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Triethylammonium 4-aminobenzenesulfonate

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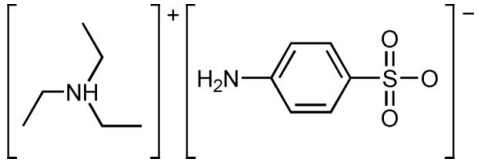
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.171; data-to-parameter ratio = 14.5.

In the title compound, $C_6H_{16}N^+\cdot C_6H_6NO_3S^-$, the NH_2 group of the 4-aminobenzenesulfonate anion forms N—H···O hydrogen bonds to O atoms of two other 4-aminobenzenesulfonate anions, generating two-dimensional layers. The triethylammonium cations lie between these layers, forming N—H···O hydrogen bonds to the sulfonate groups.

Related literature

For related literature, see: Duan *et al.* (2005); Sui *et al.* (2006).



Experimental

Crystal data

$C_6H_{16}N^+\cdot C_6H_6NO_3S^-$
M_r = 274.38
Monoclinic, $P2_1/n$
a = 13.003 (3) Å
b = 8.7648 (19) Å
c = 13.041 (3) Å
β = 101.053 (4)°
V = 1458.8 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 294 (2) K
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.956, T_{max} = 0.965
5906 measured reflections
2575 independent reflections
1770 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.171
S = 1.04
2575 reflections
178 parameters
13 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.883 (8)	2.137 (9)	2.970 (3)	157.0 (15)
N1—H1B···O1^{ii}	0.889 (7)	2.229 (8)	3.078 (3)	159.5 (18)
N2—H2A···O2^{iii}	0.901 (8)	1.852 (9)	2.752 (2)	178 (2)
N2—H2A···S1^{iii}	0.901 (8)	2.910 (10)	3.750 (2)	155.8 (18)

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

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: BI2186).

References

Bruker (1997). *SADABS* (Version 2.01), *SMART* (Version 5.044), *SAINT* (Version 5.01) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Duan, X.-M., Fan, M.-L., Zheng, P.-W. & Tu, Q.-D. (2005). *Acta Cryst.* E**61**, o3831–o3833.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sui, A.-X., Zhu, G. & Tang, Z.-X. (2006). *Acta Cryst.* E**62**, m1592–m1594.

  doi:10.1107/S1600536807022027

supplementary materials

Acta Cryst. (2007). E**63**, o2884 [**doi:10.1107/S1600536807022027**]

Triethylammonium 4-aminobenzenesulfonate

J. Li, Z.-P. Liang and H.-M. Guo

Comment

Aminobenzenesulfonic acid and its derivatives, and their complexes, are widely used in the fields of biology, catalysis and materials science. The title compound (Fig. 1) consists of triethylammonium cations and 4-aminobenzenesulfonate anions. The bond lengths and angles of the triethylammonium cation agree with those in the compound triethylammonium 4-(2-chlorobenzoyl)-3-methyl-1-(*p*-tolyl)-1*H*-pyrazol-5-olate (Duan *et al.*, 2005). The geometrical parameters of the 4-aminobenzenesulfonate anion are similar to those in a related compound (Sui *et al.*, 2006). The NH_2 group of the 4-aminobenzenesulfonate anion forms N—H···O hydrogen bonds to O atoms of two other 4-aminobenzenesulfonate anions (Table 1), generating 2-dimensional layers in the $(\bar{2}02)$ planes. The triethylammonium cations lie between these layers, forming N—H···O hydrogen bonds to the sulfonate groups (Fig. 2 and Table 1).

Experimental

4-Aminobenzenesulfonic acid (0.02 mol) and triethylamine (0.02 mol) were stirred in ethanol (10 ml) for 0.5 h. The solution was then allowed to evaporate at room temperature. Colourless single crystals of the title compound were formed after 8 d.

Refinement

H atoms bound to C atoms were positioned geometrically with C—H = 0.93–0.97 Å and refined as riding with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). H atoms bound to N atoms were located in difference Fourier maps and refined with isotropic displacement parameters, with the N—H and H···H distances restrained to be 0.90 (1) and 1.50 (1) Å, respectively. The CH_2—CH_3 distances in the triethylammonium cation were restrained to be 1.54 (1) Å, and the anisotropic displacement parameters of one methyl group (C12) were restrained to be approximately isotropic.

Figures

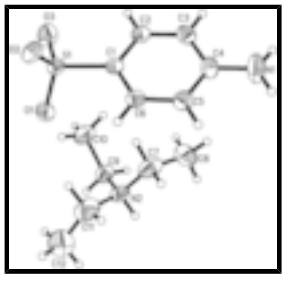

Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at 30% probability for non-H atoms.

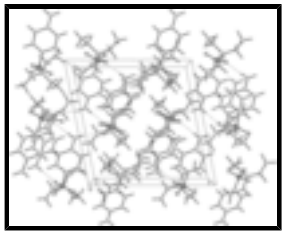

Fig. 2. The crystal packing of (I), viewed along the *b* axis. Hydrogen bonds are indicated by dashed lines.

Triethylammonium 4-aminobenzenesulfonate

Crystal data

$C_6H_{16}N^+·C_6H_6NO_3S^-$	F_{000} = 592
M_r = 274.38	D_x = 1.249 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1829 reflections
a = 13.003 (3) Å	θ = 2.5–23.6º
b = 8.7648 (19) Å	μ = 0.23 mm^{-1}
c = 13.041 (3) Å	T = 294 (2) K
β = 101.053 (4)º	Block, colourless
V = 1458.8 (6) Å^3	0.20 × 0.18 × 0.16 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	2575 independent reflections
Radiation source: fine-focus sealed tube	1770 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −11→15
T_{min} = 0.956, T_{max} = 0.965	k = −10→8
5906 measured reflections	l = −15→15

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.055	$w = 1/[\sigma^2(F_o^2) + (0.0918P)^2 + 0.6965P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.171	$(\Delta/\sigma)_{max}$ = 0.005
S = 1.04	$\Delta\rho_{max}$ = 0.77 e Å^{-3}
2575 reflections	$\Delta\rho_{min}$ = −0.36 e Å^{-3}

178 parameters
13 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.53476 (4)	0.08476 (6)	0.74545 (5)	0.04679 (15)
O1	0.58857 (13)	0.20384 (19)	0.81109 (15)	0.0704 (6)
O2	0.51159 (12)	−0.04414 (18)	0.80888 (13)	0.0597 (5)
O3	0.58690 (12)	0.0356 (2)	0.66309 (13)	0.0710 (5)
N1	0.12768 (17)	0.3574 (4)	0.54777 (18)	0.0954 (9)
C1	0.41219 (16)	0.1618 (2)	0.68650 (16)	0.0416 (5)
C2	0.37541 (17)	0.1483 (3)	0.57977 (17)	0.0486 (6)
H2	0.4149	0.0960	0.5388	0.058*
C3	0.28124 (17)	0.2116 (3)	0.53432 (18)	0.0561 (7)
H3	0.2573	0.2002	0.4628	0.067*
C4	0.22033 (17)	0.2931 (3)	0.59351 (19)	0.0552 (7)
C5	0.25780 (17)	0.3034 (3)	0.70101 (19)	0.0553 (6)
H5	0.2189	0.3550	0.7429	0.066*
C6	0.35140 (17)	0.2379 (3)	0.74524 (18)	0.0500 (6)
H6	0.3745	0.2452	0.8171	0.060*
N2	0.56177 (17)	0.6596 (2)	0.76858 (16)	0.0603 (6)
C7	0.4596 (2)	0.5954 (3)	0.7160 (3)	0.0841 (10)
H7A	0.4096	0.6059	0.7621	0.101*
H7B	0.4682	0.4874	0.7039	0.101*
C8	0.4161 (3)	0.6719 (5)	0.6135 (3)	0.1167 (14)
H8A	0.4143	0.7803	0.6236	0.175*
H8B	0.3463	0.6353	0.5876	0.175*
H8C	0.4598	0.6488	0.5640	0.175*
C9	0.64448 (19)	0.6546 (3)	0.7037 (2)	0.0642 (8)
H9A	0.7086	0.6972	0.7439	0.077*
H9B	0.6229	0.7188	0.6428	0.077*
C10	0.6674 (2)	0.4968 (3)	0.6677 (3)	0.0821 (9)
H10A	0.6866	0.4312	0.7272	0.123*

H10B	0.7241	0.5018	0.6302	0.123*
H10C	0.6061	0.4570	0.6227	0.123*
C11	0.5883 (3)	0.5882 (3)	0.8744 (3)	0.1043 (13)
H11A	0.5261	0.5885	0.9053	0.125*
H11B	0.6078	0.4827	0.8666	0.125*
C12	0.6733 (3)	0.6642 (5)	0.9464 (3)	0.1266 (7)
H12A	0.7381	0.6491	0.9228	0.190*
H12B	0.6788	0.6218	1.0151	0.190*
H12C	0.6588	0.7714	0.9484	0.190*
H1A	0.0925 (9)	0.4126 (17)	0.5859 (7)	0.072 (8)*
H1B	0.1053 (16)	0.360 (3)	0.4789 (5)	0.089 (9)*
H2A	0.5441 (14)	0.7566 (10)	0.7800 (17)	0.063 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0478 (3)	0.0379 (3)	0.0537 (3)	−0.0020 (2)	0.0074 (2)	0.0007 (3)
O1	0.0679 (10)	0.0462 (9)	0.0846 (12)	−0.0089 (8)	−0.0168 (9)	−0.0054 (9)
O2	0.0696 (9)	0.0404 (8)	0.0711 (10)	0.0057 (8)	0.0185 (8)	0.0104 (8)
O3	0.0567 (9)	0.0946 (13)	0.0660 (10)	0.0160 (9)	0.0226 (8)	−0.0002 (10)
N1	0.0629 (13)	0.159 (3)	0.0639 (14)	0.0444 (15)	0.0111 (11)	0.0076 (16)
C1	0.0452 (11)	0.0350 (11)	0.0460 (11)	−0.0065 (9)	0.0120 (9)	−0.0001 (9)
C2	0.0522 (12)	0.0486 (12)	0.0479 (12)	−0.0010 (10)	0.0168 (10)	−0.0030 (11)
C3	0.0544 (12)	0.0726 (16)	0.0413 (12)	−0.0036 (12)	0.0094 (10)	−0.0015 (12)
C4	0.0439 (11)	0.0642 (15)	0.0577 (14)	0.0018 (11)	0.0105 (10)	0.0094 (12)
C5	0.0516 (12)	0.0622 (14)	0.0557 (13)	0.0019 (11)	0.0194 (10)	−0.0042 (12)
C6	0.0552 (12)	0.0505 (13)	0.0449 (12)	−0.0002 (11)	0.0112 (10)	−0.0034 (11)
N2	0.0832 (13)	0.0315 (10)	0.0681 (13)	0.0003 (10)	0.0191 (11)	−0.0016 (10)
C7	0.0700 (16)	0.0589 (16)	0.133 (2)	−0.0122 (14)	0.0426 (16)	−0.0206 (17)
C8	0.083 (2)	0.126 (3)	0.128 (3)	−0.006 (2)	−0.013 (2)	−0.041 (3)
C9	0.0573 (13)	0.0461 (13)	0.0907 (18)	−0.0047 (11)	0.0178 (13)	−0.0009 (14)
C10	0.0773 (17)	0.0616 (17)	0.112 (2)	0.0043 (14)	0.0301 (16)	−0.0158 (17)
C11	0.167 (3)	0.0500 (16)	0.097 (2)	0.0111 (19)	0.026 (2)	0.0188 (17)
C12	0.1284 (9)	0.1245 (10)	0.1254 (10)	0.0019 (7)	0.0203 (7)	0.0000 (7)

Geometric parameters (Å, °)

S1—O3	1.4416 (18)	N2—H2A	0.901 (8)
S1—O1	1.4429 (17)	C7—C8	1.505 (4)
S1—O2	1.4653 (17)	C7—H7A	0.970
S1—C1	1.766 (2)	C7—H7B	0.970
N1—C4	1.360 (3)	C8—H8A	0.960
N1—H1A	0.883 (8)	C8—H8B	0.960
N1—H1B	0.889 (7)	C8—H8C	0.960
C1—C6	1.374 (3)	C9—C10	1.509 (3)
C1—C2	1.387 (3)	C9—H9A	0.970
C2—C3	1.371 (3)	C9—H9B	0.970
C2—H2	0.930	C10—H10A	0.960
C3—C4	1.403 (3)	C10—H10B	0.960

C3—H3	0.930	C10—H10C	0.960
C4—C5	1.396 (3)	C11—C12	1.466 (5)
C5—C6	1.369 (3)	C11—H11A	0.970
C5—H5	0.930	C11—H11B	0.970
C6—H6	0.930	C12—H12A	0.960
N2—C7	1.484 (3)	C12—H12B	0.960
N2—C9	1.491 (3)	C12—H12C	0.960
N2—C11	1.494 (4)		
O3—S1—O1	114.48 (12)	C8—C7—H7A	109.0
O3—S1—O2	111.54 (11)	N2—C7—H7B	109.0
O1—S1—O2	110.59 (11)	C8—C7—H7B	109.0
O3—S1—C1	107.70 (10)	H7A—C7—H7B	107.8
O1—S1—C1	106.05 (10)	C7—C8—H8A	109.5
O2—S1—C1	105.92 (10)	C7—C8—H8B	109.5
C4—N1—H1A	119.4 (8)	H8A—C8—H8B	109.5
C4—N1—H1B	122.9 (13)	C7—C8—H8C	109.5
H1A—N1—H1B	116.8 (13)	H8A—C8—H8C	109.5
C6—C1—C2	118.42 (19)	H8B—C8—H8C	109.5
C6—C1—S1	120.70 (16)	N2—C9—C10	114.2 (2)
C2—C1—S1	120.87 (17)	N2—C9—H9A	108.7
C3—C2—C1	120.5 (2)	C10—C9—H9A	108.7
C3—C2—H2	119.8	N2—C9—H9B	108.7
C1—C2—H2	119.8	C10—C9—H9B	108.7
C2—C3—C4	121.3 (2)	H9A—C9—H9B	107.6
C2—C3—H3	119.3	C9—C10—H10A	109.5
C4—C3—H3	119.3	C9—C10—H10B	109.5
N1—C4—C5	121.6 (2)	H10A—C10—H10B	109.5
N1—C4—C3	121.1 (2)	C9—C10—H10C	109.5
C5—C4—C3	117.4 (2)	H10A—C10—H10C	109.5
C6—C5—C4	120.5 (2)	H10B—C10—H10C	109.5
C6—C5—H5	119.8	C12—C11—N2	114.4 (3)
C4—C5—H5	119.8	C12—C11—H11A	108.7
C5—C6—C1	121.9 (2)	N2—C11—H11A	108.7
C5—C6—H6	119.0	C12—C11—H11B	108.7
C1—C6—H6	119.0	N2—C11—H11B	108.7
C7—N2—C9	114.0 (2)	H11A—C11—H11B	107.6
C7—N2—C11	107.2 (2)	C11—C12—H12A	109.5
C9—N2—C11	116.6 (2)	C11—C12—H12B	109.5
C7—N2—H2A	101.6 (12)	H12A—C12—H12B	109.5
C9—N2—H2A	110.8 (13)	C11—C12—H12C	109.5
C11—N2—H2A	105.3 (15)	H12A—C12—H12C	109.5
N2—C7—C8	113.1 (3)	H12B—C12—H12C	109.5
N2—C7—H7A	109.0		
O3—S1—C1—C6	−170.54 (18)	N1—C4—C5—C6	−179.9 (3)
O1—S1—C1—C6	−47.6 (2)	C3—C4—C5—C6	1.1 (4)
O2—S1—C1—C6	70.00 (19)	C4—C5—C6—C1	0.7 (4)
O3—S1—C1—C2	8.8 (2)	C2—C1—C6—C5	−1.7 (3)
O1—S1—C1—C2	131.77 (19)	S1—C1—C6—C5	177.65 (18)

O2—S1—C1—C2	−110.67 (19)	C9—N2—C7—C8	−56.8 (3)
C6—C1—C2—C3	0.9 (3)	C11—N2—C7—C8	172.6 (3)
S1—C1—C2—C3	−178.47 (18)	C7—N2—C9—C10	−57.7 (3)
C1—C2—C3—C4	1.0 (4)	C11—N2—C9—C10	68.1 (3)
C2—C3—C4—N1	179.1 (3)	C7—N2—C11—C12	−166.1 (3)
C2—C3—C4—C5	−1.9 (4)	C9—N2—C11—C12	64.8 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2^{i}	0.883 (8)	2.137 (9)	2.970 (3)	157.0 (15)
N1—H1B···O1^{ii}	0.889 (7)	2.229 (8)	3.078 (3)	159.5 (18)
N2—H2A···O2^{iii}	0.901 (8)	1.852 (9)	2.752 (2)	178 (2)
N2—H2A···S1^{iii}	0.901 (8)	2.910 (10)	3.750 (2)	155.8 (18)

Symmetry codes: (i) −*x*+1/2, *y*+1/2, −*z*+3/2; (ii) *x*−1/2, −*y*+1/2, *z*−1/2; (iii) *x*, *y*+1, *z*.

Fig. 1

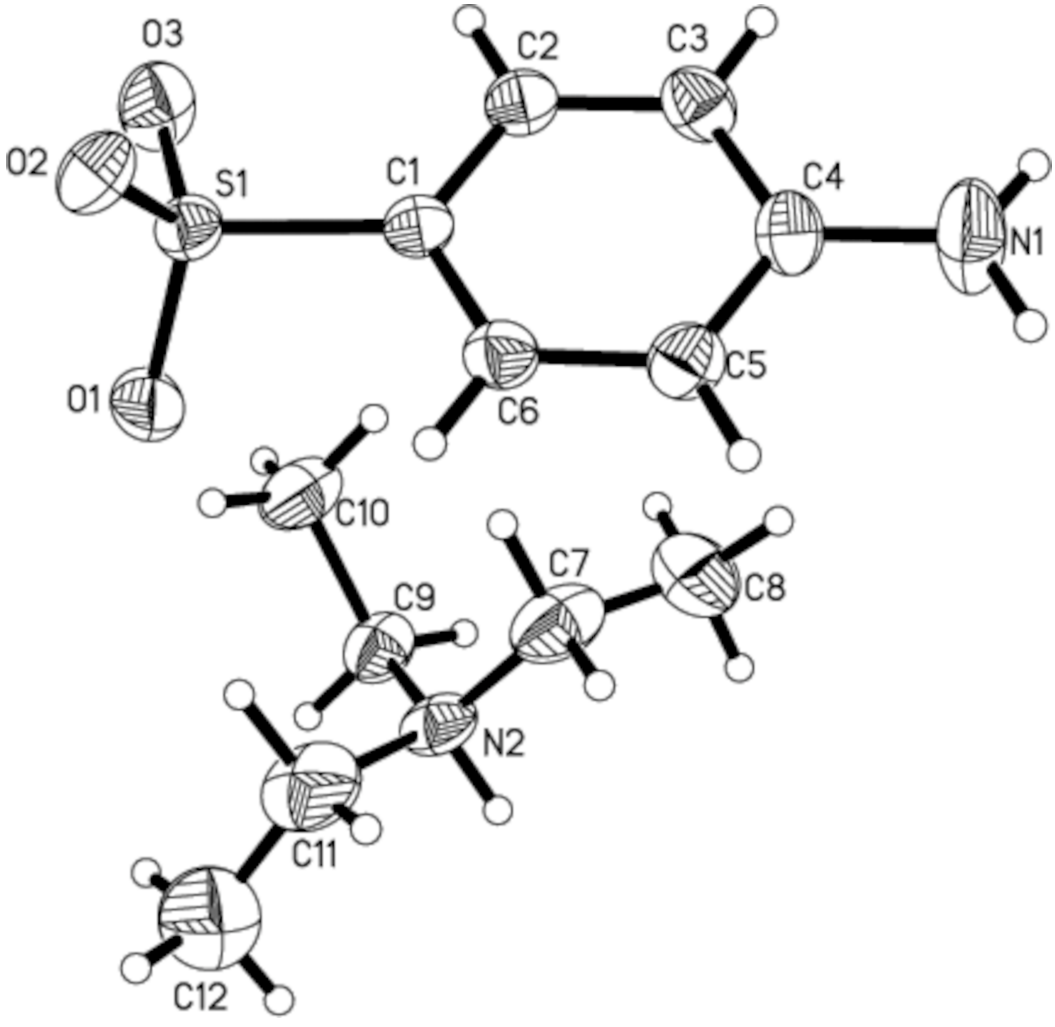

Fig. 2