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Pyridinium saccharinate

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The asymmetric unit of the title compound, $C_5H_6N^+\cdot C_7H_4NO_3S^-$, consists of two saccharinate anions and two pyridinium cations. Intermolecular N—H···O hydrogen bonds link these ions into discrete assemblies. The crystal packing is further stabilized by π–π stacking interactions.

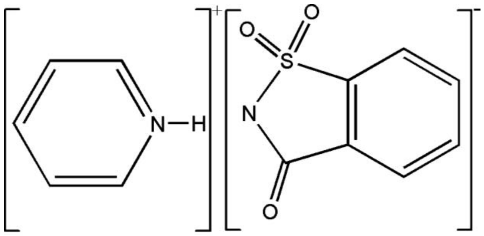
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.126
Data-to-parameter ratio = 14.0

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

Comment

Our research groups are currently investigating supramolecular structures of cocrystals containing saccharin and various organic bases. Recently, we have reported the crystal structures of ethylenediammonium, hexamethylenediammonium and ethylammonium saccharinates (Wang *et al.*, 2006*a*,*b*; Wang *et al.*, 2006). We are looking for a relation between the organic bases and solvents used in the synthesis and the crystal structures of the resulting salts. We report here the crystal structure of pyridinium saccharinate, (I).



(I)

The asymmetric unit of (I) contains two saccharinate anions and two pyridinium cations (Fig. 1). The anion geometry is similar to that observed in the earlier reported saccharinates (Wang *et al.*, 2006*a*,*b*; Wang *et al.*, 2006). The ions are linked together by intermolecular N—H···O hydrogen bonds into discrete assemblies (Table 1 and Fig. 2). Saccharinate anions and pyridinium ions form two symmetry-independent stacks running along the *a* axis, in which anions and cations alternate. The benzene ring C1–C6 is involved in π–π stacking interactions with the pyridine rings N2/C8–C12 generated by symmetry operations $(1 - x, 1 - y, -z)$ and $(x, 1 + y, z)$ and the distances between the benzene- and pyridine-ring centroids are 3.7929 (13) and 3.9774 (13) Å, respectively. In turn, the benzene ring C13–C18 interacts with the pyridinium units N4/C20–C24 at (x, y, z) and $(-1 + x, y, z)$, respectively, with a centroid-to-centroid distance of 3.7110 (13) Å (Fig. 2).

Experimental

All reagents were commercially available and of analytical grade. Saccharin (2.0 mmol, 0.376 g) was dissolved in pyridine (20 ml). The

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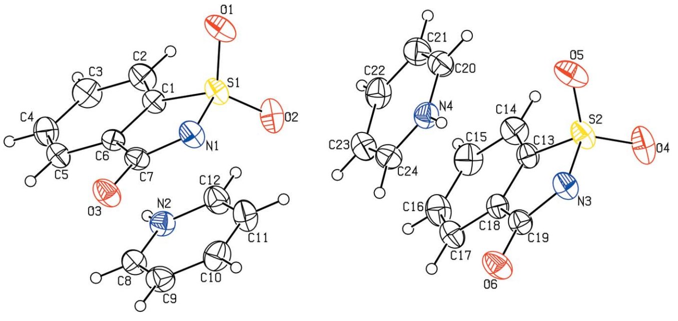

Figure 1
The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

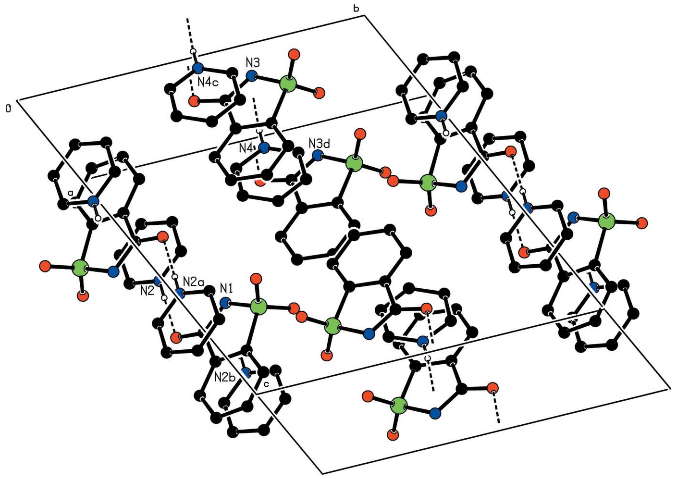

Figure 2
Perspective view of the crystal structure of (I), showing hydrogen-bond interactions (dashed lines) between ions. H atoms not involved in hydrogen bonding have been omitted for clarity.

mixture was stirred for 20 min at room temperature. The solution was filtered, and the filtrate was kept at room temperature. Colorless crystals were obtained from the filtrate after 5 d.

Crystal data

$C_5H_6N^+ \cdot C_7H_4NO_3S^-$
$M_r = 262.28$
Triclinic, $P\bar{1}$
$a = 7.4677$ (7) Å
$b = 12.9605$ (12) Å
$c = 14.1895$ (13) Å
$\alpha = 65.1760$ (10)°
$\beta = 74.752$ (2)°
$\gamma = 78.103$ (2)°
$V = 1195.35$ (19) Å^3
$Z = 4$
$D_x = 1.457$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.27$ mm^{-1}
$T = 292$ (2) K
Block, colorless
0.30 × 0.30 × 0.23 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\min} = 0.923$, $T_{\max} = 0.940$
12547 measured reflections
4678 independent reflections
3871 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.066$
$\theta_{\max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.126$
$S = 1.07$
4678 reflections
333 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0747P)^2 + 0.0707P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.33$ e Å^{-3}
$\Delta\rho_{\min} = -0.35$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1′···O3$^{\rm i}$	0.85 (1)	1.81 (1)	2.6522 (19)	172 (2)
N4—H2′···O6$^{\rm ii}$	0.86 (1)	1.78 (1)	2.641 (2)	176 (2)

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

All H atoms bonded to C atoms were placed in calculated position with C—H = 0.93 Å and were refined as riding with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. H atoms bonded to N atoms were located in difference maps and the N—H distances were restrained to 0.85 (9) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 2001); 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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