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L-Phenylalaninium 4-sulfonate

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Key indicators

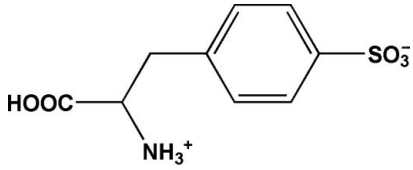
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.025
wR factor = 0.067
Data-to-parameter ratio = 15.4

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

In the crystal structure of the title compound (H_2SPA), $C_9H_{11}NO_5S$, hydrogen-bonding interactions lead to the formation of a three-dimensional network

Comment

Recently, both Werner (1991) and Escher *et al.* (1983) reported the synthesis and characterization of the ligand 4-sulfo-L-phenylalanine (H_2SPA). Xie *et al.* (2002) reported its crystal structure but involving a water solvent molecule. Here we report the crystal structure of 4-sulfo-L-phenylalanine in the zwitterionic form L-phenylalaninium 4-sulfonate, (I).



(I)

It is worth noting that the sulfonic acid H atom has moved to the amine group and this zwitterionic form of H_2SPA in acidic solution favors the structure proposed by Escher *et al.* (1983). Fig. 1 shows a perspective view of the structure, which crystallizes in the monoclinic space group $P2_1$. The asymmetric unit contains one molecule of (I).

Taking hydrogen bonding into account, H_2SPA forms a three-dimensional network. As shown in Table 2, the carboxylic acid group and the protoned amine group act as hydrogen-bond donors and sulfonate O atoms act as hydrogen-bond acceptors. Four types of hydrogen bonds are formed, and they can be divided into two groups: two strong hydrogen-bonding interactions [O5···O1 = 2.6438 (19) and N1···O1 = 2.7861 (19) Å] and two weak hydrogen-bonding

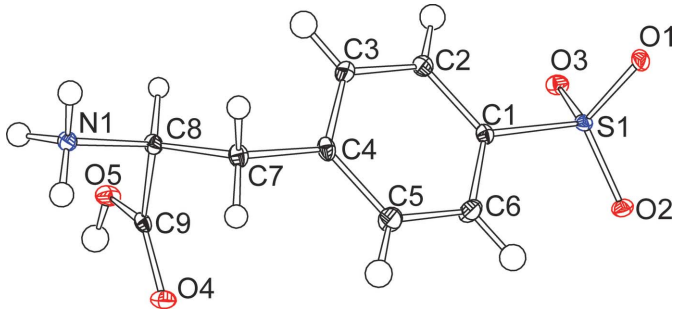


Figure 1
A view of (I) with 30% probability displacement ellipsoids; H atoms are shown as small spheres of arbitrary radii.

interactions [N1···O3 = 2.929 (2) and N1···O3 = 2.8607 (18) Å]. As shown in Fig. 2, a two-dimensional layer is formed by the two strong hydrogen-bonding interactions. The resulting layers are further linked by the two weak hydrogen-bonding interactions to complete the three-dimensional network.

Experimental

Crystals of (I) suitable for X-ray analysis were obtained from a 15 ml aqueous solution of 1 mmol 4-sulfo-L-phenylalanine powder.

Crystal data

$C_9H_{11}NO_5S$
M_r = 245.25
Monoclinic, $P2_1$
a = 5.6357 (16) Å
b = 9.177 (3) Å
c = 10.308 (3) Å
β = 98.950 (4)°
V = 526.6 (3) Å^3
Z = 2
D_x = 1.547 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 293 (2) K
Prism, white
0.30 × 0.15 × 0.08 mm

Data collection

Bruker CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan *CrystalClear* (Rigaku/MSC, 2004)
T_{min} = 0.945, T_{max} = 0.975
4021 measured reflections
2239 independent reflections
2195 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.067
S = 1.03
2239 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.0703P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Absolute structure: Flack (1983), 965 Friedel pairs
Flack parameter: −0.06 (6)

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.4397 (13)	S1—O1	1.4782 (12)
S1—O3	1.4632 (12)	S1—C1	1.7730 (16)
O2—S1—O3	113.64 (7)	O2—S1—C1	107.93 (7)
O2—S1—O1	112.72 (7)	O3—S1—C1	106.38 (7)
O3—S1—O1	110.31 (7)	O1—S1—C1	105.27 (7)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O1^{i}	0.82	1.82	2.6438 (19)	177
N1—H1A···O1^{ii}	0.89	1.91	2.7861 (19)	169
N1—H1B···O3^{iii}	0.89	2.09	2.929 (2)	157
N1—H1C···O3^{iv}	0.89	2.06	2.8607 (18)	149

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

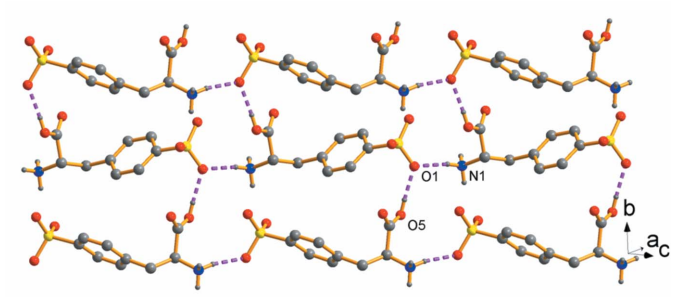


Figure 2
A view of the two-dimensional hydrogen-bonding network formed by two types of strong hydrogen bonds (dashed lines).

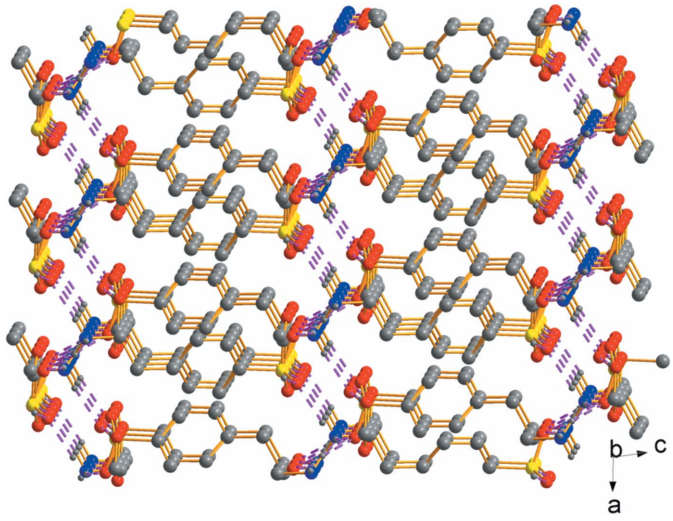


Figure 3
A view of the three-dimensional hydrogen-bonding (dashed lines) network.

All H atoms were placed at calculated positions and refined with isotropic displacement parameters, using a riding model [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C); N—H = 0.89 Å and U_{iso}(H) = 1.5U_{eq}(N); O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O)].

Data collection: *CrystalClear* (Rigaku/MSC, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Siemens, 1994); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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