organic compounds

Ammonium 4-methoxybenzenesulfonate

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The molecular structure of the title compound, $NH_4^+ \cdot C_7H_7O_4S^-$, is featureless [the methoxy C atom deviating 0.173 (6) Å from the phenyl mean plane] with interatomic distances and angles in the expected ranges. The main feature of interest is the packing mode. Hydrophilic (SO_3 and NH_4) and hydrophobic ($PhOCH_3$) parts in the structure segregate, the former interacting through a dense hydrogen-bonding scheme, leading to a well connected two-dimensional structure parallel to (100) and the latter hydrophobic groups acting as spacers for an interplanar separation of c/2 = 10.205 (2) Å. In spite of being aligned along [110], the benzene rings stack in a far from parallel fashion [viz. consecutive ring centers determine a broken line with a 164.72 (12)° zigzag angle], thus preventing any possible π–π interaction.

Related literature

For literature on the role of weak interactions in supramolecular structures, see: Desiraju (2007). For related structures, see: Fewings et al. (2001); Wang et al. (2007). For the Cambridge Structural Database, see: Allen (2002). For the synthesis, see: Porcheddu et al. (2009).

· NH_4^+
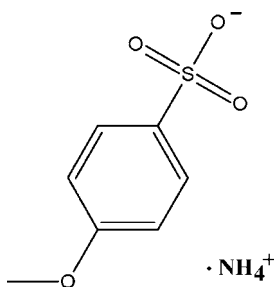
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Experimental

Crystal data

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$N\cdots$O1^i	0.88 (2)	1.99 (2)	2.851 (3)	170 (3)
N1—H4$N\cdots$O2^{ii}	0.86 (2)	1.98 (2)	2.797 (3)	160 (3)
N1—H2$N\cdots$O3^{iii}	0.88 (2)	1.98 (2)	2.824 (3)	162 (3)
N1—H3$N\cdots$O3	0.87 (2)	2.04 (2)	2.890 (3)	164 (3)

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

Data collection: CrysAlis PRO (Oxford Diffraction, 2009); cell refinement: CrysAlis PRO; data reduction: CrysAlis PRO; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2074).

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supporting information

Ammonium 4-methoxybenzenesulfonate

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S1. Comment

The study of supramolecular systems determined by weak interactions such as hydrogen bonding, π-π stacking or dipole-dipole interactions have been, and currently are, active fields of structural research due to their implications in crystal engineering, self-assembly and, above all, biological systems (Desiraju, 2007). Derivatives of the benzenesulfonate anion are extremely suited to this end due to the possibility of π-interactions between arene rings, as well as hydrogen bonding between the sulphonate groups and any H donor eventualy available (Water, ammonium, *etc*). With this latter NH_4 partner a number a structures of the sort have been published (among many others, ammonium *p*-toluenesulfonate, Fewings *et al.*, 2001, (II); ammonium 4-hydroxybenzenesulfonate, Wang *et al.*, 2007, (III), *etc*), the vast majority displaying, as expected, an extremely complex non-bonding interactions scheme. We present herein one further member in this family, ammonium 4-methoxybenzenesulfonate, $C_7H_7O_4S.H_4N$ (I), which ended up being isotructural to (II) but different from (III), in spite of the very similar formulations.

   The molecular structure in (I) (Fig 1) is featureless, with interatomic bond and angles in the expected ranges, and its main interest resides in the packing mode. Hydrophilic (SO_3, NH_4) and hydrophobic ($PhOCH_3$) parts in the structure segregate, the former one interacting through a dense H-bonding scheme (Table 1) leading to a well connected two-dimensional structure, parallell to (100) (Fig 2a) and the latter hydrophobic groups acting as spacers (Figs 2 b, 2c), for an interplanar separation of C/2 = 10.205 (2) Å. In spite of the deceiving views in Figs 2 b/2c, Ph groups stack in a far from paralell fashion, defining dihedral angles of 37° and thus preventing any possible π–π interaction.

S2. Experimental

The title compound was obtained as a byproduct in the synthesis of *N*-hydroxy-4-methoxybenzenesulfonamide, following the procedure described in Porcheddu *et al.*, 2009. A few light yellow crystals were obtained after evaporating an aceto-nitrile solution.

S3. Refinement

All H atoms were found in a difference map, though treated differently in refinement: C—H atoms were idealized and allowed to ride, with displacement parameters taken as $U_{iso}(H) = X \times U_{eq}(C)$ [$(C—H)_{methyl}$ = 0.96 A°, X = 1.5; $(C—H)_{arom}$ = 0.93 A°, X = 1.2] (CH_3 groups were also free to rotate as well). Ammonium H's were refined with restrained N—H = 0.85 (1) Å, H···H = 1.35 (2) Å distances and free isotropic displacement factors.
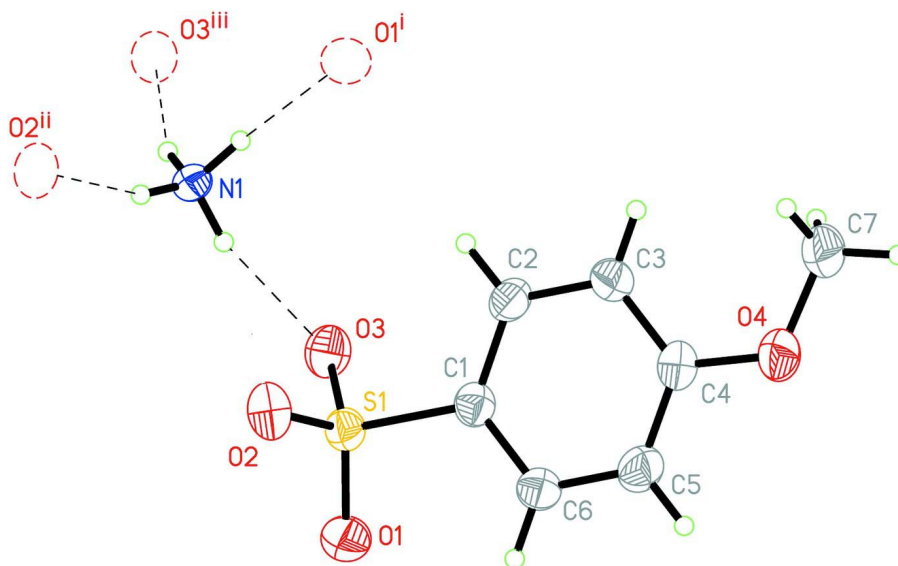
Figure 1

Ellipsoid plot of (I), drawn with displacement factors at a 50% probability level. Symmetry codes: (i) $x - 1$, y, z; (ii) $x - 1/2$, $-y + 1/2$, $-z + 1$; (iii) $x - 1/2$, $-y + 3/2$, $-z + 1$.
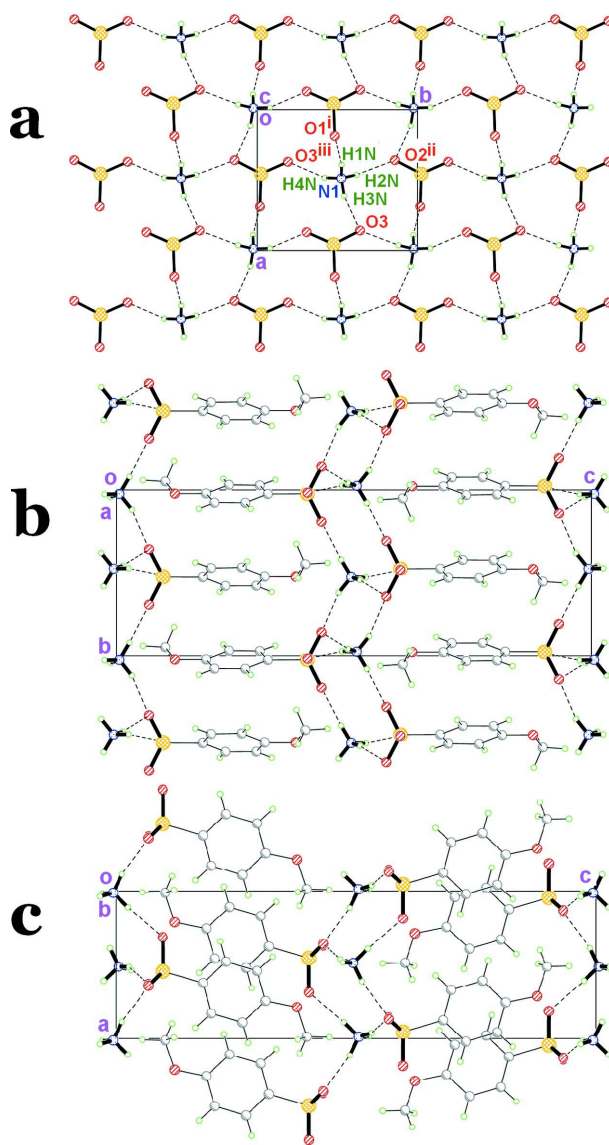
Figure 2

Packing views of (I). a) Projection paralell to (001) showing the hydrophilic part only and the H-bonding interactions taking place therein. Symmetry codes: as in Fig 1. b) A packing view with the whole structure, projected down [100]. Hydrophilic/hydrophobic parts (seen in projection) drawn in heavy/weak lining, respectively. c) Same as b) viewed along [010].

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Crystal data

$NH_4^+ \cdot C_7H_7O_4S^-$	$V = 912.4\,(2)$ Å³
$M_r = 205.23$	$Z = 4$
Orthorhombic, $P2_12_12_1$	$F(000) = 432$
Hall symbol: P 2ac 2ab	$D_x = 1.494$ Mg m⁻³
$a = 6.2664\,(12)$ Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 7.1342\,(12)$ Å	Cell parameters from 2823 reflections
$c = 20.410\,(2)$ Å	$\theta = 2.1–25.9°$

$\mu = 0.34$ mm^{-1}
$T = 298$ K

Blocks, yellow
$0.20 \times 0.10 \times 0.10$ mm

Data collection

Oxford Diffraction Gemini CCD S Ultra diffractometer	1732 independent reflections
Graphite monochromator	1548 reflections with $I > 2\sigma(I)$
ω scans, thick slices	$R_{int} = 0.050$
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)	$\theta_{max} = 26.2°$, $\theta_{min} = 2.0°$
	$h = -7 \rightarrow 6$
	$k = -8 \rightarrow 8$
$T_{min} = 0.958$, $T_{max} = 0.965$	$l = -20 \rightarrow 25$
4265 measured reflections	

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
$R[F^2 > 2\sigma(F^2)] = 0.042$	
$wR(F^2) = 0.119$	$w = 1/[\sigma^2(F_o^2) + (0.0842P)^2]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
1732 reflections	$(\Delta/\sigma)_{max} < 0.001$
135 parameters	$\Delta\rho_{max} = 0.47$ e Å^{-3}
21 restraints	$\Delta\rho_{min} = -0.36$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 637 Friedel pairs
Secondary atom site location: difference Fourier map	Absolute structure parameter: −0.11 (14)

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.

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

	x	y	z	$U_{iso}*/U_{eq}$
S1	0.95549 (11)	0.47643 (10)	0.59811 (3)	0.0305 (2)
O1	1.1864 (3)	0.4832 (4)	0.59781 (11)	0.0483 (6)
O2	0.8694 (4)	0.3085 (3)	0.56840 (11)	0.0422 (6)
O3	0.8578 (4)	0.6413 (3)	0.56824 (11)	0.0379 (6)
O4	0.7122 (4)	0.4778 (4)	0.87726 (9)	0.0426 (6)
C1	0.8765 (4)	0.4753 (4)	0.68155 (13)	0.0295 (6)
C2	0.6702 (4)	0.5282 (5)	0.69849 (13)	0.0324 (6)
H2	0.5734	0.5616	0.6660	0.039*
C3	0.6087 (4)	0.5311 (5)	0.76355 (13)	0.0338 (6)
H3	0.4713	0.5677	0.7751	0.041*
C4	0.7550 (5)	0.4783 (4)	0.81175 (13)	0.0324 (6)
C5	0.9583 (6)	0.4232 (4)	0.79423 (15)	0.0375 (7)
H5	1.0544	0.3863	0.8265	0.045*
C6	1.0207 (5)	0.4223 (4)	0.72898 (14)	0.0335 (6)
H6	1.1583	0.3864	0.7174	0.040*
C7	0.5125 (6)	0.5513 (6)	0.89746 (15)	0.0498 (8)

H7A	0.5091	0.5598	0.9444	0.075*
H7B	0.4001	0.4700	0.8828	0.075*
H7C	0.4931	0.6737	0.8789	0.075*
N1	0.4879 (3)	0.5244 (3)	0.49420 (10)	0.0264 (5)
H1N	0.391 (3)	0.526 (4)	0.5251 (9)	0.034 (8)*
H2N	0.463 (5)	0.619 (3)	0.4678 (12)	0.068 (13)*
H3N	0.612 (3)	0.542 (5)	0.5125 (10)	0.039 (9)*
H4N	0.484 (5)	0.421 (3)	0.4729 (13)	0.069 (14)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0297 (3)	0.0358 (3)	0.0261 (3)	−0.0015 (3)	0.0015 (3)	−0.0013 (3)
O1	0.0310 (11)	0.0745 (17)	0.0394 (12)	0.0018 (12)	0.0032 (9)	−0.0021 (15)
O2	0.0533 (16)	0.0399 (12)	0.0336 (12)	−0.0030 (10)	0.0042 (12)	−0.0044 (10)
O3	0.0454 (13)	0.0370 (11)	0.0313 (12)	−0.0024 (10)	−0.0004 (11)	0.0042 (10)
O4	0.0491 (12)	0.0521 (13)	0.0265 (10)	0.0068 (12)	−0.0010 (9)	0.0003 (11)
C1	0.0305 (12)	0.0307 (13)	0.0273 (13)	−0.0035 (12)	0.0009 (11)	−0.0001 (12)
C2	0.0300 (13)	0.0393 (14)	0.0279 (13)	−0.0026 (13)	−0.0045 (11)	0.0008 (14)
C3	0.0286 (13)	0.0402 (15)	0.0327 (14)	0.0001 (12)	0.0023 (11)	−0.0037 (14)
C4	0.0390 (14)	0.0313 (13)	0.0268 (13)	−0.0036 (13)	−0.0006 (11)	−0.0015 (13)
C5	0.0416 (16)	0.0377 (15)	0.0331 (15)	0.0081 (14)	−0.0069 (14)	0.0024 (12)
C6	0.0331 (15)	0.0333 (13)	0.0342 (14)	0.0060 (12)	−0.0021 (12)	−0.0019 (11)
C7	0.0438 (17)	0.076 (2)	0.0292 (15)	−0.0005 (18)	0.0048 (14)	−0.0050 (17)
N1	0.0247 (10)	0.0303 (10)	0.0241 (10)	0.0038 (9)	−0.0026 (9)	0.0019 (10)

Geometric parameters (Å, º)

S1—O2	1.447 (2)	C4—C5	1.380 (4)
S1—O1	1.448 (2)	C5—C6	1.388 (4)
S1—O3	1.459 (2)	C5—H5	0.9300
S1—C1	1.773 (3)	C6—H6	0.9300
O4—C4	1.364 (3)	C7—H7A	0.9600
O4—C7	1.418 (4)	C7—H7B	0.9600
C1—C6	1.377 (4)	C7—H7C	0.9600
C1—C2	1.390 (4)	N1—H1N	0.876 (15)
C2—C3	1.383 (4)	N1—H2N	0.877 (16)
C2—H2	0.9300	N1—H3N	0.873 (16)
C3—C4	1.396 (4)	N1—H4N	0.858 (16)
C3—H3	0.9300		
O2—S1—O1	113.48 (17)	C4—C5—C6	120.7 (3)
O2—S1—O3	109.62 (13)	C4—C5—H5	119.7
O1—S1—O3	112.99 (16)	C6—C5—H5	119.7
O2—S1—C1	107.15 (14)	C1—C6—C5	119.2 (3)
O1—S1—C1	106.45 (13)	C1—C6—H6	120.4
O3—S1—C1	106.71 (14)	C5—C6—H6	120.4
C4—O4—C7	117.2 (2)	O4—C7—H7A	109.5

C6—C1—C2	120.6 (3)	O4—C7—H7B	109.5
C6—C1—S1	119.6 (2)	H7A—C7—H7B	109.5
C2—C1—S1	119.8 (2)	O4—C7—H7C	109.5
C3—C2—C1	120.1 (3)	H7A—C7—H7C	109.5
C3—C2—H2	119.9	H7B—C7—H7C	109.5
C1—C2—H2	119.9	H1N—N1—H2N	108 (3)
C2—C3—C4	119.3 (3)	H1N—N1—H3N	108 (3)
C2—C3—H3	120.4	H2N—N1—H3N	108 (3)
C4—C3—H3	120.4	H1N—N1—H4N	111 (3)
O4—C4—C5	115.8 (3)	H2N—N1—H4N	110 (3)
O4—C4—C3	124.2 (3)	H3N—N1—H4N	111 (3)
C5—C4—C3	120.0 (3)		

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O1^i	0.88 (2)	1.99 (2)	2.851 (3)	170 (3)
N1—H4*N*···O2^{ii}	0.86 (2)	1.98 (2)	2.797 (3)	160 (3)
N1—H2*N*···O3^{iii}	0.88 (2)	1.98 (2)	2.824 (3)	162 (3)
N1—H3*N*···O3	0.87 (2)	2.04 (2)	2.890 (3)	164 (3)

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