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Ethylammonium saccharinate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.113
Data-to-parameter ratio = 16.4

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

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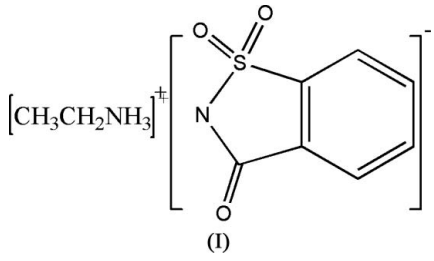
The asymmetric unit of the title compound, $C_2H_8N^+\cdot C_7H_4NO_3S^-$, contains a saccharinate anion and a protonated ethylamine cation. Intermolecular N—H···O hydrogen bonds link these ions into a two-dimensional framework structure. The crystal packing is further stabilized by weak intermolecular C—H···O hydrogen bonds

Comment

Our research groups are currently investigating supramolecular structures of cocrystals containing saccharin and various organic bases (Wang *et al.*, 2006*a*,*b*). We have attempted to find relationships between the crystal structure and type of organic base and solvents used in the synthesis, reaction temperature, reaction times and so on. Here we report the crystal structure of the title compound, (I).



(I)

The asymmetric unit of (I) contains an ethylammonium cation and a saccharinate anion (Fig. 1), both of which show normal values for bond lengths and angles (Wardell *et al.*, 2005). Intermolecular N—H···O hydrogen bonds (Table 1) link these ions into a two-dimensional framework. The crystal packing (Fig. 2) is further stabilized by weak intermolecular C—H···O hydrogen bonds (Table 1).

Experimental

All reagents were commercially available and of analytical grade. Saccharin (2.0 mmol, 0.376 g) was dissolved in 20 ml ethylamine. The mixture was stirred for 20 min at room temperature. The solution was filtered and the filtrate was kept at room temperature. Colourless prismatic crystals were obtained from the filtrate after 3 d.

Crystal data

$C_2H_8N^+\cdot C_7H_4NO_3S^-$
M_r = 228.27
Monoclinic, $P2_1/n$
a = 9.6355 (9) Å
b = 11.2251 (10) Å
c = 10.5563 (10) Å
β = 112.1380 (10)°
V = 1057.59 (17) Å^3
Z = 4
D_x = 1.434 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 292 (2) K
Prism, colourless
0.20 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.943, T_{max} = 0.944
5187 measured reflections
2276 independent reflections
2047 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.113
S = 1.06
2276 reflections
139 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0731P)^2 + 0.1108P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.039 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*C*···O1^{i}	0.89	2.39	3.0833 (18)	136
N2—H2*C*···O1^{ii}	0.89	2.30	3.0373 (18)	140
N2—H2*B*···O3^{iii}	0.89	1.90	2.7832 (17)	174
N2—H2*A*···O2^{iv}	0.89	2.01	2.8733 (19)	162
C2—H2···O3^{v}	0.93	2.55	3.383 (2)	150
C5—H5···O3^{vi}	0.93	2.50	3.415 (2)	168

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

All H atoms were placed in calculated position, with C—H = 0.93–0.97 Å and N—H = 0.89 Å, and were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(N).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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References

Bruker (2001). *SAINT-Plus* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

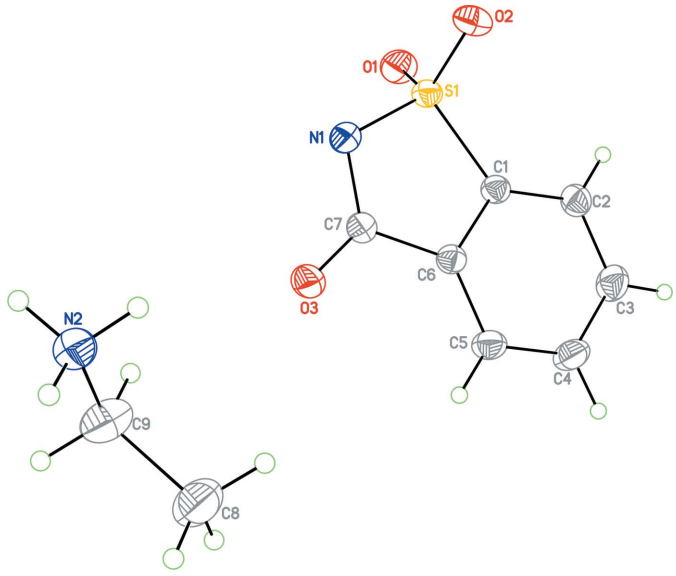

Figure 1
The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

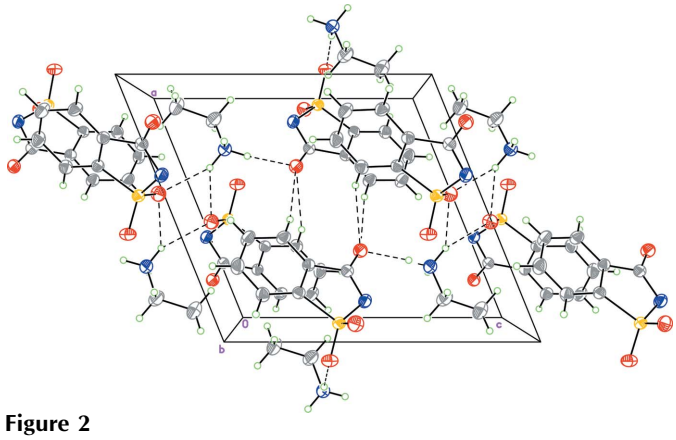

Figure 2
Perspective view of the crystal packing along the *b* axis, showing the linkage of the ions by hydrogen-bonding interactions (dashed lines).

Sheldrick, G. M. (2001). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Wang, Z.-L., Wei, L.-H., Li, M.-X. & Niu, J.-Y. (2006*a*). *Acta Cryst.* E**62**, o1058–o1059.
Wang, Z.-L., Wei, L.-H., Li, M.-X. & Niu, J.-Y. (2006*b*). *Acta Cryst.* E**62**, o1314–o1316.
Wardell, J. L., Low, J. N. & Glidewell, C. (2005). *Acta Cryst.* E**61**, o1944–o1946.