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2-Aminobenzothiazolium toluene-*p*-sulfonate

Wei-Xing Ma,* Bao-Hua Qian, Qing-Qing Liu, Hong-Yu Ge and Xing-You Xu

Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China
Correspondence e-mail: weixingma650528@163.com

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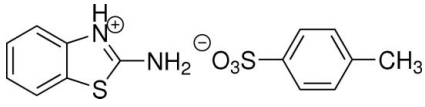
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.061; wR factor = 0.163; data-to-parameter ratio = 13.6.

The title compound, $C_7H_7N_2S^+\cdot C_7H_7O_3S^-$, was studied for its potential to form supramolecular constructs. Intermolecular N—H···O hydrogen bonds link each cation to two anions and each anion, in turn, to two cations, forming infinite one-dimensional chains. There are weak π–π stacking interactions of 3.577 (6) Å between the salt chains, involving the benzene and thiazole rings of neighbouring cations.

Related literature

For related literature, see: Biradha & Mahata (2005); Fuller (1996); Ma *et al.* (2006); Ren *et al.* (2000).



Experimental

Crystal data

$C_7H_7N_2S^+\cdot C_7H_7O_3S^-$
M_r = 322.39
Monoclinic, $P2_1/c$
a = 7.5140 (13) Å
b = 29.878 (3) Å
c = 6.8937 (12) Å
β = 107.661 (2)°
V = 1474.7 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 298 (2) K
0.63 × 0.42 × 0.12 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.800, T_{max} = 0.957
7447 measured reflections
2591 independent reflections
1864 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.164
S = 1.08
2591 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3	0.86	1.91	2.764 (5)	171
N2—H2A···O1	0.86	2.01	2.798 (5)	152
N2—H2B···O2^{i}	0.86	1.90	2.737 (5)	165

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2174).

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supplementary materials

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2-Aminobenzothiazolium toluene-*p*-sulfonate

W.-X. Ma, B.-H. Qian, Q.-Q. Liu, H.-Y. Ge and X.-Y. Xu

Comment

We are interested in sulfonate complexes as they have been shown to form supramolecular constructs (Biradha & Mahata, 2005; Fuller, 1996). We report here the synthesis and structure study on one such sulfonate.

Fig. 1 shows the molecular structure of the title compound. It crystallized as a 1:1 salt with a thiazole cation and a sulfonate anion. Bond distances and angles are similar to those found in 2-aminobenzothiazole complexed with Zn (Ma *et al.*, 2006) and in the toluene-*p*-sulfonate in HMASPS, (Ren *et al.*, 2000). Intermolecular N—H···O hydrogen bonds link each cation to two anions and each anion, in turn, to two cations forming infinite one dimensional chains. There are weak π–π stacking interactions with a *Cg*1 (C1,C2,C3,N1,S1) to *Cg*2 (C1,C2,C3,C4,C5,C6,C7) (x, 0.5 − y, 1/2 + z) distance of 3.577 (6) Å between the salt chains (Fig. 2)

Experimental

A solution of toluene-*p*-sulfonate (0.7608 g, 4 mmol), 2-aminobenzothiazole (1.200 g, 4 mmol) and 40 ml me thanol was refluxed for 3 h, then cooled. Colourless single crystals of th title compound suitable for X-ray diffraction were crystallized from the methanol solution.

Refinement

All of the hydrogen atoms were placed in the calculated positions, assigned by fixed isotropic thermal parameters at 1.5 times the equivalent isotropic U of the atoms to which they are attached.

Figures

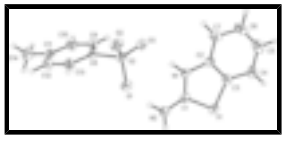

Fig. 1. Molecular structure showing 30% probability displacement ellipsoids.

Fig. 2. A perspective view of the crystal packing of (I). The hydrogen-bond contacts and π–π stacking interactions are shown as dashed lines. Hydrogen atoms have been ommited for clarity. i = 1 + x, y, z; ii = x, 0.5 − y, 1/2 + z

2-Aminobenzothiazolium toluene-*p*-sulfonate

Crystal data

$C_7H_7N_2S^+·C_7H_7O_3S^-$ $F_{000} = 672$

M_r = 322.39	D_x = 1.452 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.5140 (13) Å	Cell parameters from 2309 reflections
b = 29.878 (3) Å	θ = 2.8–25.2º
c = 6.8937 (12) Å	μ = 0.37 mm^{-1}
β = 107.661 (2)º	T = 298 (2) K
V = 1474.7 (4) Å^3	Column, colourless
Z = 4	0.63 × 0.42 × 0.12 mm

Data collection

Brucker SMART 1000 CCD area-detector diffractometer	2591 independent reflections
Radiation source: fine-focus sealed tube	1864 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −8→8
T_{min} = 0.800, T_{max} = 0.957	k = −35→29
7447 measured reflections	l = −8→8

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.061	H-atom parameters constrained
$wR(F^2)$ = 0.164	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 3.0209P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max} < 0.001$
2591 reflections	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
190 parameters	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	1.13486 (15)	0.21913 (4)	0.52219 (19)	0.0453 (3)
S2	0.45495 (15)	0.11448 (4)	0.40956 (19)	0.0446 (3)
N1	0.7878 (5)	0.20196 (12)	0.4315 (5)	0.0413 (9)
H1	0.6838	0.1876	0.4043	0.050*
N2	0.9729 (5)	0.13840 (13)	0.4832 (6)	0.0501 (10)
H2A	0.8771	0.1211	0.4600	0.060*
H2B	1.0831	0.1271	0.5122	0.060*
O1	0.6440 (4)	0.10003 (11)	0.5173 (5)	0.0510 (9)
O2	0.3394 (4)	0.11641 (12)	0.5440 (6)	0.0611 (10)
O3	0.4537 (4)	0.15591 (10)	0.2988 (6)	0.0565 (9)
C1	0.9510 (5)	0.18143 (15)	0.4746 (6)	0.0382 (10)
C2	0.7965 (6)	0.24824 (15)	0.4334 (6)	0.0407 (10)
C3	0.9779 (6)	0.26377 (15)	0.4800 (7)	0.0422 (11)
C4	1.0162 (8)	0.30909 (16)	0.4901 (7)	0.0540 (13)
H4	1.1386	0.3195	0.5256	0.065*
C5	0.8679 (9)	0.33834 (19)	0.4459 (8)	0.0689 (16)
H5	0.8902	0.3690	0.4475	0.083*
C6	0.6881 (9)	0.32317 (19)	0.3998 (8)	0.0663 (16)
H6	0.5906	0.3437	0.3730	0.080*
C7	0.6487 (7)	0.27792 (18)	0.3922 (8)	0.0559 (13)
H7	0.5262	0.2677	0.3603	0.067*
C8	0.3596 (5)	0.07252 (15)	0.2294 (7)	0.0401 (11)
C9	0.3183 (7)	0.08006 (16)	0.0232 (8)	0.0525 (13)
H9	0.3325	0.1085	−0.0252	0.063*
C10	0.2556 (7)	0.04505 (17)	−0.1108 (9)	0.0592 (14)
H10	0.2264	0.0503	−0.2499	0.071*
C11	0.2353 (6)	0.00273 (16)	−0.0441 (9)	0.0529 (13)
C12	0.2767 (7)	−0.00441 (17)	0.1615 (9)	0.0579 (14)
H12	0.2643	−0.0330	0.2093	0.070*
C13	0.3365 (6)	0.03009 (16)	0.2980 (8)	0.0505 (12)
H13	0.3613	0.0249	0.4366	0.061*
C14	0.1721 (8)	−0.0356 (2)	−0.1911 (10)	0.0791 (19)
H14A	0.2714	−0.0570	−0.1702	0.119*
H14B	0.1395	−0.0244	−0.3281	0.119*
H14C	0.0653	−0.0497	−0.1688	0.119*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0317 (6)	0.0540 (7)	0.0460 (7)	−0.0058 (5)	0.0057 (5)	0.0002 (6)
S2	0.0284 (6)	0.0480 (7)	0.0547 (8)	−0.0007 (5)	0.0087 (5)	−0.0036 (6)
N1	0.0296 (18)	0.050 (2)	0.040 (2)	−0.0028 (16)	0.0037 (16)	−0.0023 (18)
N2	0.037 (2)	0.048 (2)	0.063 (3)	−0.0004 (17)	0.0125 (19)	0.000 (2)
O1	0.0312 (16)	0.058 (2)	0.057 (2)	−0.0002 (14)	0.0036 (15)	0.0011 (17)

O2	0.0385 (18)	0.082 (3)	0.066 (2)	−0.0028 (17)	0.0209 (17)	−0.019 (2)
O3	0.0467 (19)	0.0432 (19)	0.069 (2)	−0.0056 (15)	0.0025 (17)	−0.0003 (17)
C1	0.032 (2)	0.049 (3)	0.031 (2)	−0.0015 (19)	0.0059 (19)	0.000 (2)
C2	0.042 (2)	0.046 (3)	0.031 (2)	0.003 (2)	0.0080 (19)	0.002 (2)
C3	0.047 (3)	0.046 (3)	0.030 (2)	−0.001 (2)	0.006 (2)	−0.001 (2)
C4	0.069 (3)	0.051 (3)	0.035 (3)	−0.012 (3)	0.005 (2)	−0.003 (2)
C5	0.104 (5)	0.053 (3)	0.052 (4)	0.004 (3)	0.027 (3)	−0.002 (3)
C6	0.088 (4)	0.058 (4)	0.051 (3)	0.035 (3)	0.019 (3)	0.015 (3)
C7	0.051 (3)	0.070 (4)	0.043 (3)	0.016 (3)	0.008 (2)	0.007 (3)
C8	0.025 (2)	0.043 (3)	0.049 (3)	−0.0001 (18)	0.0079 (19)	0.004 (2)
C9	0.052 (3)	0.041 (3)	0.062 (3)	−0.003 (2)	0.014 (3)	0.004 (3)
C10	0.062 (3)	0.059 (3)	0.057 (3)	−0.001 (3)	0.018 (3)	−0.007 (3)
C11	0.036 (2)	0.047 (3)	0.076 (4)	0.004 (2)	0.017 (2)	−0.010 (3)
C12	0.054 (3)	0.041 (3)	0.077 (4)	−0.003 (2)	0.018 (3)	0.006 (3)
C13	0.045 (3)	0.047 (3)	0.057 (3)	0.000 (2)	0.011 (2)	0.006 (2)
C14	0.064 (4)	0.071 (4)	0.100 (5)	−0.003 (3)	0.021 (3)	−0.035 (4)

Geometric parameters (Å, °)

S1—C1	1.735 (4)	C5—H5	0.9300
S1—C3	1.745 (5)	C6—C7	1.382 (8)
S2—O2	1.451 (3)	C6—H6	0.9300
S2—O3	1.453 (3)	C7—H7	0.9300
S2—O1	1.454 (3)	C8—C9	1.379 (7)
S2—C8	1.757 (5)	C8—C13	1.382 (6)
N1—C1	1.322 (5)	C9—C10	1.380 (7)
N1—C2	1.384 (6)	C9—H9	0.9300
N1—H1	0.8600	C10—C11	1.370 (7)
N2—C1	1.295 (6)	C10—H10	0.9300
N2—H2A	0.8600	C11—C12	1.372 (7)
N2—H2B	0.8600	C11—C14	1.507 (7)
C2—C7	1.382 (6)	C12—C13	1.376 (7)
C2—C3	1.382 (6)	C12—H12	0.9300
C3—C4	1.382 (6)	C13—H13	0.9300
C4—C5	1.376 (7)	C14—H14A	0.9600
C4—H4	0.9300	C14—H14B	0.9600
C5—C6	1.368 (8)	C14—H14C	0.9600
C1—S1—C3	90.3 (2)	C5—C6—H6	119.4
O2—S2—O3	113.1 (2)	C7—C6—H6	119.4
O2—S2—O1	111.5 (2)	C6—C7—C2	118.1 (5)
O3—S2—O1	111.77 (19)	C6—C7—H7	121.0
O2—S2—C8	106.6 (2)	C2—C7—H7	121.0
O3—S2—C8	107.5 (2)	C9—C8—C13	119.3 (5)
O1—S2—C8	105.9 (2)	C9—C8—S2	121.9 (4)
C1—N1—C2	115.0 (4)	C13—C8—S2	118.6 (4)
C1—N1—H1	122.5	C8—C9—C10	119.4 (5)
C2—N1—H1	122.5	C8—C9—H9	120.3
C1—N2—H2A	120.0	C10—C9—H9	120.3
C1—N2—H2B	120.0	C11—C10—C9	121.7 (5)

H2A—N2—H2B	120.0	C11—C10—H10	119.2
N2—C1—N1	124.5 (4)	C9—C10—H10	119.2
N2—C1—S1	123.6 (3)	C10—C11—C12	118.5 (5)
N1—C1—S1	111.9 (3)	C10—C11—C14	121.3 (6)
C7—C2—C3	120.5 (4)	C12—C11—C14	120.2 (5)
C7—C2—N1	127.3 (4)	C11—C12—C13	121.0 (5)
C3—C2—N1	112.2 (4)	C11—C12—H12	119.5
C4—C3—C2	121.1 (4)	C13—C12—H12	119.5
C4—C3—S1	128.3 (4)	C12—C13—C8	120.1 (5)
C2—C3—S1	110.6 (3)	C12—C13—H13	119.9
C5—C4—C3	118.0 (5)	C8—C13—H13	119.9
C5—C4—H4	121.0	C11—C14—H14A	109.5
C3—C4—H4	121.0	C11—C14—H14B	109.5
C6—C5—C4	121.2 (5)	H14A—C14—H14B	109.5
C6—C5—H5	119.4	C11—C14—H14C	109.5
C4—C5—H5	119.4	H14A—C14—H14C	109.5
C5—C6—C7	121.2 (5)	H14B—C14—H14C	109.5
C2—N1—C1—N2	179.1 (4)	N1—C2—C7—C6	−179.1 (5)
C2—N1—C1—S1	−0.1 (5)	O2—S2—C8—C9	128.9 (4)
C3—S1—C1—N2	−179.3 (4)	O3—S2—C8—C9	7.3 (4)
C3—S1—C1—N1	−0.1 (3)	O1—S2—C8—C9	−112.3 (4)
C1—N1—C2—C7	179.3 (4)	O2—S2—C8—C13	−55.1 (4)
C1—N1—C2—C3	0.3 (6)	O3—S2—C8—C13	−176.7 (3)
C7—C2—C3—C4	1.1 (7)	O1—S2—C8—C13	63.7 (4)
N1—C2—C3—C4	−179.8 (4)	C13—C8—C9—C10	−0.4 (7)
C7—C2—C3—S1	−179.4 (4)	S2—C8—C9—C10	175.6 (4)
N1—C2—C3—S1	−0.3 (5)	C8—C9—C10—C11	−0.8 (7)
C1—S1—C3—C4	179.7 (5)	C9—C10—C11—C12	0.8 (7)
C1—S1—C3—C2	0.2 (4)	C9—C10—C11—C14	−178.2 (5)
C2—C3—C4—C5	−2.0 (7)	C10—C11—C12—C13	0.3 (7)
S1—C3—C4—C5	178.6 (4)	C14—C11—C12—C13	179.3 (4)
C3—C4—C5—C6	2.0 (8)	C11—C12—C13—C8	−1.4 (7)
C4—C5—C6—C7	−1.2 (9)	C9—C8—C13—C12	1.5 (7)
C5—C6—C7—C2	0.2 (8)	S2—C8—C13—C12	−174.6 (4)
C3—C2—C7—C6	−0.2 (7)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3	0.86	1.91	2.764 (5)	171
N2—H2A···O1	0.86	2.01	2.798 (5)	152
N2—H2B···O2^{i}	0.86	1.90	2.737 (5)	165

Symmetry codes: (i) *x*+1, *y*, *z*.

Fig. 1

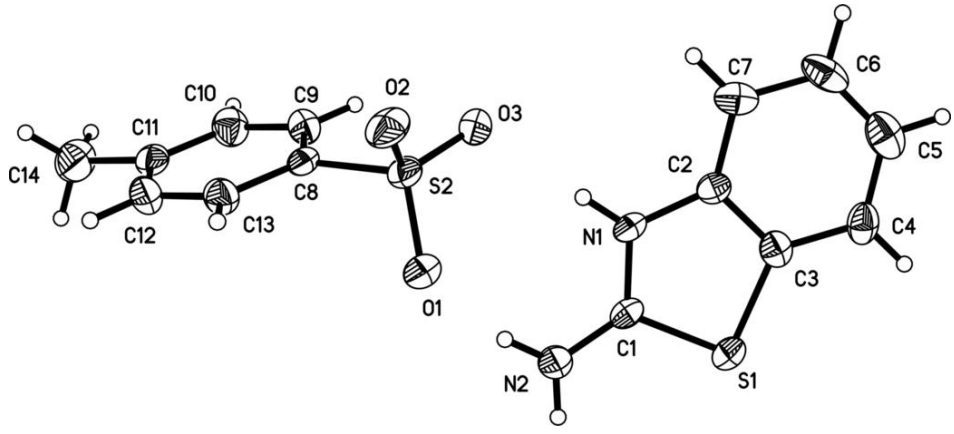

Fig. 2