Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Methylpyridinium saccharinate

Zi-Liang Wang,[a]* Ming-Xue Li,[a] Lin-Heng Wei[b] and Jing-Ping Wang[a]

[a]Institute of Molecular and Crystal Engineering, College of Chemistry and Chemical Engineering, Henan University, Kaifeng 475001, People's Republic of China, and [b]College of Environment and Planning, Henan University, Kaifeng 475001, People's Republic of China

Correspondence e-mail: zlwang@henu.edu.cn

Received 19 April 2006
Accepted 1 May 2006

Key indicators

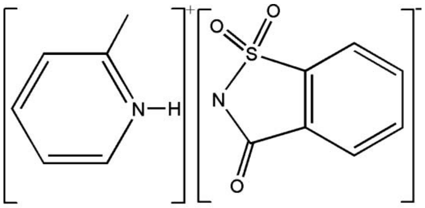
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.127
Data-to-parameter ratio = 16.2

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

The asymmetric unit of the title compound, $C_6H_8N^+\cdot C_7H_4NO_3S^-$, is composed of two saccharinate anions and two 2-methylpyridinium cations. These ions are linked into a supermolecular structure by intermolecular N—H···O hydrogen bonds. In addition, π–π interactions are observed between saccharinate anions and 2-methylpyridinium cations.

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 the relationships between the observed crystal structure and the type of organic base and solvents used in the synthesis, the reaction temperature, the reaction time, and so on. Here we report the title salt of saccharin, (I), incorporating the organic base 2-methylpyridine.


(I)

The asymmetric unit of (I) is composed of two saccharinate anions and two 2-methylpyridinium cations (Fig. 1). These ions are linked together by intermolecular N—H···O hydrogen bonds (Table 1). The crystal packing is further stabilized by π–π interactions between pyridinium and saccharinate ions (Fig. 2).

Experimental

All reagents were commercially available and of analytical grade. Saccharin (2.0 mmol, 0.376 g) was dissolved in 20 ml 2-methylpyridine and the 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

$C_6H_8N^+\cdot C_7H_4NO_3S^-$	$Z = 8$
$M_r = 276.31$	$D_x = 1.429$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 15.5187$ (13) Å	$\mu = 0.26$ mm^{-1}
$b = 10.6596$ (9) Å	$T = 292$ (2) K
$c = 16.2842$ (13) Å	Block, colorless
$\beta = 107.553$ (2)°	0.30 × 0.30 × 0.25 mm
$V = 2568.4$ (4) Å^3	

doi:10.1107/S1600536806016023

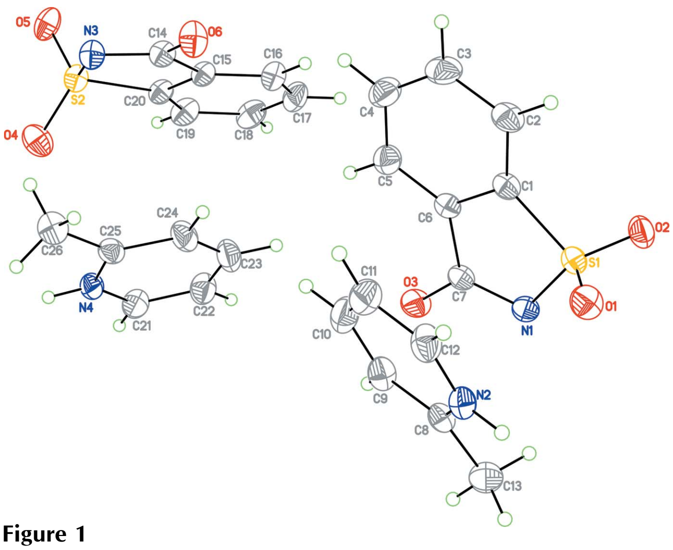


Figure 1
The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: none
15255 measured reflections
5598 independent reflections
4565 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.042$
$\theta_{\rm max} = 27.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.127$
$S = 1.05$
5598 reflections
345 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0792P)^2 + 0.0218P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.002$
$\Delta\rho_{\rm max} = 0.22$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.40$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2$A\cdots$O1$^{\rm i}$	0.86	1.79	2.6463 (18)	179
N4—H4$A\cdots$O4$^{\rm ii}$	0.86	1.78	2.6413 (18)	176

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

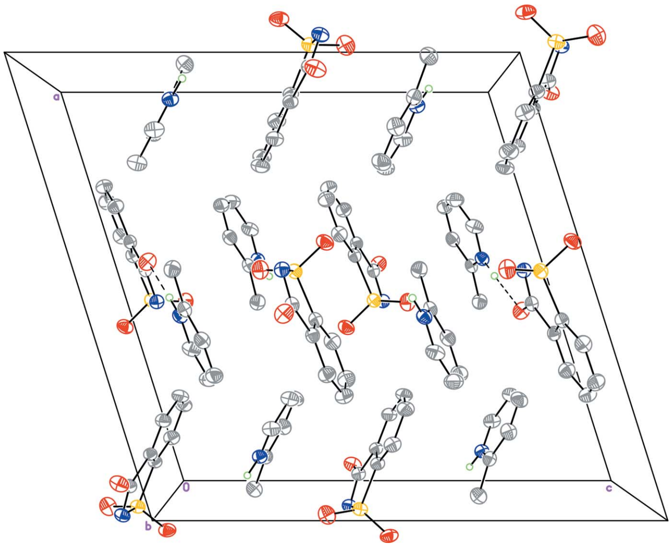


Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines. H atoms not involving hydrogen bonds have been omitted for clarity.

All H atoms were placed in calculated positions, with C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and N—H = 0.86Å, and were refined as riding, with $U_{\rm iso} = xU_{\rm eq}$(C), where $x = 1.5$ for methyl and $x = 1.2$ for aromatic H atoms, and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(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*.

This work was supported by the Basic Research Foundation for Natural Science of Henan University (No. 04YBRW053).

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.

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.