

Zwitterionic 2-(methylamino)ethanesulfonic acid

Author

Kalaitzis, JA, Leone, PD, Quinn, RJ, Healy, PC

Published

2003

Journal Title

ACTA Crystallographica Section E - Structure Reports Online

DOI

[10.1107/S160053680300895X](https://doi.org/10.1107/S160053680300895X)

Rights statement

© The Author(s) 2003. For information about this journal please refer to the journal's website. All articles published in Acta Crystallographica Section E are open access and distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited. See <http://creativecommons.org/licenses/by/2.0/uk/legalcode>

Downloaded from

<http://hdl.handle.net/10072/6334>

Link to published version

<http://journals.iucr.org/e/journalhomepage.html>

Griffith Research Online

<https://research-repository.griffith.edu.au>

John A. Kalaitzis, Priscila de Almeida Leone, Ronald J. Quinn and Peter C. Healy*

School of Science, Griffith University, Nathan, Brisbane 4111, Australia

Correspondence e-mail:
p.healy@mailbox.gu.edu.au

Key indicators

Single-crystal X-ray study
 $T = 295\text{ K}$
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>.

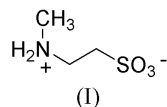
Zwitterionic 2-(methylamino)ethanesulfonic acid

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 (MN^+), (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*

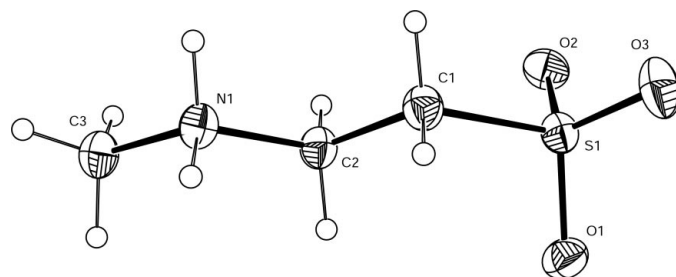


Figure 1

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

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
 Görbitz, C. H., Prydz, K. & Ugland, S. (2000). *Acta Cryst.* **C56**, e23–e24.
 Molecular Structure Corporation (1999). *MSC/AFC-7 Diffractometer Control Software*. Windows Version 1.02. MSC, 9009 New Trails Drive, The Woodlands, TX 77381, USA.
 Molecular Structure Corporation (1997–2001). *TEXSAN for Windows*. Version 1.06. MSC, 9009 New Trails Drive, The Woodlands, TX 77381, USA.
 North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
 Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
 Spek, A. L. (1980–2001). *PLATON for Windows*. Version 121201. University of Utrecht, The Netherlands.
 Yin, M., Palmer, H. R., Fyfe-Johnson, A. L., Bedford, J. J., Smith, R. A. J. & Yancey, P. H. (2000). *Physiol. Biochem. Zool.* **73**, 629–637.