

De-Suo Yang

Department of Chemistry and Chemical
Engineering, Baoji College of Arts and Sciences,
Baoji 721007, People's Republic of ChinaCorrespondence e-mail:
desuoyang@yahoo.com.cn

Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.066
 wR factor = 0.198
Data-to-parameter ratio = 13.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Bis(pyridinium-4-olate) succinic acid

In the title compound, $2\text{C}_5\text{H}_5\text{NO}\cdot\text{C}_4\text{H}_6\text{O}_4$, a phenolic proton is transferred to the pyridine N atom, yielding a zwitterionic pyridinium-4-olate. The succinic acid molecule lies about a centre of symmetry which also generates the second pyridinium-4-olate molecule. The crystal structure is stabilized by intermolecular $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming a network structure.

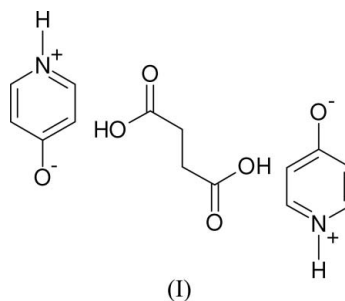
Received 13 December 2005

Accepted 19 December 2005

Online 23 December 2005

Comment

Proton transfer in molecular associations confers considerable stability in the structure-forming process (Smith *et al.*, 2004, 2004*a,b*; Moghimi *et al.*, 2004). In order to study the role of proton-exchange compounds in the construction of net-like structures, we have prepared the title compound, (I), and its structure is reported here.



In the reaction with succinic acid a phenolic proton is transferred to the pyridine N atom, forming a zwitterionic pyridinium-4-olate. The structure of (I) thus has half of a neutral succinic acid residue and one pyridinium-4-olate molecule in the asymmetric unit, as the succinic acid molecule lies on a centre of symmetry located at the mid-point of the

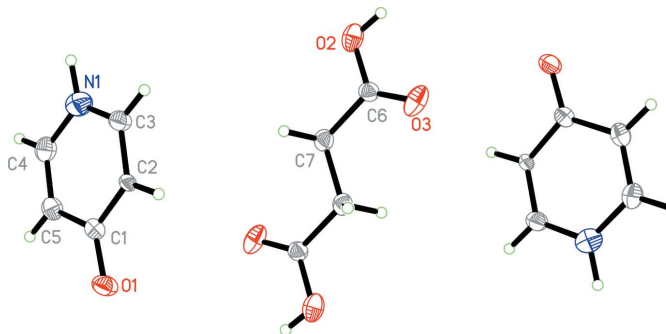


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to the equivalent labelled atoms by the symmetry operation $(1-x, 2-y, 2-z)$.

C7—C7ⁱ bond (see Fig. 1 for symmetry code). All bond lengths in the molecules are within normal ranges (Allen *et al.*, 1987).

In the crystal structure, intermolecular O—H···O hydrogen bonds link succinic acid molecules to two adjacent pyridinium-4-olate residues along the *a* axis. The structure is further stabilized by a number of C—H···O hydrogen bonds (Table 1), forming a network parallel to the *ac* plane (Fig. 2).

Experimental

Pyridin-4-ol (0.2 mmol, 19.1 mg) and succinic acid (0.1 mmol, 11.8 mg) were dissolved in distilled water (10 ml). The mixture was heated under reflux to form a clear colourless solution. Crystals of the title compound were grown by gradual evaporation of water over a period of one week at room temperature.

Crystal data

2C ₅ H ₅ NO·C ₄ H ₆ O ₄	$D_x = 1.423 \text{ Mg m}^{-3}$
$M_r = 308.29$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 1725 reflections
$a = 8.559 (2) \text{ \AA}$	$\theta = 2.5\text{--}26.6^\circ$
$b = 5.178 (1) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$c = 16.387 (3) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\beta = 97.891 (2)^\circ$	Plate, colourless
$V = 719.4 (3) \text{ \AA}^3$	$0.34 \times 0.20 \times 0.07 \text{ mm}$
$Z = 2$	

Data collection

Bruker SMART APEX area-detector diffractometer	1464 independent reflections
φ and ω scans	1146 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.022$
$T_{\text{min}} = 0.963$, $T_{\text{max}} = 0.992$	$\theta_{\text{max}} = 26.5^\circ$
5307 measured reflections	$h = -10 \rightarrow 10$
	$k = -6 \rightarrow 6$
	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1263P)^2 + 0.2431P]$
$R[F^2 > 2\sigma(F^2)] = 0.066$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.198$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.53 \text{ e \AA}^{-3}$
1464 reflections	$\Delta\rho_{\text{min}} = -0.43 \text{ e \AA}^{-3}$
106 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O2—H2···O1 ⁱ	0.84 (3)	1.796 (16)	2.611 (2)	163 (4)
C2—H2A···O1 ⁱⁱ	0.93	1.86	2.792 (2)	178 (3)
C3—H3···O3 ⁱⁱⁱ	0.93	2.48	3.340 (2)	154 (3)
C4—H4···O2 ^{iv}	0.93	2.52	3.360 (2)	150 (3)

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

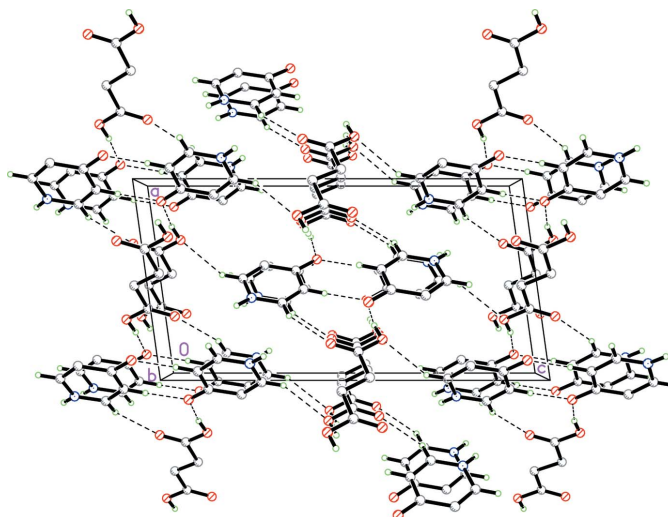


Figure 2

The crystal packing of (I). Intermolecular hydrogen bonds are drawn as dashed lines.

Atoms H1 and H2, attached to N1 and O2, respectively, were located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.97 (1) \AA and the O—H distance restrained to 0.84 (1) \AA . The other H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 \AA , and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXL97.

Financial assistance from the Baoji College of Arts and Sciences research funds is gratefully acknowledged.

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bruker (2002). SMART, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
- Moghimi, A., Sharif, M. A. & Aghabozorg, H. (2004). *Acta Cryst.* **E60**, o1790–o1792.
- Sheldrick, G. M. (1997a). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). SHELXTL. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Smith, G., Wermuth, U. D. & Healy, P. C. (2004a). *Acta Cryst.* **E60**, o1257–o1259.
- Smith, G., Wermuth, U. D. & Healy, P. C. (2004b). *Acta Cryst.* **E60**, o1040–o1042.
- Smith, G., Wermuth, U. D., Young, D. J. & White, J. M. (2004). *Acta Cryst.* **E60**, o2014–o2016.