The chemistry of salts containing $(H_2PO_4^-)_n$ aggregates is close to clathrate chemistry and appears very attractive. Indeed, the controlled formation of $(H_2PO_4^-)_n$ or $(H_2PO_4.S)_n^{n-}$ aggregates using the previous chemical reactions (1), (2), (3) and (4) is an important step in the crystal engineering of acentric materials having a layer structure for non-linear optical applications.

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Absolute Configuration of Two Bases Co-crystallized with (+)-Tartaric Acid: (R)-1-[3-(4-Chlorophenyl)-3-hydroxy-3-(2-pyridyl)propyl]pyrrolidinium (+)-Tartrate 2-Propanol Hemihydrate and (S)-2-[1-Hydroxy-1-(4-methoxyphenyl)ethyl]pyridinium (+)-Tartrate

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Abstract. (1) $C_{18}H_{22}ClN_2O^+.C_4H_5O_6^-.C_3H_8O.\frac{1}{2}H_2O$, $M_r = 536.08$, monoclinic, $P2_1$, $a = 13.738$ (3), $b = 15.037$ (5), $c = 7.012$ (2) Å, $\beta = 103.26$ (2)°, $V = 1409.9$ (5) Å^3, $Z = 2$, $D_x = 1.260$ Mg m^{-3}, $\lambda(Mo\ K\alpha) = 0.71069$ Å, $\mu = 0.181$ mm^{-1}, $F(000) = 570$, $T = 295$ K, $R = 0.041$, $wR = 0.047$ for 1606 reflections [$I > 3\sigma(I)$]. (2) $C_{14}H_{16}NO_2^+.C_4H_5O_6^-$, $M_r = 379.37$, monoclinic, $P2_1$, $a = 16.036$ (2), $b = 7.839$ (2), $c = 7.548$ (1) Å, $\beta = 102.97$ (1)°, $V = 924.6$ (5) Å^3, $Z = 2$, $D_x = 1.367$ Mg m^{-3}, $\lambda(Mo\ K\alpha) = 0.71069$ Å, $\mu = 0.101$ mm^{-1}, $F(000) = 400$, $T = 295$ K, $R = 0.046$, $wR = 0.055$ for 1613 reflections [$I > 3\sigma(I)$]. The absolute configurations of the bases in (1) and (2) were determined by referring to the known absolute configuration of the co-crystallized (+)-tartrate anion. In both structures the carboxyl groups of the (+)-tartrate anions are *anti*. In both, the molecular packing is dominated by hydrogen bonds including a bifurcated system from the protonated N atoms.

Introduction. Some α-substituted pyridine derivatives exhibit important pharmacological activities and a

few are used in human medicine. A series of such compounds in enantiomerically pure form has been synthesized (Berova, 1987; Bojadziev, Kojić-Prodić & Berova, 1987). For some of them the absolute configuration could not be determined by chemical correlation. The absolute configuration of two selected derivatives, reported in this paper, and their CD measurements were used to determine the chiroptical properties of nine related compounds (Berova, Bojadziev, Bresciani-Pahor, Ivanov, Kojić-Prodić, Rakovska, Ružić-Toroš & Snatzke, 1991).

Experimental. Both samples were crystallized from 2-propanol at ambient temperature. The crystals of (1) were found to include one molecule of solvent and half a molecule of H_2O. Preliminary cell dimensions and space groups were determined from oscillation and Weissenberg photographs with Cu $K\alpha$ radiation; final cell dimensions were refined from diffractometer measurements using 25 reflections with $9 < \theta < 15°$ for (1) and 20 reflections with $10 < \theta < 16°$ for (2). Intensities were measured on an Enraf–Nonius CAD-4F diffractometer in the $\omega/2\theta$ scan mode, $1 + 0.35\tan\theta$, with graphite-mono-

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chromated Mo $K\alpha$ radiation. $2\theta_{max} = 54°$, h $0\rightarrow 12$, k $0\rightarrow 18$, l $-8\rightarrow 8$ for (I) and h $0\rightarrow 17$, k $0\rightarrow 10$, $l-9$ $\rightarrow 9$ for (2). 1606 independent reflections for (1) and 1613 for (2) having $I > 3\sigma(I)$ were recorded in the range $2\cdot5 < \theta < 27°$. Crystal dimensions were $0\cdot2 \times 0\cdot3 \times 0\cdot4$ mm for (1) and $0\cdot3 \times 0\cdot4 \times 0\cdot3$ mm for (2). Lorentz–polarization corrections were applied. The structures were solved by direct methods, *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). The H atoms of the phenyl, pyridyl, and pyrrolidinyl moieties were placed at the stereochemically expected positions. Subsequent difference Fourier syntheses located the remaining H atoms. Full-matrix least-squares refinement minimized $\Sigma w(|F_o| - |F_c|)^2$ with $w^{-1} = \sigma^2(F_o) + (0\cdot02F_o)^2 + 1$ (Killean & Lawrence, 1969). Scale factor, atomic coordinates, and anisotropic thermal parameters were refined for non-H atoms in both structures, except that the water oxygen in (1) was treated as isotropic and of site occupancy $0\cdot5$. The H atoms were included in structure factor calculations. The residual electron density observed was $-0\cdot3 < \Delta\rho < 0\cdot2$ e Å^{-3}. Δ/σ_{max} $0\cdot29$ for (1) and $0\cdot15$ for (2). Final $R = 0\cdot047$, $wR = 0\cdot050$ for 1606 observed reflections for (1) and $R = 0\cdot046$, $wR = 0\cdot055$ for 1613 observed reflections for (2). Scattering factors were according to *International Tables for X-ray Crystallography* (1974, Vol. IV), with corrections for anomalous dispersion. Table 1 lists the final atomic parameters for (1) and (2).* Calculations were carried out on PDP 11-44 with programs from *SDP* (B. A. Frenz & Associates Inc., 1985) at Università di Trieste and on an IBM 4341 with routines from Nardelli (1983) at the University Computing Centre in Zagreb.

Discussion. Interatomic distances, bond angles and selected torsion angles of both structures [(1), (2)] are listed in Table 2. Figs. 1(*a*) and 1(*b*) show the base in (1) and (2) respectively. The absolute configurations of the bases in both structures were determined by referring to the known absolute configuration of the co-crystallized (+)-tartrate anion; in both structures the chiral centre is C1 with an R configuration in (1) and S in (2). The (+)-tartrate anions of (1) and (2) with the atom numbering are given in Fig. 2. Molecular packing *via* hydrogen bonds is shown in Figs. 3(*a*) and 3(*b*).

The location of protons in difference Fourier maps indicated that in (1) there is a pyrrolidinium cation and in (2) a pyridinium cation; tartaric acid must

Table 1. *Positional parameters and isotropic thermal parameters with e.s.d.'s in parentheses*

$$B_{eq} = (4/3)[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2)$$
$$+ ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)].$$

	x	y	z	B_{eq} (Å^2)
(1)				
Cl	0·7178 (1)	−0·243	0·0815 (3)	6·21 (4)
O1	0·7902 (3)	0·6749 (3)	0·0241 (6)	5·2 (1)
C1	0·8211 (4)	−0·6325 (4)	0·2112 (8)	4·3 (1)
C2	0·7686 (4)	−0·6756 (4)	0·3573 (8)	4·6 (1)
C3	0·6554 (4)	−0·6742 (4)	0·2878 (8)	4·3 (1)
C1*A*	0·7951 (4)	−0·5339 (3)	0·1779 (8)	3·8 (1)
C2*A*	0·7628 (4)	−0·4999 (4)	−0·0074 (8)	4·8 (1)
C3*A*	0·7396 (4)	−0·4098 (4)	−0·0378 (9)	4·9 (1)
C4*A*	0·7493 (4)	−0·3562 (2)	0·1204 (9)	4·4 (1)
C5*A*	0·7819 (4)	−0·3867 (4)	0·3039 (9)	5·0 (1)
C6*A*	0·8049 (5)	−0·4759 (4)	0·3339 (9)	5·0 (1)
N1*B*	0·9697 (4)	−0·6422 (4)	0·4757 (9)	6·8 (2)
C2*B*	0·9344 (4)	−0·6413 (4)	0·2843 (9)	4·9 (1)
C3*B*	0·9957 (5)	−0·6449 (5)	0·153 (1)	6·8 (2)
C4*B*	1·0980 (5)	−0·6519 (5)	0·233 (1)	8·2 (2)
C5*B*	1·1345 (5)	−0·6553 (5)	0·429 (1)	8·0 (2)
C6*B*	1·0681 (5)	−0·6485 (6)	0·544 (1)	8·2 (2)
N1*C*	0·6069 (3)	−0·7284 (3)	0·4182 (6)	4·0 (1)
C2*C*	0·6139 (6)	−0·6913 (4)	0·620 (1)	6·5 (2)
C3*C*	0·5329 (5)	−0·7410 (6)	0·6902 (9)	7·1 (2)
C4*C*	0·4555 (5)	−0·7624 (7)	0·510 (1)	9·4 (3)
C5*C*	0·4974 (4)	−0·7429 (5)	0·3394 (9)	5·3 (1)
C7	0·5823 (4)	−0·0170 (4)	0·9530 (7)	4·2 (1)
O71	0·5082 (3)	0·0080 (4)	0·8377 (6)	7·1 (1)
O72	0·6634 (3)	−0·0467 (3)	0·9132 (5)	4·80 (9)
C8	0·5851 (4)	−0·0158 (4)	1·1691 (7)	4·0 (1)
O8	0·4964 (3)	0·0200 (4)	1·1973 (6)	6·9 (1)
C9	0·6753 (4)	0·0369 (4)	1·2805 (6)	3·3 (1)
O9	0·6745 (3)	0·1239 (2)	1·2047 (5)	4·15 (8)
C10	0·6778 (4)	0·0393 (4)	1·4974 (7)	3·6 (1)
O101	0·6883 (3)	0·1103 (2)	1·5880 (5)	4·35 (9)
O102	0·6712 (3)	−0·0370 (3)	1·5713 (5)	5·4 (1)
C11	0·8920 (5)	−0·9117 (5)	−0·027 (1)	6·2 (2)
O11*	0·8040 (3)	−0·8590 (2)	−0·0417 (5)	4·07 (8)
C12*	0·9483 (6)	−0·8848 (8)	−0·169 (1)	10·0 (3)
C13*	0·9501 (6)	−0·9062 (6)	0·181 (1)	9·9 (3)
O33†	0·3855 (6)	0·0317 (7)	1·467 (1)	6·4 (2)*
(2)				
C1	0·6775 (2)	0·715	0·0523 (5)	3·34 (8)
O1	0·7133 (2)	0·5487 (4)	0·0885 (4)	3·70 (6)
C2	0·6595 (3)	0·7536 (8)	−0·1493 (6)	4·9 (1)
C1*A*	0·5982 (2)	0·7169 (5)	0·1333 (5)	2·83 (7)
C2*A*	0·5991 (2)	0·6282 (6)	0·2912 (5)	3·54 (8)
C3*A*	0·5287 (2)	0·6273 (7)	0·3703 (5)	3·59 (9)
C4*A*	0·4562 (2)	0·7185 (6)	0·2877 (5)	3·46 (8)
O4*A*	0·3828 (2)	0·7268 (6)	0·3524 (4)	5·31 (8)
C5*A*	0·4545 (2)	0·8072 (6)	0·1295 (6)	3·93 (9)
C6*A*	0·5247 (2)	0·8070 (6)	0·0530 (6)	3·59 (9)
C7*A*	0·3822 (3)	0·648 (1)	0·5202 (7)	6·5 (1)
N1*B*	0·8062 (3)	0·7855 (6)	0·2768 (8)	8·0 (1)
C2*B*	0·7412 (2)	0·8469 (6)	0·1572 (5)	3·19 (8)
C3*B*	0·7365 (3)	1·0187 (7)	0·1395 (6)	4·8 (1)
C4*B*	0·7983 (4)	1·1217 (7)	0·2453 (6)	5·7 (1)
C5*B*	0·8620 (3)	1·0530 (8)	0·3675 (8)	6·6 (1)
C6*B*	0·8669 (3)	0·8834 (8)	0·380 (1)	10·4 (2)
C7	0·8645 (2)	0·4172 (5)	0·6383 (4)	2·79 (7)
O71	0·7926 (2)	0·4411 (5)	0·5479 (3)	4·64 (7)
O72	0·9340 (2)	0·4312 (5)	0·5833 (3)	3·51 (6)
C8	0·8782 (2)	0·3672 (5)	0·8369 (4)	2·80 (7)
O8	0·7981 (2)	0·3424 (4)	0·8835 (3)	3·69 (6)
C9	0·9285 (2)	0·5068 (5)	0·9566 (4)	2·39 (6)
O9	0·8803 (2)	0·6590 (4)	0·9315 (3)	3·09 (5)
C10	0·9515 (2)	0·4503 (5)	1·1550 (4)	2·48 (6)
O101	1·0086 (2)	0·3472 (5)	1·2034 (4)	4·83 (7)
O102	0·9080 (2)	0·5141 (4)	1·2591 (3)	3·41 (5)

* Atoms of solvent molecule 2-propanol.
† Oxygen atom of water molecule, site occupancy 0·5.

therefore be present in each as the monoanion. Differences in bond distances and angles of chemically analogous moieties of both structures are below the limit of 4σ. The C8—O8 value of $1\cdot387$ (7) Å in the hydroxylic group of the (+)-tartrate anion (1)

Table 2. Bond distances (Å), bond angles (°) and selected torsional angles (°)

		(1)	(2)
C1	C4A	1·762 (6)	
O1	C1	1·433 (7)	1·426 (5)
C1	C2	1·527 (8)	1·514 (5)
C1	C1A	1·529 (8)	1·529 (5)
C1	C2B	1·528 (8)	1·542 (5)
C2	C3	1·520 (8)	
C1A	C2A	1·372 (8)	1·378 (5)
C1A	C6A	1·382 (8)	1·391 (5)
C2A	C3A	1·396 (8)	1·391 (5)
C3A	C4A	1·353 (9)	1·388 (5)
C4A	C5A	1·343 (8)	1·377 (5)
C4A	O4A		1·373 (4)
O4A	C7A		1·413 (6)
C5A	C6A	1·382 (9)	1·376 (5)
N1B	C2B	1·318 (9)	1·307 (5)
N1B	C6B	1·331 (9)	1·343 (6)
C2B	C3B	1·384 (10)	1·354 (6)
C3B	C4B	1·392 (12)	1·385 (7)
C4B	C5B	1·352 (13)	1·327 (7)
C5B	C6B	1·355 (12)	1·334 (9)
N1C	C2C	1·506 (8)	
N1C	C5C	1·495 (7)	
N1C	C3	1·490 (7)	
C2C	C3C	1·513 (11)	
C3C	C4C	1·490 (11)	
C4C	C5C	1·470 (10)	
C7	O71	1·205 (7)	1·215 (4)
C7	O72	1·290 (7)	1·278 (4)
C7	C8	1·507 (8)	1·517 (4)
C8	O8	1·387 (7)	1·418 (4)
C8	C9	1·526 (7)	1·529 (5)
C9	O9	1·411 (6)	1·411 (4)
C9	C10	1·514 (7)	1·526 (4)
C10	O101	1·234 (6)	1·215 (4)
C10	O102	1·270 (7)	1·264 (4)
C11	O11	1·430 (8)	
C11	C12	1·453 (11)	
C11	C13	1·491 (12)	
O1	C1	C2	109·8 (5)	110·7 (3)
O1	C1	C1A	106·3 (5)	105·5 (3)
O1	C1	C2B	109·5 (5)	108·8 (3)
C2	C1	C1A	112·6 (5)	114·3 (3)
C2	C1	C2B	109·9 (5)	109·7 (3)
C1A	C1	C2B	108·7 (4)	107·6 (3)
C1	C2	C3	112·6 (5)	
C1	C4A	C3A	118·3 (5)	
C1	C4A	C5A	119·6 (5)	
C3A	C4A	O4A		124·2 (3)
O4A	C4A	C5A		115·6 (3)
C4A	O4A	C7A		118·5 (2)
C2B	N1B	C6B	118·3 (7)	123·5 (5)
C1	C2B	N1B	116·8 (7)	116·2 (4)
C1	C2B	C3B	120·6 (7)	126·9 (4)
C2C	N1C	C5C	104·1 (5)	
C2C	N1C	C3	115·7 (5)	
C5C	N1C	C3	113·9 (4)	
N1C	C2C	C3C	103·2 (6)	
C2C	C3C	C4C	105·5 (6)	
C3C	C4C	C5C	108·1 (6)	
N1C	C5C	C4C	106·1 (6)	
C2	C3	N1C	111·3 (4)	
O71	C7	O72	127·0 (6)	126·2 (3)
O71	C7	C8	119·6 (7)	120·2 (3)
O72	C7	C8	113·4 (5)	113·6 (3)
C7	C8	O8	109·1 (5)	110·0 (3)
C7	C8	C9	110·6 (5)	109·8 (3)
O8	C8	C9	111·2 (5)	109·8 (2)
C8	C9	O9	110·7 (4)	109·0 (2)
C8	C9	C10	110·9 (4)	110·6 (3)
O9	C9	C10	110·7 (4)	112·4 (3)
C9	C10	O101	120·7 (5)	119·2 (3)
C9	C10	O102	113·6 (5)	116·7 (3)
O101	C10	O102	125·6 (5)	124·1 (3)
O11	C11	C12	111·7 (7)	
O11	C11	C13	107·2 (7)	
C12	C11	C13	113·8 (7)	
O1	C1	C2	C3	-56·1 (6)	
C1A	C1	C2	C3	62·2 (6)	
C2B	C1	C2	C3	-176·5 (5)	
O1	C1	C1A	C2A	-8·6 (7)	35·2 (4)
C2	C1	C1A	C2A	-128·8 (6)	157·1 (4)
C2B	C1	C1A	C2A	109·2 (6)	-80·8 (4)

Table 2 (cont.)

				(1)	(2)
O1	C1	C2B	N1B	-151·5 (5)	-10·5 (5)
C2	C1	C2B	N1B	-30·9 (7)	-131·6 (4)
C1A	C1	C2B	N1B	92·7 (6)	103·4 (4)
C1	C2	C3	N1C	171·5 (5)	
C3A	C4A	O4A	C7A		4·5 (6)
C5C	N1C	C2C	C3C	36·3 (6)	
C6C	N1C	C2C	C3C	162·1 (5)	
C2C	N1C	C5C	C4C	-30·1 (6)	
C3	N1C	C5C	C4C	-157·1 (5)	
C2C	N1C	C3	C2	69·5 (6)	
C5C	N1C	C3	C2	-169·9 (5)	
N1C	C2C	C3C	C4C	-29·1 (7)	
C2C	C3C	C4C	C5C	10·9 (8)	
C3C	C4C	C5C	N1C	11·9 (7)	
O71	C7	C8	O8	-2·5 (8)	4·8 (5)
O71	C7	C8	C9	-125·1 (6)	-116·2 (4)
C7	C8	C9	O9	56·1 (6)	62·2 (5)
C7	C8	C9	C10	179·3 (5)	-173·7 (3)
O8	C8	C9	O9	-65·3 (6)	-58·9 (4)
O8	C8	C9	C10	58·0 (6)	65·2 (4)
C8	C9	C10	O101	-130·0 (5)	75·3 (4)

Table 3. Hydrogen bonds (Å) for (1) and (2)

D—H···A	D···A	Symmetry operation on A
(1)		
O1—HO1···O11	2·820 (6)	x, y, z
O9—HO9···O11	2·762 (5)	x, y + 1, z + 1
O72—HO72···O102	2·429 (5)	x, y, z - 1
O11—HO11···O101	2·755 (5)	x, y + 1, z + 2
*O8—HO8···O33	2·692 (11)	x, y, z
*O33—H2O33···O71	2·779 (10)	x, y, z - 1
N1C—HN1C···O9	2·945 (6)	x, y - 1, z - 1
N1C—HN1C···O101	2·818 (6)	x, y - 1, z - 1
(2)		
O72—HO72···O102	2·475 (3)	x, y, z - 1
O1—HO1···O8	2·794 (4)	x, y, z - 1
O9—HO9···O101	2·684 (5)	$-x + 2, y + \frac{1}{2}, -z + 2$
N1B—HN1B···O102	2·703 (6)	x, y, z - 1
O8—HO8···O4A	3·177 (4)	x + 1, y, z + 1
O8—HO8···O71	2·631 (3)	x, y, z
N1B—HN1B···O9	3·253 (6)	x, y, z - 2

* O33, H1O33, H2O33: water molecule with pp = 0·5.

deviates considerably from that of a C—O single bond. It might be explained by somewhat higher temperature movement of O8 and its function in the system of hydrogen bonds. The O8 hydroxyl group acts as the proton donor to the water molecule with the population parameter being 0·5. The O8—HO8 was normalized to a value of 0·983 Å using the program GSTAT89 (Motherwell, Murray-Rust, Raferty, Allen & Doyle, 1989).

In the syntheses of suitable salts of bases (1) and (2) the (+)-tartaric acid was used as an internal standard for determination of the absolute configuration at C1 of these two bases. During the structure determination the (+)-tartrate anions were selected and according to this the sense of chirality at C1 was assigned. In both structures the carboxyl groups of the tartrate anions are anti to each other; the torsion angles C7—C8—C9—C10 are 179·3 (5)° in (1) and -173·7 (3)° in (2). This finding is in accord with the literature (Kroon, 1982). The C=O bonds labelled as O71 (in both structures) are in an eclipsed position to

(a)

(b)

Fig. 1. The *ORTEP* (Johnson, 1970) drawing of the base (a) in structure (1) and (b) in structure (2) with the atom-numbering scheme. Thermal ellipsoids are drawn at the 50% probability level.

(1)   (2)

Fig. 2. The *ORTEP* (Johnson, 1970) drawing of (+)-tartrate anions in (1) and (2), and solvent molecule 2-propanol in (1) with the atom-numbering scheme.

the α-hydroxyl O atoms (O8) [(O8—C8—C7—O71 $-2\cdot5$ (8) (1); $4\cdot8$ (5)° (2)].

Hydrogen bonds. In both structures the molecular packing is dominated by very extensive hydrogen bonds [Figs. 3(a) and 3(b) and Table 3]. The system of hydrogen bonds is even more complex in structure (1) due to the presence of a solvent molecule (2-propanol) and a water molecule (occupancy = 0·50). In both structures there are bifurcated hydrogen bonds joining the protonated N atoms of the base moieties to the (+)-tartrate anions.

(a)

(b)

Fig. 3. A view of (a) the structure of (1) and (b) the structure of (2) along b illustrating the hydrogen bonds.

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Structures of Ethylammonium Hydrogen Succinate and Diethylammonium Hydrogen Succinate at 110 K

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Abstract. $C_2H_5NH_3^+.C_4H_5O_4^-$, $M_r = 163\cdot17$, triclinic, $P\bar{1}$, $a = 8\cdot293$ (1), $b = 9\cdot342$ (6), $c = 10\cdot934$ (2) Å, $\alpha = 88\cdot94$ (3), $\beta = 89\cdot39$ (1), $\gamma = 84\cdot46$ (2)°, $V = 842\cdot9$ (8) Å^3, $Z = 4$, $D_x = 1\cdot286$ g cm^{-3}, λ(Mo $K\bar{\alpha}$) $= 0\cdot71073$ Å, $\mu = 1\cdot008$ cm^{-1}, $F(000) = 352$, $T = 110$ K, $R = 0\cdot052$ for 1885 observed reflections. $(C_2H_5)_2NH_2^+.C_4H_5O_4^-$, $M_r = 191\cdot23$, orthorhombic, *Pban*, $a = 12\cdot661$ (2), $b = 10\cdot125$ (1), $c = 8\cdot031$ (1) Å, $V = 1029\cdot5$ (5) Å^3, $Z = 4$, $D_x = 1\cdot234$ g cm^{-3}, λ(Mo $K\bar{\alpha}$) $= 0\cdot71073$ Å, $\mu = 0\cdot918$ cm^{-1}, $F(000) = 416$, $T = 110$ K, $R = 0\cdot040$ for 2007 observed reflections. In both compounds the hydrogen succinate ions are linked by very short hydrogen bonds resulting in infinite chains. In ethylammonium hydrogen succinate the chains are formed by two distinct succinate entities which alternate in the structure. They are connected by two short hydrogen bonds, both asymmetric. One hydrogen bond with length $2\cdot483$ (4) Å is between a carboxylic acid group and a carboxylate group, while the other short hydrogen bond with length $2\cdot456$ (4) Å is between two half ionized, but not identical, COO groups. Diethylammonium hydrogen succinate contains a crystallographically symmetric short hydrogen bond with length $2\cdot4370$ (7) Å. The H atom in the short hydrogen bond seems to be best described by two equally populated sites on each side of the center of the

bond. The chains of anions are interconnected by longer hydrogen bonds to the cations in both compounds.

Introduction. The crystal structure determinations of ethylammonium hydrogen succinate (1) and diethylammonium hydrogen succinate (2) have been performed as a continuation of earlier studies of acid salts of malonic acid and succinic acid with special interest in the hydrogen bonding (Kalsbeek & Larsen, 1991). Acid salts of carboxylic acids and dicarboxylic acids have been extensively investigated structurally (Speakman, 1972) and spectroscopically (Hadži, 1965).

One of the main subjects of the research work is to understand the nature of the very short crystallographically symmetric hydrogen bonds linking the anions in infinite chains. Is the H atom effectively centered or is there a dynamical or statistical disorder? The first situation indicates a single minimum potential function for the H atom, the second a double minimum potential function.

Experimental. Suitable crystals for the diffraction studies of (1) and (2) were obtained by slow evaporation from aqueous solutions which contained equivalent molar amounts of succinic acid and the