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2,6-Dimethylpyridinium saccharinate

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The asymmetric unit of the title compound, $C_7H_{10}N^+\cdot C_7H_4NO_3S^-$, is composed of one saccharinate anion and one 2,6-dimethylpyridinium cation. They are linked by an N—H···O hydrogen bond. Furthermore, π–π interactions are observed between saccharinate anions and 2,6-dimethylpyridinium cations.

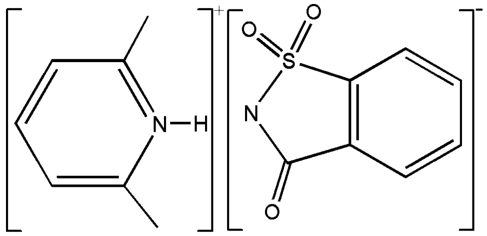
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.140
Data-to-parameter ratio = 14.6

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 the supramolecular structures of co-crystals containing saccharin and various organic bases (Wang *et al.*, 2006*a*, 2006*b*). We are attempting to establish the relationship between the crystal structures obtained and the type of organic base and solvents used in the synthesis, the reaction temperature, reaction times and so on. Here, we report the title salt, (I), of saccharin with the organic base 2,6-dimethylpyridine.



(I)

The asymmetric unit of (I) consists of one saccharinate anion and one protonated 2,6-dimethylpyridinium cation (Fig. 1). They are linked together by an N—H···O hydrogen bond (Table 1, Fig. 1). Moreover, π–π stacking interactions are observed between the C1–C6 rings at (x, y, z) and (x, $\frac{1}{2} - y$, $-\frac{1}{2} + z$) and the pyridinium rings at (x, y, z) and ($x, \frac{1}{2} - y, \frac{1}{2} + z$), with centroid-to-centroid distances of 3.6125 (13) and 3.9696 (14) Å, respectively (Fig. 2).

Experimental

All reagents were commercially available and of analytical grade. Saccharin (2.0 mmol, 0.376 g) was dissolved in 2,6-dimethylpyridine (20 ml) and the mixture was stirred for 20 min. The solution was filtered, and the filtrate was kept at room temperature. Colourless crystals of (I) were obtained from the filtrate after 6 d.

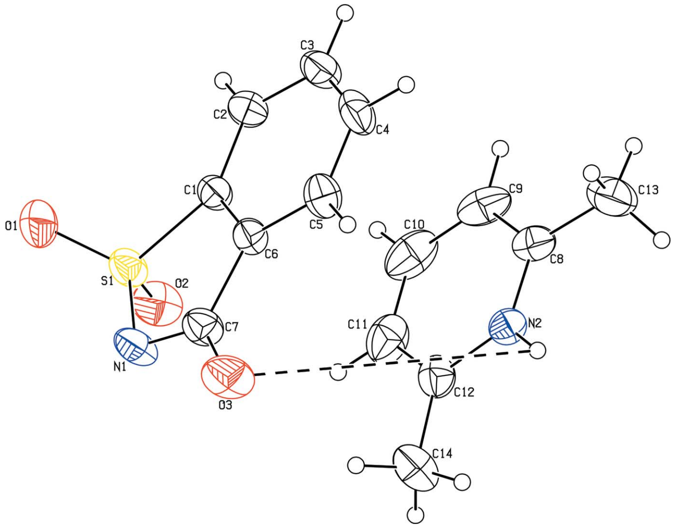


Figure 1
A drawing of the title molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The hydrogen bond is shown as a dashed line.

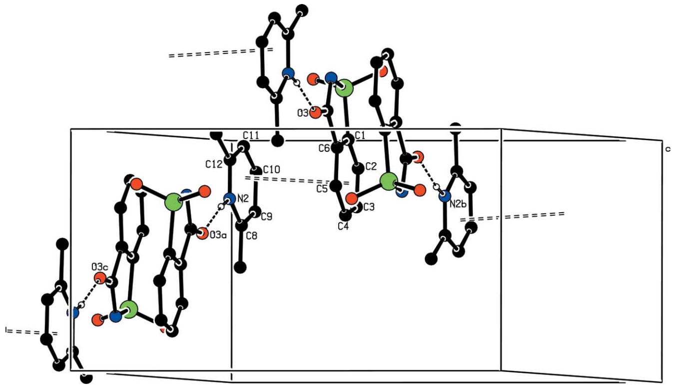


Figure 2
A packing diagram for (I). Hydrogen bonds and π–π stacking interactions are shown as dashed lines. H atoms not involved in the hydrogen bonding have been omitted for clarity [Symmetry codes: (a) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (b) $x, \frac{1}{2} - y, -\frac{1}{2} + z$; (c) $x, \frac{1}{2} - y, \frac{1}{2} + z$].

Crystal data

$C_7H_{10}N^+\cdot C_7H_4NO_3S^-$
$M_r = 290.33$
Monoclinic, $P2_1/c$
$a = 12.5366$ (18) Å
$b = 8.2522$ (11) Å
$c = 14.710$ (2) Å
$\beta = 113.674$ (2)°
$V = 1393.7$ (3) Å^3
$Z = 4$
$D_x = 1.384$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.24$ mm^{-1}
$T = 292$ (2) K
Block, colourless
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Thin–slice ω scans
Absorption correction: none
5910 measured reflections
2726 independent reflections
2093 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.067$
$\theta_{\rm max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.140$
$S = 1.04$
2726 reflections
187 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0826P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.29$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.23$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···O3	0.84 (1)	1.83 (1)	2.657 (2)	168 (2)

Atom H1 was located in a difference synthesis and refined isotropically [N—H = 0.84 (1) Å]. The remaining H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{\rm iso} = xU_{\rm eq}$(C), where $x = 1.5$ for methyl H and $x = 1.2$ for aromatic H.

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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