—H9	109.27
S1—C1—H1	109.01	H8—C3—H9	109.29
O1—S1—C1—C2	-59.98 (18)	C3—N1—C2—C1	175.97 (19)
O2—S1—C1—C2	58.72 (18)	S1—C1—C2—N1	180.00 (15)
O3—S1—C1—C2	178.94 (16)		

Symmetry codes: (i) $x+1/2, -y+1/2, -z+1$; (ii) $-x+1/2, -y, z+1/2$; (iii) $-x+1/2, -y, z-1/2$; (iv) $x+1/2, -y+1/2, -z+2$; (v) $x, y, z-1$; (vi) $x+1, y, z$; (vii) $x-1/2, -y+1/2, -z+1$; (viii) $x-1/2, -y+1/2, -z+2$; (ix) $x, y, z+1$; (x) $x-1, y, z$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H5 \cdots O1 ⁱⁱ	0.85	2.13	2.862 (3)	144
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