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# Ammonium 4-hydroxybenzenesulfonate

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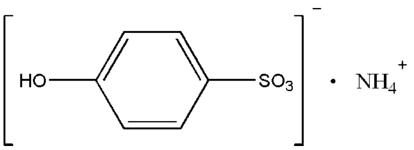
Key indicators: single-crystal X-ray study; $T$ = 223 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.031; $wR$ factor = 0.085; data-to-parameter ratio = 12.3.

The title compound, $NH_4^+\cdot C_6H_5SO_4^-$, consists of a 4-hydroxybenzenesulfonate anion and an ammonium cation which are linked together through O—H···O and N—H···O hydrogen bonds, resulting in the formation of an intricate three-dimensional hydrogen-bond network.

## Related literature

For related literature, see: Bu *et al.* (2000); Chen *et al.* (2004); Gunderman *et al.* (1997); Jin *et al.* (2004); Kosnic *et al.* (1992); Francis *et al.* (2003); Rombke *et al.* (2003); Schreuer (1999); Sharma *et al.* (2005); Yang & Chen (2003).



## Experimental

### *Crystal data*

$NH_4^+\cdot C_6H_5O_4S^-$
$M_r$ = 191.21
Monoclinic, $P2_1/c$
$a$ = 10.227 (2) Å
$b$ = 7.1414 (13) Å
$c$ = 11.461 (2) Å
$\beta$ = 100.163 (4)°
$V$ = 823.9 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.37 mm$^{-1}$
$T$ = 223 (2) K
0.40 × 0.38 × 0.35 mm

### *Data collection*

Rigaku Mercury diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.863, $T_{max}$ = 0.879
7537 measured reflections
1498 independent reflections
1442 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.085
$S$ = 1.11
1498 reflections
122 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O3$^{i}$ | 0.82 | 1.89 | 2.6930 (17) | 164 |
| N1—H1$A$···O2$^{ii}$ | 0.849 (9) | 1.984 (10) | 2.829 (2) | 173 (2) |
| N1—H1$B$···O1$^{iii}$ | 0.848 (9) | 2.148 (10) | 2.977 (2) | 165.6 (17) |
| N1—H1$C$···O4 | 0.848 (9) | 2.075 (12) | 2.873 (2) | 156.6 (18) |
| N1—H1$C$···O3$^{iv}$ | 0.848 (9) | 2.630 (17) | 3.151 (2) | 120.9 (16) |
| N1—H1$D$···O3$^{v}$ | 0.834 (9) | 2.143 (10) | 2.952 (2) | 163.7 (18) |
| N1—H1$D$···O4$^{iv}$ | 0.834 (9) | 2.575 (18) | 3.009 (2) | 113.7 (15) |

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2207).

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# supplementary materials

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# Ammonium 4-hydroxybenzenesulfonate

**K.-W. Wang, W.-J. Feng, H.-Y. Li, L.-L. Ma and Z.-M. Jin**

## Comment

Hydroxybenzene sulfonic acid is a useful intermediate in dye stuff and chemical synthesis(Yang *et al.*, 2003). Many crystalline compounds of 4-hydroxybenzene sulfonic acid have been previously reported (Kosnic *et al.*, 1992; Bu *et al.*, 2000; Jin *et al.*, 2004). Moreover, there are numerous examples of metal benzenesulfonate molecular complexes (Schreuer, 1999; Rombke *et al.*, 2003).

The 4-hydroxybenzenesulfonate anion is linked to the ammonium cation by strong N—H···O hydrogen bond (Fig. 1, Table 1). The S—O distances are comparable to those previously reported for sulfonates (Gunderman *et al.*, 1997; Chen *et al.*, 2004; Sharma *et al.*, 2005).

The packing arrangement in the crystal structure is governed by the occurrence of strong O—H···O and N—H···O hydrogen bonds between anions and cations resulting in the formation of an intricated three dimensionnal hydrogen bond network (Table 1, Fig. 2). Moreover, weak slipped π-π stacking exists between symmetry related rings ($1 - x, -y, -z$) with a centroid to centroid distances of 3.621 (1)Å and an interplanar distance of 3.40 Å resulting in an offset angle of 20.1°. This π-π stackings further stabilize the structure.

## Experimental

4-hydroxybenzene sulfonic acid and famotidine in a 1:1 molar ratio were mixed and dissolved in sufficient acetone by heating to a temperature at which a clear solution resulted. Ammonium cations were split up from molecules of famotidine in the course. Thus crystals of (I) were formed by gradual evaporation of acetone over a period of three days at 298 K.

## Refinement

H atoms attaching to O and N atoms were deduced from difference Fourier maps, and incorporated in refinement freely. Others were placed in calculated positions and allowed to ride on their parent atoms at distances of 0.94Å for aromatic group, with $U_{iso}(H) = 1.2 U_{eq}(C)$.

## Figures

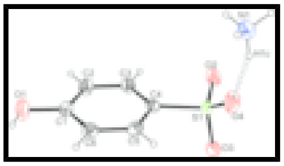

Fig. 1. The asymmetric unit of (I) with atom-labelling scheme. Ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii. Hydrogen bond is shown as dashed line.

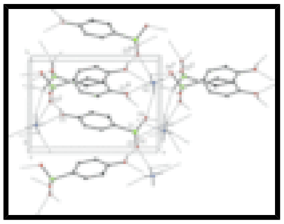

Fig. 2. Partial packing view showing the intricated hydrogen bonds network. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) 1 − *x*, 1/2 + *y*, 3/2 − *z*; (ii) 2 − *x*, 1 − *y*, 1 − *z*; (iii) 1 − *x*, 1 − *y*, 1 − *z*; (iv) *x*, 1 + *y*, *z*; (v) 2 − *x*, 1/2 + *y*, 3/2 − *z*].

## Ammonium 4-hydroxybenzenesulfonate

### *Crystal data*

| | |
|---|---|
| $NH_4^+\cdot C_6H_5O_4S^-$ | $F_{000} = 400$ |
| $M_r = 191.21$ | $D_x = 1.541$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>$\lambda = 0.71070$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 3236 reflections |
| $a = 10.227$ (2) Å | $\theta = 3.4$–$25.3$° |
| $b = 7.1414$ (13) Å | $\mu = 0.37$ mm$^{-1}$ |
| $c = 11.461$ (2) Å | $T = 223$ (2) K |
| $\beta = 100.163$ (4)° | Block, colourless |
| $V = 823.9$ (3) Å$^3$ | 0.40 × 0.38 × 0.35 mm |
| $Z = 4$ | |

### *Data collection*

| | |
|---|---|
| Rigaku Mercury diffractometer | $R_{int} = 0.020$ |
| Radiation source: fine-focus sealed tube | $\theta_{max} = 25.4$° |
| Monochromator: graphite | $\theta_{min} = 3.4$° |
| $T = 223(2)$ K | $h = -12\rightarrow12$ |
| ω scans | $k = -8\rightarrow8$ |
| Absorption correction: multi-scan (ABSCOR; Higashi, 1995) | $l = -13\rightarrow13$ |
| $T_{min} = 0.863$, $T_{max} = 0.879$ | Standard reflections: .; |
| 7537 measured reflections | every . reflections |
| 1498 independent reflections | intensity decay: . |
| 1442 reflections with $I > 2\sigma(I)$ | |

### *Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.031$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.085$ | $w = 1/[\sigma^2(F_o^2) + (0.0457P)^2 + 0.4222P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |

| | |
|---|---|
| $S = 1.11$ | $(\Delta/\sigma)_{\max} < 0.001$ |
| 1498 reflections | $\Delta\rho_{\max} = 0.27$ e Å$^{-3}$ |
| 122 parameters | $\Delta\rho_{\min} = -0.37$ e Å$^{-3}$ |
| 9 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

### *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* | $U_{\text{iso}}$*/$U_{\text{eq}}$ |
|---|---|---|---|---|
| S1 | 0.81650 (4) | 0.20307 (6) | 0.62303 (3) | 0.02096 (16) |
| O1 | 0.25361 (12) | 0.3946 (2) | 0.60586 (11) | 0.0341 (3) |
| H1 | 0.2415 | 0.4491 | 0.6660 | 0.051* |
| O2 | 0.82941 (12) | 0.1392 (2) | 0.50524 (11) | 0.0355 (3) |
| O3 | 0.83397 (12) | 0.04653 (17) | 0.70710 (11) | 0.0305 (3) |
| O4 | 0.90302 (12) | 0.35765 (19) | 0.66613 (12) | 0.0366 (3) |
| C1 | 0.38589 (16) | 0.3607 (2) | 0.61239 (14) | 0.0224 (4) |
| C2 | 0.42366 (17) | 0.2668 (2) | 0.51755 (15) | 0.0255 (4) |
| H2 | 0.3600 | 0.2316 | 0.4530 | 0.031* |
| C3 | 0.55608 (16) | 0.2257 (2) | 0.51934 (14) | 0.0230 (4) |
| H3 | 0.5815 | 0.1626 | 0.4560 | 0.028* |
| C4 | 0.65111 (16) | 0.2784 (2) | 0.61549 (14) | 0.0188 (3) |
| C5 | 0.61402 (17) | 0.3763 (2) | 0.70918 (14) | 0.0224 (4) |
| H5 | 0.6780 | 0.4140 | 0.7729 | 0.027* |
| C6 | 0.48144 (17) | 0.4175 (2) | 0.70732 (14) | 0.0231 (4) |
| H6 | 0.4563 | 0.4833 | 0.7698 | 0.028* |
| N1 | 0.95300 (15) | 0.7327 (2) | 0.59472 (14) | 0.0264 (3) |
| H1A | 1.0222 (13) | 0.765 (3) | 0.5683 (17) | 0.040* |
| H1B | 0.8939 (15) | 0.717 (3) | 0.5336 (12) | 0.040* |
| H1C | 0.959 (2) | 0.6279 (17) | 0.6300 (15) | 0.040* |
| H1D | 0.9321 (19) | 0.817 (2) | 0.6380 (14) | 0.040* |

### *Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0168 (2) | 0.0235 (3) | 0.0229 (3) | −0.00103 (15) | 0.00433 (16) | 0.00343 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1 | 0.0196 (6) | 0.0514 (9) | 0.0306 (7) | 0.0073 (6) | 0.0025 (5) | −0.0118 (6) |
| O2 | 0.0244 (7) | 0.0572 (9) | 0.0272 (7) | 0.0025 (6) | 0.0106 (5) | −0.0036 (6) |
| O3 | 0.0263 (7) | 0.0293 (7) | 0.0381 (7) | 0.0082 (5) | 0.0118 (5) | 0.0131 (5) |
| O4 | 0.0242 (7) | 0.0309 (7) | 0.0511 (8) | −0.0080 (5) | −0.0033 (6) | 0.0033 (6) |
| C1 | 0.0195 (8) | 0.0240 (8) | 0.0238 (8) | 0.0034 (6) | 0.0040 (6) | 0.0015 (7) |
| C2 | 0.0207 (9) | 0.0331 (9) | 0.0215 (8) | −0.0006 (7) | 0.0001 (7) | −0.0055 (7) |
| C3 | 0.0228 (9) | 0.0269 (9) | 0.0197 (8) | 0.0004 (7) | 0.0051 (7) | −0.0036 (7) |
| C4 | 0.0183 (8) | 0.0185 (8) | 0.0199 (8) | −0.0006 (6) | 0.0041 (6) | 0.0033 (6) |
| C5 | 0.0237 (8) | 0.0240 (8) | 0.0179 (8) | −0.0004 (7) | −0.0009 (6) | −0.0015 (6) |
| C6 | 0.0274 (9) | 0.0239 (8) | 0.0183 (8) | 0.0039 (7) | 0.0046 (6) | −0.0017 (6) |
| N1 | 0.0240 (8) | 0.0280 (8) | 0.0278 (8) | −0.0002 (6) | 0.0064 (6) | 0.0008 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—O4 | 1.4461 (13) | C3—C4 | 1.387 (2) |
| S1—O2 | 1.4528 (13) | C3—H3 | 0.9300 |
| S1—O3 | 1.4661 (12) | C4—C5 | 1.389 (2) |
| S1—C4 | 1.7624 (16) | C5—C6 | 1.384 (2) |
| O1—C1 | 1.363 (2) | C5—H5 | 0.9300 |
| O1—H1 | 0.8200 | C6—H6 | 0.9300 |
| C1—C6 | 1.388 (2) | N1—H1A | 0.849 (9) |
| C1—C2 | 1.389 (2) | N1—H1B | 0.848 (9) |
| C2—C3 | 1.382 (2) | N1—H1C | 0.848 (9) |
| C2—H2 | 0.9300 | N1—H1D | 0.834 (9) |
| O4—S1—O2 | 113.99 (8) | C3—C4—C5 | 120.15 (15) |
| O4—S1—O3 | 111.18 (8) | C3—C4—S1 | 119.22 (12) |
| O2—S1—O3 | 110.54 (8) | C5—C4—S1 | 120.42 (12) |
| O4—S1—C4 | 107.93 (8) | C6—C5—C4 | 119.70 (15) |
| O2—S1—C4 | 107.10 (7) | C6—C5—H5 | 120.1 |
| O3—S1—C4 | 105.63 (7) | C4—C5—H5 | 120.1 |
| C1—O1—H1 | 109.5 | C5—C6—C1 | 120.15 (15) |
| O1—C1—C6 | 123.06 (15) | C5—C6—H6 | 119.9 |
| O1—C1—C2 | 116.95 (15) | C1—C6—H6 | 119.9 |
| C6—C1—C2 | 119.99 (15) | H1A—N1—H1B | 105.1 (16) |
| C3—C2—C1 | 119.87 (15) | H1A—N1—H1C | 115 (2) |
| C3—C2—H2 | 120.1 | H1B—N1—H1C | 104.9 (16) |
| C1—C2—H2 | 120.1 | H1A—N1—H1D | 109.4 (16) |
| C2—C3—C4 | 120.11 (15) | H1B—N1—H1D | 111.5 (17) |
| C2—C3—H3 | 119.9 | H1C—N1—H1D | 111.2 (16) |
| C4—C3—H3 | 119.9 | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O3$^{i}$ | 0.82 | 1.89 | 2.6930 (17) | 164 |
| N1—H1A···O2$^{ii}$ | 0.849 (9) | 1.984 (10) | 2.829 (2) | 173 (2) |
| N1—H1B···O1$^{iii}$ | 0.848 (9) | 2.148 (10) | 2.977 (2) | 165.6 (17) |
| N1—H1C···O4 | 0.848 (9) | 2.075 (12) | 2.873 (2) | 156.6 (18) |

| | | | | |
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| N1—H1C···O3$^{iv}$ | 0.848 (9) | 2.630 (17) | 3.151 (2) | 120.9 (16) |
| N1—H1D···O3$^{v}$ | 0.834 (9) | 2.143 (10) | 2.952 (2) | 163.7 (18) |
| N1—H1D···O4$^{iv}$ | 0.834 (9) | 2.575 (18) | 3.009 (2) | 113.7 (15) |

Symmetry codes: (i) $-x+1, y+1/2, -z+3/2$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+2, y+1/2, -z+3/2$; (v) $x, y+1, z$.

**Fig. 1**

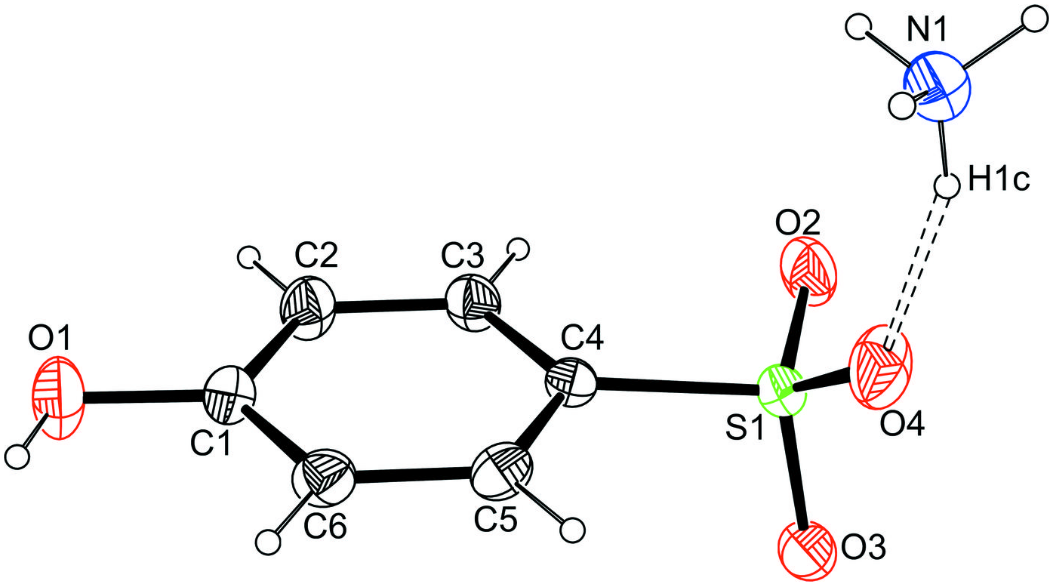

**Fig. 2**