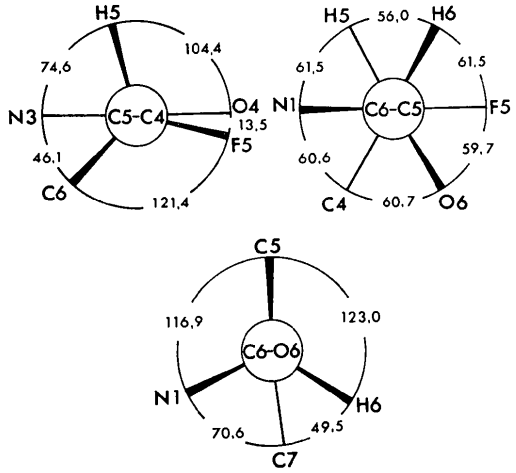

Fig. 3. Torsion angles in the form of Newman projections.

170 (3) for N(3)–H(3)···O(2^{i}) and 117·3 (8)° for C(2)–O(2)···H(3^{i}). The symmetry operation, i, is at ($\frac{1}{2}-x$, y,z).

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N-Succinopyridine

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Abstract. $C_9H_9NO_4$, M.W. 195·17, orthorhombic, $P2_12_12_1$, $a=7{\cdot}775$ (2), $b=14{\cdot}974$ (3), $c=7{\cdot}730$ (2) Å, $Z=4$, $D_m=1{\cdot}442$, $D_x=1{\cdot}439$ g cm^{-3}. The final R was 0·032 for 1037 reflexions [$I>3\sigma(I)$]. The molecular dimensions agree well with the aspartic acid structures. In the crystals the carbonyl and the negatively charged O atoms approach the positions *ortho* and *para* with respect to the N atom of the pyridinium moiety.

Introduction. Unexpectedly, maleic acid reacts with pyridine in water to produce *N*-succinopyridine. Oscillation and Weissenberg photographs showed that the crystals belonged to the space group $P2_12_12_1$. The systematic absences were: $h00$: $h=2n+1$; $0k0$: $k=2n+1$; $00l$: $l=2n+1$. A single crystal, 0·23 × 0·25 × 0·43 mm, was mounted on a Picker FACS-1 diffractometer and graphite-monochromatized Mo $K\alpha$ radiation ($\lambda=0{\cdot}70926$ Å) was used to measure intensities up to $2\theta=55°$ by θ–2θ scan mode for hkl and $hk\bar{l}$ reflexions. After averaging these two independent sets, 1037 out of 1221 reflexions had $I>3\sigma(I)$. The intensities were reduced to structure amplitudes by the Lorentz and polarization factors and then to E's by a Wilson (1942) plot ($B=3{\cdot}21$ Å^2). The structure was solved by direct methods (Karle & Karle, 1966). The atomic parameters, arbitrarily describing the L-enantiomer, were refined by full-matrix least squares. The weighting scheme was $w=[2|F_o|^{1/2}/\sigma(I)]$. The final R and R_w were 0·032 and 0·031, respectively.† The maximum shift for the non-

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† A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31497 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Positional and thermal parameters*

(*a*) The parameters (× 10^4) for the non-hydrogen atoms

The anisotropic temperature factor parameters, U_{ij}, are in the form: $T=\exp[-2\pi^2(U_{11}h^2a^{*2}+\ldots+2U_{12}hka^*b^*+\ldots)]$.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(1)	8203 (2)	1013 (1)	4448 (3)	219 (8)	306 (8)	419 (9)	−15 (6)	−58 (7)	24 (7)
C(2)	6363 (2)	1354 (1)	4080 (2)	254 (8)	305 (8)	289 (7)	7 (6)	−13 (6)	5 (7)
C(3)	5083 (2)	596 (1)	4324 (3)	240 (8)	331 (8)	396 (9)	16 (7)	−0 (7)	53 (7)
C(4)	3239 (2)	920 (1)	4194 (3)	266 (8)	380 (9)	362 (8)	18 (8)	28 (7)	28 (8)
N(5)	6204 (2)	1750 (1)	2317 (2)	252 (6)	272 (7)	337 (7)	17 (6)	−2 (5)	15 (5)
C(6)	5995 (4)	2634 (1)	2155 (3)	531 (13)	275 (9)	477 (10)	52 (9)	2 (9)	15 (7)
C(7)	5898 (5)	3012 (2)	531 (4)	814 (21)	360 (10)	590 (14)	75 (12)	0 (14)	167 (9)
C(8)	6013 (5)	2490 (2)	−917 (3)	688 (17)	659 (15)	430 (11)	112 (15)	47 (11)	212 (11)
C(9)	6221 (5)	1581 (2)	−717 (3)	785 (18)	582 (13)	341 (10)	126 (14)	47 (11)	−4 (9)
C(10)	6314 (4)	1222 (1)	912 (3)	596 (14)	352 (9)	356 (9)	106 (10)	11 (10)	−12 (7)
O(1)	8524 (2)	888 (1)	5994 (2)	422 (8)	467 (7)	410 (8)	51 (7)	−108 (6)	44 (6)
O(2)	9153 (2)	856 (1)	3165 (3)	246 (7)	764 (12)	516 (9)	74 (8)	5 (6)	49 (8)
O(3)	2839 (2)	1693 (1)	4447 (3)	345 (8)	414 (8)	732 (11)	83 (7)	59 (8)	−25 (7)
O(4)	2161 (2)	289 (1)	3767 (3)	265 (7)	479 (9)	853 (12)	5 (7)	−52 (7)	−63 (8)

Table 1 (*cont.*)

(*b*) The parameters (× 10^3) for the hydrogen atoms

	x	y	z	U_{iso}
H(2)	615 (5)	179 (2)	481 (4)	43 (7)
H(31)	524 (4)	34 (2)	542 (4)	39 (6)
H(32)	529 (4)	14 (2)	346 (3)	34 (6)
H(4)	121 (7)	52 (3)	365 (5)	62 (10)
H(6)	584 (6)	291 (2)	319 (5)	55 (8)
H(7)	569 (7)	359 (3)	42 (6)	76 (12)
H(8)	596 (6)	283 (3)	−209 (5)	67 (10)
H(9)	642 (5)	120 (2)	−175 (5)	57 (9)
H(10)	645 (4)	61 (2)	111 (3)	37 (7)

hydrogen atomic parameters was 0·05 of the corresponding e.s.d. in the final refinement cycle. Scattering factors for C, N and O were taken from Cromer & Mann (1968) and for H from Stewart, Davidson & Simpson (1965). The programs were from the X-RAY 70 system (Stewart, Kundell & Baldwin, 1970). The atomic parameters are listed in Table 1. The atomic numbering, the bond lengths and angles are shown in Fig. 1.

Discussion. When maleic acid is mixed with pyridine in water, pyridinium maleate had been expected to crystallize, but the *E* map showed that an unexpected reaction had taken place. The pyridinium moiety had added to the double bond of maleic acid to produce the title compound. A stereoscopic view of the molecule is shown in Fig. 2. The bond lengths and angles around C(1) are similar to those for negatively charged carboxyl groups (Hahn, 1957). The molecule thus exists as a zwitterion in the crystals. This charged system is similar to that of aspartic acid. In fact the bond lengths and angles agree better with those of L-aspartic acid (Derissen, Endeman & Peerdeman, 1968) and DL-aspartic acid (Rao, 1973) than with those of succinic acid derivatives (Broadley, Cruickshank, Morrison, Robertson & Shearer, 1959; McAdam, Currie & Speakman, 1971; Klapper & Küppers, 1973; Schouwstra, 1972, 1973). Also the torsion angles C(1)–C(2)–C(3)–C(4), and O(2)–C(1)–C(2)–N(5) are 173·1°

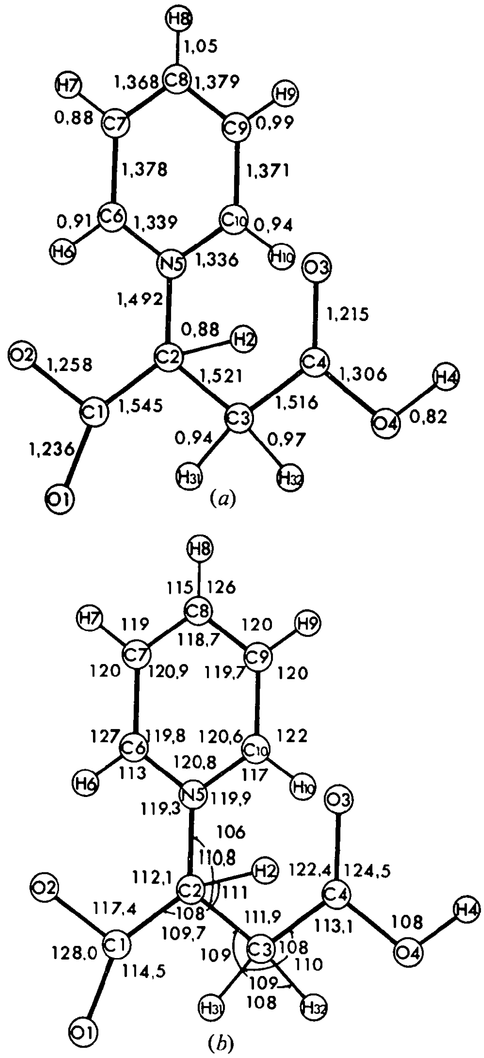

Fig. 1. (*a*) Bond lengths (Å). The e.s.d.'s of the bonds between the non-hydrogen atoms are 0·002–0·004 Å and those of the bonds including the hydrogen atoms are 0·04 Å. (*b*) Bond angles (°). The e.s.d.'s are 0·2° between the non-hydrogen atoms and 2° for the angles involving the hydrogen atoms.

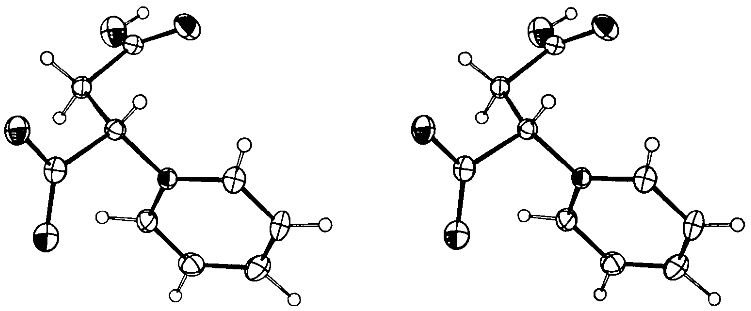

Fig. 2. A stereoscopic view of the molecule.

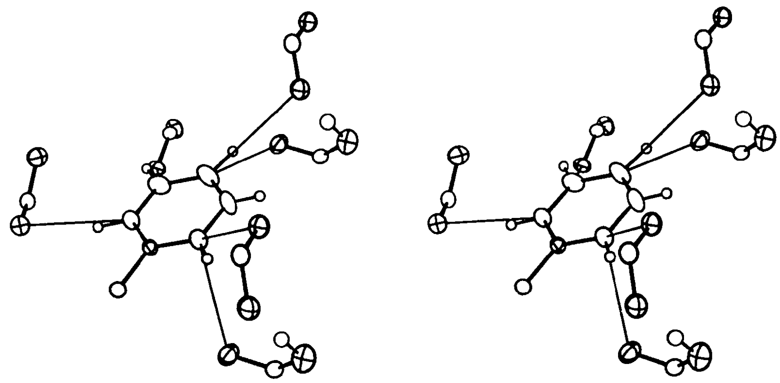

Fig. 3. A stereoscopic view of the environment around the pyridinium moiety.

and −20·7°, respectively, close to the corresponding angles of the aspartic acid structures.

A hydrogen bond is formed between O(4) and O(2) of the molecule translated by one unit cell along **a**. The distances are 2·531 (2) between these O atoms and 1·72 (5) Å between H(4) and O(2). The angle O(4)–H(4)···O(2) is 171 (4)°.

A stereoscopic view of the environment around the positively charged pyridine ring is shown in Fig. 3. The intermolecular contacts were scanned within a 3·5 Å radius from each of the C atoms of the pyridine ring. The distances are listed in Table 2. The carbonyl and the negatively charged O atoms are oriented primarily towards both of the *ortho* C atoms and the *para* C atom of the pyridine ring (*ortho* and *para* with respect to the positively charged N atom). This suggests that these C atoms are involved in the charge delocalization and have a slight positive charge on them.

Table 2. *The intermolecular distances* (Å) *around the pyridinium moiety*

$C(6)\cdots O(3^{i})$	3·157 (3) Å
$C(6)\cdots O(1^{ii})$	3·262 (3)
$C(8)\cdots O(3^{iii})$	3·311 (3)
$C(8)\cdots O(2^{iv})$	3·354 (3)
$C(9)\cdots O(1^{v})$	3·278 (3)
$C(10)\cdots O(1^{vi})$	3·162 (3)

(i) $0{\cdot}5+x, 0{\cdot}5-y, 1{\cdot}0-z$
(ii) $x-0{\cdot}5, 0{\cdot}5-y, 1{\cdot}0-z$
(iii) $0{\cdot}5+x, 0{\cdot}5-y, -z$
(iv) $x-0{\cdot}5, 0{\cdot}5-y, -z$
(v) $1{\cdot}5-x, -y, 0{\cdot}5+z$

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