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# 3-Ammonio-4-methoxybenzenesulfonate

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**Key indicators**

Single-crystal X-ray study
*T* = 295 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.028
*wR* factor = 0.084
Data-to-parameter ratio = 11.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

3–Amino-4-methoxybenzenesulfonic acid exists in the solid state in the zwitterionic form as 3-ammonio-4-methoxybenzenesulfonate, $C_7H_9NO_4S$. The zwitterions are linked by the ammonium H atoms into a layer structure.

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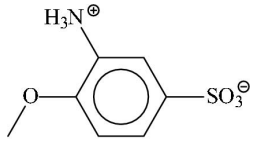
## Comment

3-Amino-4-hydroxybezenesulfonic acid, like a number of arenesulfonic acids, adopts a layer structure in which the aromatic rings stack into sheets; the sulfonate groups are located on the top and bottom of the layers (Gunderman & Squattrito, 1996). The title compound, (I), which has a methoxy substituent in place of the hydroxy substituent, also adopts a layer structure in which the zwitterions are linked to each other by hydrogen bonds (Fig. 1). The ammonium unit serves as the donor site for three hydrogen bonds; however, two of the three sulfonate O atoms are engaged in hydrogen bonding (Table 2). The negative charge appears to be delocalized over only two of the three O atoms, as the O atom that is not engaged in the interactions is nearest to the S atom.




(I)

## Experimental

The title compound was recovered unchanged in an unsuccessful reaction with calcium nitrate hexahydrate. The calcium salt (0.82 g, 3 mmol) was mixed with methoxybenzenesulfonic acid (1.22 g, 6 mmol) in water. Colorless prismatic crystals separated from the solution after several days. Analysis calculated for $C_7H_9NO_4S$: C 41.37, H 4.46, N 6.89%; found C 41.33, H 4.48, N 6.87%.

*Crystal data*

$C_7H_9NO_4S$
$M_r$ = 203.21
Triclinic, $P\overline{1}$
$a$ = 7.321 (2) Å
$b$ = 8.234 (2) Å
$c$ = 8.354 (2) Å
$\alpha$ = 62.05 (3)°
$\beta$ = 65.34 (3)°
$\gamma$ = 74.04 (3)°
$V$ = 402.3 (1) Å$^3$
$Z$ = 2
$D_x$ = 1.678 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 3869 reflections
$\theta$ = 3.1–27.5°
$\mu$ = 0.38 mm$^{-1}$
$T$ = 295 (2) K
Prism, colorless
0.34 × 0.26 × 0.19 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.810, $T_{max}$ = 0.931
3979 measured reflections
1830 independent reflections
1713 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.011
$\theta_{max}$ = 27.5°
$h = -9 \rightarrow 8$
$k = -10 \rightarrow 10$
$l = -10 \rightarrow 10$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.084
$S$ = 1.04
1830 reflections
154 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 0.1821P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| S1—O1 | 1.465 (1) | O4—C4 | 1.354 (2) |
| S1—O2 | 1.464 (1) | O4—C7 | 1.434 (2) |
| S1—O3 | 1.445 (1) | N1—C3 | 1.457 (2) |
| S1—C1 | 1.771 (2) | | |
| O1—S1—O2 | 111.1 (1) | C2—C1—C6 | 120.4 (1) |
| O1—S1—O3 | 114.4 (1) | C2—C1—S1 | 120.0 (1) |
| O2—S1—O3 | 112.6 (1) | C6—C1—S1 | 119.5 (1) |
| C1—S1—O1 | 105.0 (1) | C2—C3—N1 | 120.4 (1) |
| C1—S1—O2 | 105.4 (1) | C4—C3—N1 | 117.9 (1) |
| C1—S1—O3 | 107.6 (1) | O4—C4—C5 | 125.9 (1) |
| C4—O4—C7 | 117.8 (1) | O4—C4—C3 | 115.1 (1) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*n*1···O1$^{i}$ | 0.86 (1) | 1.98 (1) | 2.829 (2) | 171 (2) |
| N1—H1*n*2···O2$^{ii}$ | 0.86 (1) | 1.93 (1) | 2.770 (2) | 169 (2) |
| N1—H1*n*3···O1$^{iii}$ | 0.86 (1) | 2.10 (1) | 2.878 (2) | 151 (2) |

Symmetry codes: (i) $x, 1+y, z-1$; (ii) $-x, 1-y, 1-z$; (iii) $1-x, 1-y, 1-z$.

All H atoms were refined with distance restraints of N—H = 0.85 (1) Å and C—H = 0.95 (1) Å.

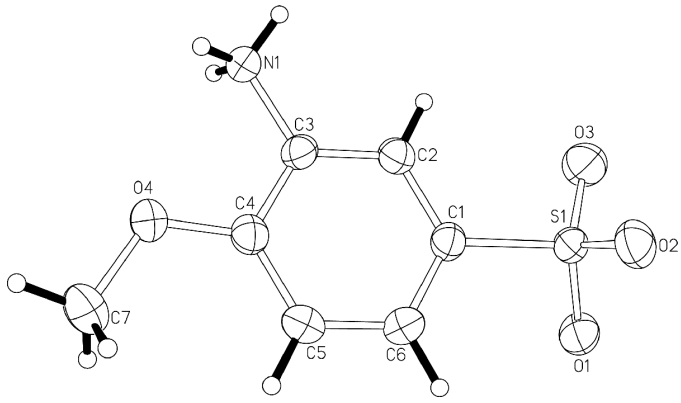



**Figure 1**
*ORTEPII* (Johnson, 1976) plot of (I). Displacement ellipsoids are drawn at the 70% probability level and H atoms are drawn as spheres of arbitrary radii.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO;* data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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## References

Gunderman, B. J. & Squattrito, P. J. (1996). *Acta Cryst.* C**52**, 940–942.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.