Table 2. *Selected geometric parameters* (Å, °)

Host molecule			
S(1)—C(3)	1.701 (7)	C(4)—C(5)	1.381 (9)
S(1)—C(4)	1.697 (8)	C(4)—C(6)	1.489 (11)
S(2)—C(9)	1.715 (7)	C(6)—C(7)	1.464 (14)
S(2)—C(10)	1.715 (6)	C(8)—C(9)	1.361 (9)
S(3)—C(15)	1.698 (7)	C(8)—C(11)	1.422 (9)
S(3)—C(16)	1.723 (7)	C(10)—C(11)	1.359 (8)
O(1)—C(6)	1.250 (10)	C(10)—C(12)	1.469 (9)
O(2)—C(12)	1.210 (8)	C(12)—C(13)	1.508 (10)
O(3)—C(18)	1.225 (9)	C(14)—C(15)	1.357 (9)
C(1)—C(2)	1.508 (9)	C(14)—C(17)	1.445 (9)
C(1)—C(8)	1.519 (9)	C(16)—C(17)	1.371 (9)
C(1)—C(14)	1.519 (9)	C(16)—C(18)	1.475 (9)
C(2)—C(3)	1.356 (10)	C(18)—C(19)	1.487 (11)
C(2)—C(5)	1.424 (10)		
Guest molecule			
C(20)—Cl(1)	1.687 (9)	C(20)—Cl(2)′	1.642 (13)
C(20)—Cl(2)	1.719 (11)	C(20)—Cl(3)′	1.733 (14)
C(20)—Cl(3)	1.742 (12)	C(20)—Cl(4)′	1.686 (13)
C(20)—Cl(4)	1.627 (10)		
Host molecule			
C(3)—S(1)—C(4)	90.9 (3)	O(2)—C(12)—C(10)	121.4 (6)
C(9)—S(2)—C(10)	91.5 (3)	O(2)—C(12)—C(13)	122.5 (6)
C(15)—S(3)—C(16)	91.5 (3)	C(10)—C(12)—C(13)	116.0 (6)
C(2)—C(1)—C(8)	112.4 (5)	C(1)—C(14)—C(15)	125.9 (6)
C(2)—C(1)—C(14)	112.9 (5)	C(1)—C(14)—C(17)	122.1 (5)
C(8)—C(1)—C(14)	110.3 (5)	C(15)—C(14)—C(17)	112.0 (6)
C(1)—C(2)—C(3)	122.7 (6)	S(3)—C(15)—C(14)	113.1 (5)
C(1)—C(2)—C(5)	126.0 (6)	S(3)—C(16)—C(17)	112.2 (5)
C(3)—C(2)—C(5)	111.2 (6)	O(1)—C(6)—C(4)	117.4 (8)
S(1)—C(3)—C(2)	113.8 (5)	O(1)—C(6)—C(7)	122.8 (8)
S(1)—C(4)—C(5)	112.7 (5)	C(4)—C(6)—C(7)	119.8 (7)
S(1)—C(4)—C(6)	120.7 (6)	C(1)—C(8)—C(9)	126.1 (6)
C(5)—C(4)—C(6)	126.6 (7)	C(1)—C(8)—C(11)	122.6 (5)
C(2)—C(5)—C(4)	111.5 (6)	C(16)—C(18)—C(19)	120.0 (6)
C(9)—C(8)—C(11)	111.3 (5)	S(3)—C(16)—C(18)	121.9 (5)
S(2)—C(9)—C(8)	112.5 (5)	C(17)—C(16)—C(18)	125.9 (6)
S(2)—C(10)—C(11)	111.3 (5)	C(14)—C(17)—C(16)	111.3 (6)
S(2)—C(10)—C(12)	118.5 (4)	O(3)—C(18)—C(16)	117.8 (6)
C(11)—C(10)—C(12)	130.2 (6)	O(3)—C(18)—C(19)	122.2 (6)
C(8)—C(11)—C(10)	113.4 (5)		
Guest molecule			
Cl(1)—C(20)—Cl(2)	105.3 (6)	Cl(1)—C(20)—Cl(2)′	107.0 (6)
Cl(1)—C(20)—Cl(3)	110.6 (6)	Cl(1)—C(20)—Cl(3)′	101.3 (7)
Cl(1)—C(20)—Cl(4)	111.6 (6)	Cl(1)—C(20)—Cl(4)′	122.2 (8)
Cl(2)—C(20)—Cl(3)	105.1 (6)	Cl(2)′—C(20)—Cl(3)′	109.9 (9)
Cl(2)—C(20)—Cl(4)	111.8 (6)	Cl(2)′—C(20)—Cl(4)′	111.6 (8)
Cl(3)—C(20)—Cl(4)	112.0 (7)	Cl(3)′—C(20)—Cl(4)′	103.8 (9)

The structure was solved by direct methods with the program *SOLVER* (Gabe, Le Page, Charland, Lee & White, 1989) and refined by full-matrix least squares using the *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989) system of programs. All the non-H atoms were refined with anisotropic displacement parameters. All positions and displacement parameters of the H atoms were calculated. The CCl_4 solvent is partially disordered. Cl(1) and C(20) are ordered but there are two orientations of the remaining Cl atoms, a major (65%) and a minor (35%).

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71621 (33 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: CD1049]

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Structures of the Choline Ion in Different Crystal Surroundings

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Abstract

The crystal structures of four choline salts have been determined: choline (*S*)-*N*-acetylserinate, $C_5H_{14}NO^+.C_5H_8NO_4^-$, choline (*R*,*R*)-hydrogentartrate, $C_5H_{14}NO^+.C_4H_5O_6^-$, choline (±)-*N*-acetylphenylalaninate, $C_5H_{14}NO^+.C_{11}H_{12}NO_3^-$, and dicholine phthalate, $2C_5H_{14}NO^+.C_8H_4O_4^{2-}$. In these compounds the choline ion adopts two different conformations, extended and folded, both of which are low-energy conformations. In all four crystal structures, the hydroxy group of the choline ion is involved in a hydrogen bond to a carboxylate group. Short contacts between the quaternary ammonium groups and the carboxylate groups are not observed, but there are many weak contacts.

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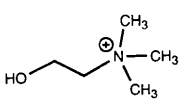
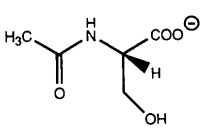
Comment

Acetylcholine is a neurotransmitter in the peripheral as well as in the central nervous system. As the detailed molecular structures of the cholinergic receptors are still unknown, there is interest in the construction of models of the interactions between macromolecules and acetylcholine or related compounds. Crystallographic studies of choline salts have been performed in order to obtain information which would contribute to the reliability of such models. Studies of some salts of *N*-acetylated amino acids and choline and related compounds have been presented (Jensen, 1990).

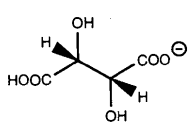
The crystal structure determinations of choline (*S*)-*N*-acetylserinate (SERCHO), choline (*R*,*R*)-hydrogentartrate (BITART), choline (±)-*N*-acetylphenylalaninate (PHECHO) and dicholine phthalate (TALCHO) have been carried out in order to study possible preferred contacts to the quaternary ammonium group of choline and structurally related compounds.



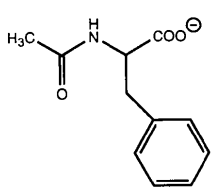
Choline



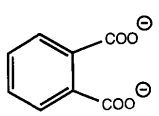
(*S*)-*N*-Acetylserinate



(*R*,*R*)-Hydrogentartrate



dl-*N*-Acetylphenylalaninate



Phthalate

Different conformations of the choline ion are observed (Fig. 1): folded conformations with the torsion angle O—C—C—N being −66.4 (2), −73.5 (2), ± 63.4 (5) and 65.0 (2)°, and an extended conformation with the torsion angle O—C—C—N being 170.9 (1)°. The magnitude of the O—C—C bond angle varies from 107.8 (1) (TALCHO) to 115.1 (1)° (SERCHO, PHECHO, BITART and TALCHO). This great variation in the magnitude of the O—C—C angle has also been found for choline esters (Jensen, 1984), and it was observed that the O—C—C angle is small in extended conformers.

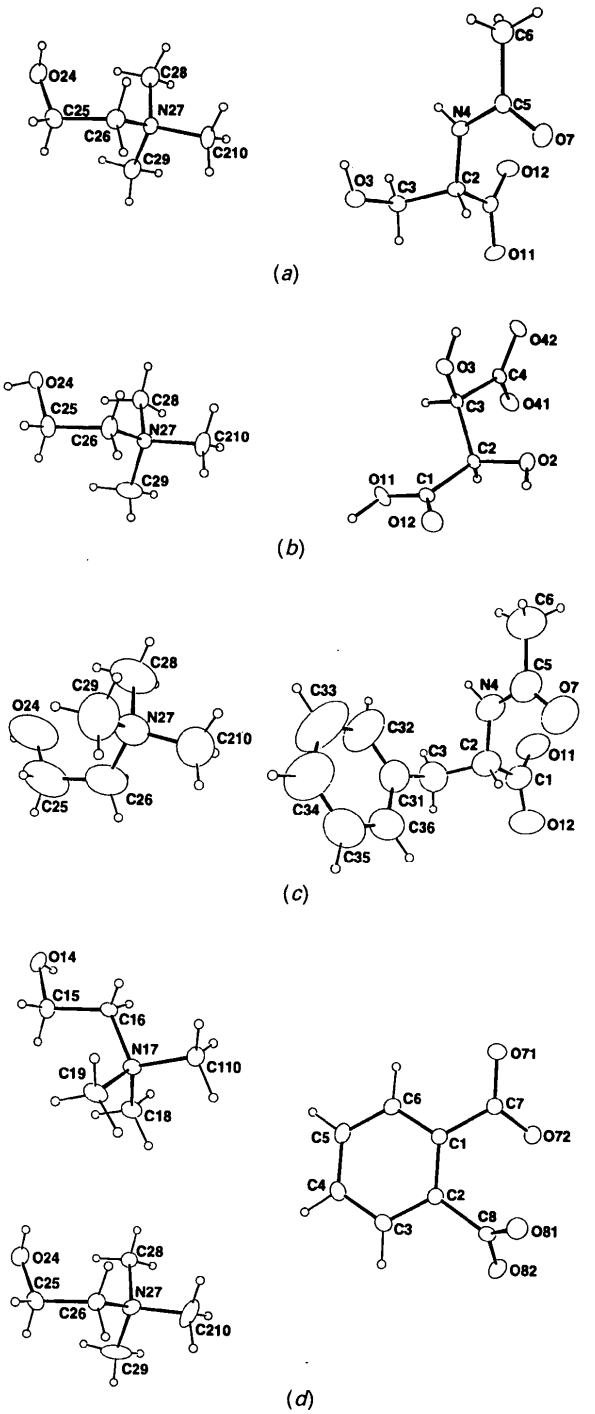


Fig. 1. The ions of the four title compounds with atomic labelling and displacement ellipsoids at the 50% probability level (*ORTEP*II; Johnson, 1976) are shown. The five independent choline ions are oriented in a mutual way. The figure shows (*a*) SERCHO, (*b*) BITART, (*c*) PHECHO and (*d*) TALCHO.

The choline fragments O—C—C—N(C)$_3$, as present in the CSD (Cambridge Structural Database, 1992), have been analyzed. 59 different fragments

were found and a list of refcodes have been deposited. Fig. 2 shows the variation in the bond angle in correlation with the torsion angles. Very few structures are observed in the extended conformation and the O—C—C bond angles for these structures are in the range 100–105°. The present structure determination of a choline ion in the extended conformation produced a larger O—C—C bond angle of 107.8 (1)°. In this choline ion, the O—C—C—N angle is approximately *anti*, but the H—O—C—C angle is *gauche*. The three extended fragments in the CSD are all fully extended (C—O—C—C *anti*, O—C—C—N *anti*). For one structure (ACTART10; Jensen, 1982) the data in the CSD give some very unusual angles (O—C—C—N −10°, O—C—C 125°). This structure is disordered and only some of the atomic positions are thus stored in the database. Care should be taken with more or less automatic use of the CSD.

All bond lengths within the choline ions are in the expected ranges (Frydenvang, Jensen & Nielsen, 1992) (Table 2). The H—O—C—C angle varies due to different hydrogen-bond patterns in the different crystal surroundings (Figs. 1 and 3). The structure of PHECHO is based on data measured at room temperature. Bond lengths and angles are, therefore, of lower accuracy and systematic errors due to large displacement parameters give rise to bond lengths which are too short.

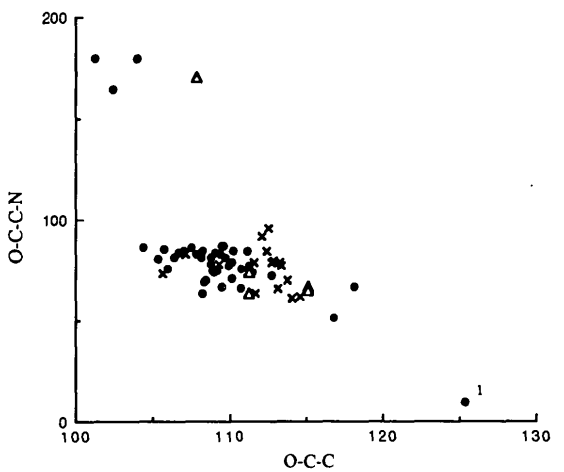


Fig. 2. The variations in the O—C—C bond angle compared to the O—C—C—N angle are shown; the results were derived from the Cambridge Structural Database and the present structure determinations. Symbols used are: the angle (C—O—C—C) *anti* ●, or *gauche* x, and the present structure determinations Δ. The label 1 indicates the data for ACTART10 (Jensen, 1982).

The crystal packing in SERCHO is dominated by hydrogen bonds. The choline ion donates a hydrogen bond to the carboxylate group of serine (O—H···O). The hydroxy and the amide group of the serine ion form hydrogen bonds to the carboxylate groups of neighbouring serine ions. Many weak contacts from the quaternary ammonium group to O atoms are observed. The shortest one involves the carbonyl O atom of the amide and is well below the sum of the van der Waals radii, O7···C29 $(1-x, \frac{1}{2}+y, \frac{1}{2}-z)$ 3.176 (2) Å. No especially short contact to the carboxylate group of serine is observed [shortest O11···C28 $(\frac{1}{2}+x, \frac{3}{2}-y, 1-z)$ 3.301 (2) Å].

The choline ion in BITART donates a hydrogen bond to the carboxylate of the bitartrate. Furthermore, a weak contact [O3···O24 2.891 (2) Å] between the choline ion and the hydroxy group (O3) of the bitartrate may be classified as a hydrogen bond [H3···O24 2.21 (4) Å], or could be a result of crystal packing. The bitartrate ions are connected into strands by hydrogen bonds from the carboxylic acid group in one ion to the carboxylate group in another ion. Many weak contacts are observed from the quaternary ammonium group to O atoms. The shortest contacts to a carboxylate group are O12···C210 $(x+2, y+1, z)$ 3.389 (2) Å and O41···C29 $(x+1, y, z+1)$ 3.484 (3) Å, which are both approximately the sum of the van der Waals radii.

The choline ion in PHECHO donates a hydrogen bond to the carboxylate group of phenylalanine. Another hydrogen bond is observed between two phenylalanine ions (the amide NH to the carboxylate). Many contacts are observed from the quaternary ammonium group to O atoms. The shortest contact is to the carbonyl O atom of the amide group, C210···O7 $(1-x, \frac{1}{2}+y, \frac{3}{2}-z)$ 3.250 (4) Å, well below the sum of the van der Waals radii. The shortest contact to a carboxylate group is C210···O12 $(1-x, y-\frac{1}{2}, \frac{3}{2}-z)$ 3.347 (5) Å.

In TALCHO, neighbouring benzene rings are roughly perpendicular to one other. Each phthalate ion is connected *via* hydrogen bonds to the carboxylate groups of two crystallographically independent choline ions. The quaternary ammonium groups form many weak contacts to both hydroxy and carboxylate O atoms. Many contacts, well below the sum of the van der Waals radii, to aromatic as well as aliphatic C atoms, are also found. No single strong contact to a quaternary ammonium group is observed.

The hydroxy group of all four choline ions is involved in hydrogen bonds to the carboxylate groups of the counter ions; the dimensions of the nearly linear hydrogen bonds are very similar. The C—O bond of the carboxylate group is always elongated when the O atom accepts a hydrogen bond. No special short contacts from the quaternary ammonium group to the carboxylate groups are observed,

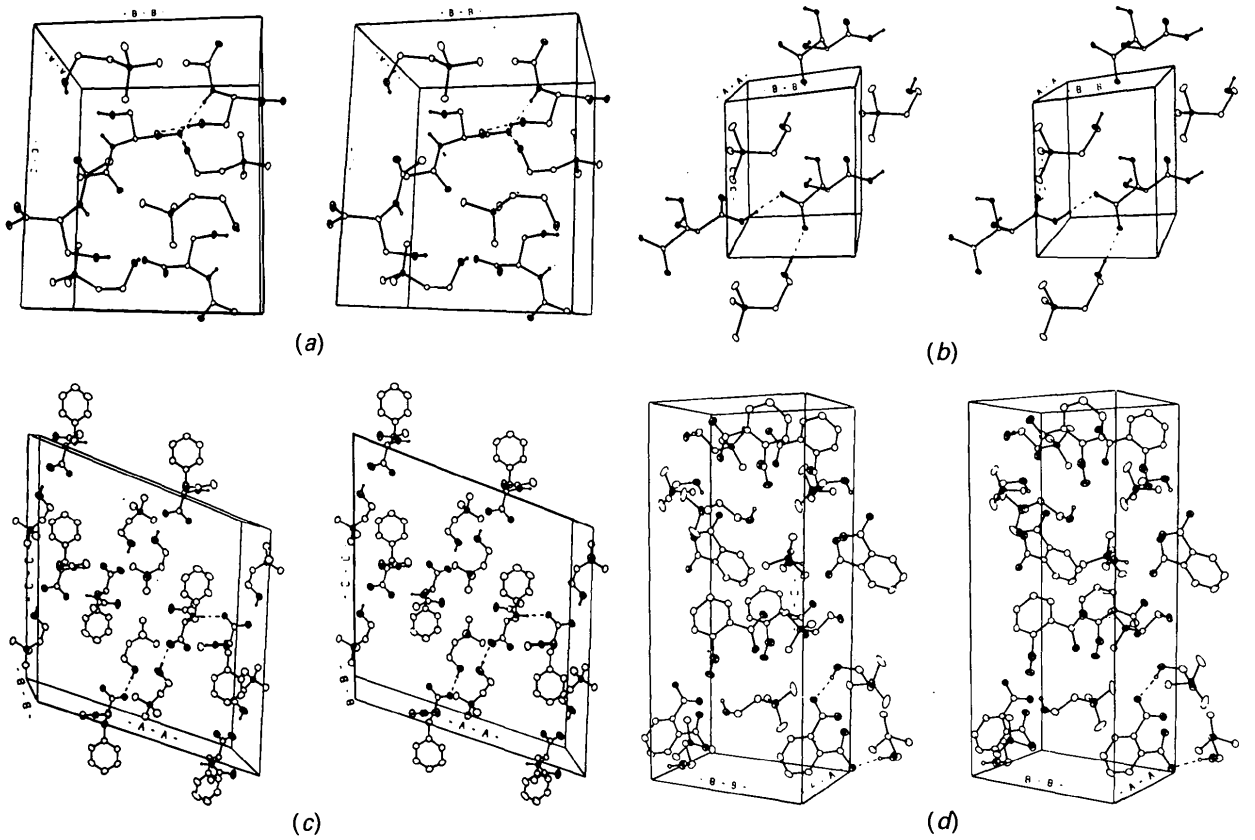


Fig. 3. Stereo drawings of the unit cells of the four title compounds. O and N atoms appear as filled circles and H atoms connected to O and N atoms are shown. The figure shows (*a*) SERCHO (horizontal *y*, vertical *z* and *x* into the plane of the paper), (*b*) BITART (horizontal *y*, vertical *z* and *x* into the plane of the paper), (*c*) PHECHO (horizontal *x*, vertical *z* and *y* into the plane of the paper) and (*d*) TALCHO (horizontal *y*, vertical *z* and *x* into the plane of the paper).

but electrostatic interactions between the groups may still be of some importance. This type of contact is expected at the receptor site where an aspartic acid group is known to be present and of importance for the binding characteristics of the receptor (Fraser, Wang, Robinson, Gocayne & Venter, 1989). The shortest contacts to the ammonium group involve amide O atoms, which are present everywhere in proteins.

Experimental

SERCHO, PHECHO and TALCHO have been prepared as follows using strictly stoichiometric amounts of the acids, silver nitrate and choline iodide. The acid was dissolved in water and added to a suspension of freshly precipitated silver oxide, washed to neutral reaction. Finally, a solution of choline iodide in water was added. The precipitated silver iodide was removed and the water evaporated. The residue was dried by repeated additions of toluene and ethanol, followed by evaporation. Extremely hygroscopic single crystals were obtained when dry acetone was added to the freshly prepared salts. Single crystals of BITART were obtained by the slow cooling of a hot ethanol/water solution of the compound.

SERCHO

Crystal data

$C_5H_{14}NO^+.C_5H_8NO_4^-$
M_r = 250.3
Orthorhombic
$P2_12_12_1$
a = 9.997 (2) Å
b = 10.347 (2) Å
c = 12.680 (1) Å
V = 1311.7 (6) Å^3
Z = 4
D_x = 1.267 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71073 Å
Cell parameters from 18 reflections
θ = 15.85-20.05°
μ = 0.09 mm^{-1}
T = 105 K
Prism
0.3 × 0.3 × 0.2 mm
Colourless
M.p. = 389.5-390.5 K (hot stage microscope)

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
8402 measured reflections
7571 independent reflections
3795 observed reflections [$I \geq 3\sigma(I)$]
R_{int} = 0.014
θ_{max} = 40°
$h = 0 \rightarrow 18$
$k = 0 \rightarrow 18$
$l = -22 \rightarrow 22$
3 standard reflections
frequency: 166.7 min
intensity variation: −4.0%

Refinement

Refinement on F
$R = 0.041$
$wR = 0.043$
$S = 0.696$
3795 reflections
215 parameters
$w = 1/[\sigma^2(F) + 0.0004F^2]$
$(\Delta/\sigma)_{max} = 0.03$
$\Delta\rho_{max} = 0.526$ e Å^{-3}
$\Delta\rho_{min} = -0.588$ e Å^{-3}
Atomic scattering factors from *SDP* (B. A. Frenz & Associates, Inc., 1982)

BITART

Crystal data

$C_5H_{14}NO^+.C_4H_5O_6^-$
$M_r = 253.3$
Triclinic
$P\bar{1}$
$a = 6.228$ (1) Å
$b = 6.819$ (1) Å
$c = 7.494$ (1) Å
$\alpha = 95.42$ (2)°
$\beta = 99.48$ (1)°
$\gamma = 108.99$ (1)°
$V = 293.0$ (2) Å^3
$Z = 1$
$D_x = 1.435$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 18 reflections
$\theta = 19.52$-22.35°
$\mu = 0.12$ mm^{-1}
$T = 122$ K
Prism
0.35 × 0.3 × 0.2 mm
Colourless
M.p. = 418.5-419.5 K (hot stage microscope)

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
7713 measured reflections
7710 independent reflections
3856 observed reflections $[I \geq 5\sigma(I)]$
$R_{int} = 0.057$
$\theta_{max} = 40$°
$h = -12 \rightarrow 13$
$k = -14 \rightarrow 13$
$l = -16 \rightarrow 15$
3 standard reflections
frequency: 166.7 min
intensity variation: −1.9%

Refinement

Refinement on F
$R = 0.053$
$wR = 0.074$
$S = 1.797$
3856 reflections
208 parameters
$w = 1/[\sigma^2(F) + 0.0009F^2]$
$(\Delta/\sigma)_{max} = 0.13$
$\Delta\rho_{max} = 0.582$ e Å^{-3}
$\Delta\rho_{min} = -0.622$ e Å^{-3}
Atomic scattering factors from *SDP* (B. A. Frenz & Associates, Inc., 1982)

PHECHO

Crystal data

$C_5H_{14}NO^+.C_{11}H_{12}NO_3^-$
$M_r = 310.4$
Monoclinic
$I2/a$
$a = 21.438$ (3) Å
$b = 8.161$ (1) Å
$c = 21.655$ (6) Å
$\beta = 109.98$ (2)°
$V = 3561$ (2) Å^3
$Z = 8$
$D_x = 1.158$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 18 reflections
$\theta = 15.11$-20.62°
$\mu = 0.08$ mm^{-1}
$T = 295$ K
Prism
0.5 × 0.25 × 0.25 mm
Colourless
M.p. = 416-419 K (hot stage microscope)

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
6950 measured reflections
3140 independent reflections
1337 observed reflections $[I \geq 3\sigma(I)]$
$R_{int} = 0.013$
$\theta_{max} = 25$°
$h = 0 \rightarrow 25$
$k = -9 \rightarrow 9$
$l = -25 \rightarrow 24$
3 standard reflections
frequency: 166.7 min
intensity variation: −1.9%

Refinement

Refinement on F
$R = 0.041$
$wR = 0.061$
$S = 1.331$
1337 reflections
202 parameters
$w = 1/[\sigma^2(F) + 0.0016F^2]$
$(\Delta/\sigma)_{max} = 0.20$
$\Delta\rho_{max} = 0.166$ e Å^{-3}
$\Delta\rho_{min} = -0.130$ e Å^{-3}
Atomic scattering factors from *SDP* (B. A. Frenz & Associates, Inc., 1982)

TALCHO

Crystal data

$2C_5H_{14}NO^+.C_8H_4O_4^{2-}$
$M_r = 372.5$
Orthorhombic
$P2_12_12_1$
$a = 7.951$ (2) Å
$b = 10.6133$ (9) Å
$c = 23.421$ (4) Å
$V = 1976.5$ (9) Å^3
$Z = 4$
$D_x = 1.252$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 16.30$-19.55°
$\mu = 0.09$ mm^{-1}
$T = 105$ K
Prism
0.3 × 0.2 × 0.2 mm
Colourless
M.p. = 401-404 K (hot stage microscope)

Data collection

Enraf-Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
7085 measured reflections
6180 independent reflections
3751 observed reflections $[I \geq 5\sigma(I)]$
$R_{int} = 0.014$
$\theta_{max} = 31$°
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 15$
$l = -33 \rightarrow 32$
3 standard reflections
frequency: 166.7 min
intensity variation: none

Refinement

Refinement on F
$R = 0.031$
$wR = 0.039$
$S = 0.96$
3751 reflections
363 parameters
$w = 1/[\sigma^2(F) + 0.0009F^2]$
$(\Delta/\sigma)_{max} = 0.34$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Atomic scattering factors from *SDP* (B. A. Frenz & Associates, Inc., 1982)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
SERCHO				
C1	0.4615 (1)	1.0063 (1)	0.1897 (1)	1.17 (2)
O12	0.3901 (1)	1.10274 (9)	0.21211 (8)	1.56 (2)
O11	0.5841 (1)	1.0096 (1)	0.16971 (9)	1.97 (2)
C2	0.3897 (1)	0.8744 (1)	0.1917 (1)	1.12 (2)
C3	0.3565 (1)	0.8418 (1)	0.3066 (1)	1.35 (2)
O3	0.2735 (1)	0.73122 (9)	0.31676 (9)	1.65 (2)
N4	0.4666 (1)	0.7706 (1)	0.14598 (9)	1.17 (2)
C5	0.4656 (1)	0.7447 (1)	0.0423 (1)	1.22 (2)
C6	0.5556 (2)	0.6352 (2)	0.0094 (1)	1.81 (2)
O7	0.3962 (1)	0.8043 (1)	−0.02122 (8)	1.88 (2)
O24	0.3736 (1)	0.88249 (9)	0.68604 (9)	1.69 (2)
C25	0.3634 (2)	0.8256 (1)	0.5857 (1)	1.73 (2)
C26	0.3020 (1)	0.6914 (1)	0.5842 (1)	1.44 (2)
N27	0.3814 (1)	0.5853 (1)	0.63708 (9)	1.23 (2)
C28	0.3794 (2)	0.5995 (2)	0.7552 (1)	1.81 (2)
C29	0.5240 (2)	0.5852 (2)	0.6001 (1)	2.02 (3)
C210	0.3195 (2)	0.4586 (1)	0.6079 (1)	1.84 (3)
BITART				
C1	1.338	0.880	0.801	0.98 (2)
O11	1.3172 (2)	1.0623 (2)	0.8470 (2)	1.40 (2)
O12	1.4830 (2)	0.8498 (2)	0.7216 (2)	1.66 (2)
C2	1.1605 (2)	0.7020 (2)	0.8631 (2)	0.84 (2)
O2	1.1935 (2)	0.5094 (2)	0.8246 (2)	1.21 (2)
C3	0.9135 (2)	0.6816 (2)	0.7741 (2)	0.80 (2)
O3	0.8816 (2)	0.6381 (2)	0.5818 (2)	1.08 (2)
C4	0.7410 (2)	0.5148 (2)	0.8543 (2)	0.96 (2)
O41	0.7665 (3)	0.5387 (3)	1.0249 (2)	1.60 (2)
O42	0.5840 (2)	0.3709 (2)	0.7398 (2)	1.37 (2)
O24	0.5143 (2)	0.3938 (3)	0.2750 (2)	1.61 (2)
C25	0.3200 (3)	0.4609 (3)	0.2539 (3)	1.74 (3)
C26	0.1600 (3)	0.3677 (3)	0.3784 (3)	1.50 (3)
N27	0.0145 (2)	0.1374 (2)	0.3270 (2)	1.08 (2)
C28	0.1631 (3)	0.0030 (3)	0.3402 (3)	1.68 (3)
C29	−0.1289 (4)	0.0891 (4)	0.1373 (3)	2.32 (4)
C210	−0.1419 (3)	0.0881 (3)	0.4625 (3)	1.98 (3)
PHECHO				
O24	0.4703 (1)	0.9271 (5)	0.7230 (1)	10.5 (1)
C25	0.4221 (2)	0.9047 (7)	0.7519 (2)	8.6 (1)
C26	0.4490 (2)	0.8127 (2)	0.8147 (2)	6.2 (1)
N27	0.5040 (1)	0.8902 (3)	0.8700 (1)	4.47 (6)
C28	0.5681 (2)	0.8857 (6)	0.8572 (2)	7.6 (1)
C29	0.4879 (2)	1.0601 (5)	0.8819 (2)	7.0 (1)
C210	0.5123 (2)	0.7943 (5)	0.9307 (2)	5.97 (9)
C1	0.3705 (1)	0.8661 (4)	0.5656 (1)	4.39 (7)
O11	0.33336 (9)	0.8012 (3)	0.5913 (1)	6.00 (6)
O12	0.4236 (1)	0.9381 (3)	0.5957 (1)	6.90 (6)
C2	0.3532 (1)	0.8601 (4)	0.4909 (1)	4.21 (7)
C3	0.3280 (1)	1.0254 (4)	0.4596 (1)	4.89 (8)
N4	0.3057 (1)	0.7328 (3)	0.4593 (1)	4.19 (6)
C5	0.3231 (1)	0.5825 (4)	0.4504 (1)	4.61 (8)
C6	0.2680 (2)	0.4653 (5)	0.4179 (2)	6.6 (1)
O7	0.3814 (1)	0.5380 (3)	0.4677 (1)	7.13 (7)
C31	0.3267 (1)	1.0392 (4)	0.3901 (2)	4.85 (8)
C32	0.2711 (2)	1.0080 (8)	0.3386 (2)	9.5 (1)
C33	0.2721 (2)	1.013 (1)	0.2749 (2)	13.5 (2)
C34	0.3286 (2)	1.0557 (8)	0.2627 (2)	10.4 (2)
C35	0.3843 (2)	1.0893 (5)	0.3138 (2)	6.5 (1)
C36	0.3837 (2)	1.0806 (4)	0.3769 (2)	5.36 (9)
TALCHO				
C1	0.8536 (2)	−0.0965 (1)	0.57541 (6)	1.09 (2)
C2	0.7703 (2)	−0.1813 (1)	0.61149 (6)	1.04 (2)
C3	0.7779 (2)	−0.3106 (1)	0.59877 (7)	1.32 (3)
C4	0.8639 (2)	−0.3541 (1)	0.55139 (7)	1.61 (3)
C5	0.9446 (2)	−0.2698 (2)	0.51528 (7)	1.85 (3)
C6	0.9380 (2)	−0.1420 (2)	0.52730 (7)	1.49 (3)
C7	0.8683 (2)	0.0420 (1)	0.59062 (7)	1.09 (2)
O71	0.8794 (2)	0.1197 (1)	0.54979 (5)	1.75 (2)
O72	0.8745 (1)	0.0693 (1)	0.64244 (5)	1.44 (2)
C8	0.6719 (2)	−0.1383 (1)	0.66346 (6)	1.14 (2)
O81	0.5461 (1)	−0.0704 (1)	0.65605 (5)	1.54 (2)
O82	0.7225 (2)	−0.1798 (1)	0.71125 (5)	1.62 (2)
O14	0.2729 (1)	0.1537 (1)	0.41563 (5)	1.62 (2)
C15	0.1014 (2)	0.1690 (2)	0.43074 (7)	1.50 (3)
C16	0.0180 (2)	0.2484 (1)	0.38459 (6)	1.06 (2)
N17	−0.1590 (2)	0.2921 (1)	0.39774 (5)	1.10 (2)
C18	−0.1563 (2)	0.3944 (2)	0.44196 (7)	1.60 (3)
C19	−0.2671 (2)	0.1851 (2)	0.41812 (7)	1.55 (3)
C110	−0.2315 (2)	0.3451 (2)	0.34341 (7)	1.42 (3)
O24	0.1539 (2)	0.5428 (1)	0.19869 (5)	1.76 (2)
C25	0.0673 (2)	0.4283 (2)	0.20530 (7)	1.67 (3)
C26	0.1530 (2)	0.3326 (1)	0.24325 (7)	1.23 (2)
N27	0.3201 (2)	0.2814 (1)	0.22213 (6)	1.41 (2)
C28	0.4558 (2)	0.3805 (1)	0.22375 (7)	1.33 (3)
C29	0.3066 (2)	0.2288 (2)	0.16327 (8)	2.72 (3)
C210	0.3710 (2)	0.1786 (2)	0.2631 (1)	2.72 (4)

Table 2. *Bond lengths* (Å), *bond angles* (°) *and torsion angles* (°) *for the four structure determinations*

For the choline ion

	SERCHO	BITART	PHECHO	TALCHO	
	x = 2	x = 2	x = 2	x = 1	x = 2
Hx4—Ox4	0.82 (2)	0.75 (5)	0.79 (3)	0.82 (2)	0.76 (2)
Ox4—Cx5	1.406 (2)	1.418 (3)	1.389 (5)	1.419 (2)	1.406 (2)
Cx5—Cx6	1.518 (2)	1.508 (3)	1.487 (6)	1.522 (2)	1.512 (2)
Cx6—Nx7	1.512 (2)	1.510 (2)	1.502 (4)	1.514 (2)	1.518 (2)
Nx7—Cx8	1.506 (2)	1.498 (2)	1.493 (5)	1.501 (2)	1.507 (2)
Nx7—Cx9	1.500 (2)	1.493 (3)	1.472 (5)	1.502 (2)	1.491 (2)
Nx7—Cx10	1.497 (2)	1.507 (3)	1.489 (5)	1.506 (2)	1.509 (2)
Hx4—Ox4—Cx5	104 (1)	101 (4)	115 (2)	103 (2)	111 (2)
Ox4—Cx5—Cx6	115.1 (1)	111.3 (2)	111.2 (3)	107.8 (1)	115.1 (1)
Cx5—Cx6—Nx7	116.5 (1)	117.0 (2)	118.0 (3)	115.5 (1)	116.3 (1)
Cx6—Nx7—Cx8	111.3 (1)	111.3 (1)	111.3 (3)	110.4 (1)	111.6 (1)
Cx6—Nx7—Cx9	111.2 (1)	111.6 (2)	111.7 (2)	111.4 (1)	111.9 (1)
Cx6—Nx7—Cx10	108.0 (1)	106.6 (2)	107.9 (3)	107.4 (1)	106.6 (1)
Cx8—Nx7—Cx9	108.9 (1)	108.8 (2)	109.9 (3)	109.6 (1)	109.6 (1)
Cx8—Nx7—Cx10	109.0 (1)	108.9 (2)	108.1 (3)	108.6 (1)	107.2 (1)
Cx9—Nx7—Cx10	108.4 (1)	109.7 (2)	107.8 (3)	109.4 (1)	109.7 (1)
Hx4—Ox4—Cx5—Cx6	−66 (2)	174 (4)	144 (2)	71 (2)	−58 (2)
Ox4—Cx5—Cx6—Nx7	−66.4 (2)	−73.5 (2)	63.4 (5)	−170.9 (1)	−65.0 (2)
Cx5—Cx6—Nx7—Cx8	71.9 (2)	65.9 (2)	−73.5 (4)	73.1 (2)	69.3 (2)
Cx5—Cx6—Nx7—Cx9	−49.7 (2)	−55.8 (2)	49.8 (4)	−49.0 (2)	−53.9 (3)
Cx5—Cx6—Nx7—Cx10	−168.4 (1)	−175.5 (2)	168.0 (3)	−168.7 (1)	−173.9 (1)

For the counter ions

	SERCHO	PHECHO
C1—O11	1.252 (2)	1.235 (4)
C1—O12	1.259 (2)	1.249 (3)
C1—C2	1.543 (2)	1.533 (4)
C2—C3	1.531 (2)	1.524 (5)
C2—N4	1.442 (2)	1.452 (4)
N4—C5	1.342 (2)	1.316 (4)
C5—O7	1.229 (2)	1.232 (4)
C5—C6	1.505 (2)	1.495 (4)
C3—O3	1.419 (2)	
C3—C31		1.500 (5)
C31—C32		1.350 (4)
C32—C33		1.389 (6)
C33—C34		1.369 (7)
C34—C35		1.350 (5)
C35—C36		1.372 (6)
C31—C36		1.387 (5)
O11—C1—O12	125.4 (1)	125.4 (3)
O11—C1—C2	118.9 (1)	120.1 (2)
O12—C1—C2	115.8 (1)	114.5 (3)
C1—C2—C3	108.1 (1)	111.3 (3)
C1—C2—N4	113.9 (1)	113.5 (3)
C3—C2—N4	109.6 (1)	109.8 (2)
C2—N4—C5	122.6 (1)	123.2 (2)
N4—C5—C6	114.7 (1)	116.6 (3)
N4—C5—O7	123.1 (1)	122.6 (3)
C6—C5—O7	122.2 (1)	120.8 (3)
C2—C3—O3	113.0 (1)	
C2—C3—C31		113.3 (3)
C3—C31—C32		121.6 (3)
C3—C31—C36		120.6 (2)

C31—C32—C33		120.5 (4)
C32—C33—C34		120.9 (4)
C33—C34—C35		119.2 (4)
C34—C35—C36		119.9 (4)
C35—C36—C31		121.8 (3)
C36—C31—C32		117.8 (3)
O11—C1—C2—C3	108.3 (1)	105.3 (3)
O11—C1—C2—N4	−13.7 (2)	−19.1 (4)
O12—C1—C2—C3	−69.6 (1)	−75.4 (3)
O12—C1—C2—N4	168.4 (1)	160.2 (3)
C1—C2—C3—O3	171.6 (1)	
C1—C2—C3—C31		165.5 (3)
N4—C2—C3—O3	−63.8 (1)	
N4—C2—C3—C31		−68.1 (3)
C1—C2—N4—C5	−86.0 (2)	−89.1 (3)
C3—C2—N4—C5	152.8 (1)	145.7 (3)
C2—N4—C5—C6	178.3 (1)	179.1 (3)
C2—N4—C5—O7	−2.4 (2)	−0.7 (5)
C2—C3—O3—H3	85 (1)	
C2—C3—C31—C32		95.3 (5)
C2—C3—C31—C36		−83.0 (4)
C3—C31—C32—C33		−176.5 (5)
C3—C31—C36—C35		178.1 (3)
C31—C32—C33—C34		−3 (1)
C32—C33—C34—C35		2 (1)
C33—C34—C35—C36		−0.0 (8)
C34—C35—C36—C31		−0.6 (6)
C35—C36—C31—C32		−0.3 (6)
C36—C31—C32—C33		1.8 (8)

BITART

C1—O11	1.311 (2)	C4—O41	1.250 (2)
C1—O12	1.218 (2)	C4—O42	1.263 (2)
C1—C2	1.523 (1)	C4—C3	1.535 (2)
C2—O2	1.405 (2)	C3—O3	1.411 (2)
C2—C3	1.528 (2)		
O11—C1—O12	126.1 (1)	O41—C4—O42	127.0 (2)
O11—C1—C2	112.06 (9)	C3—C4—O41	116.9 (1)
O12—C1—C2	121.8 (1)	C3—C4—O42	116.1 (1)
C1—C2—C3	110.8 (1)	C2—C3—C4	109.0 (1)
C1—C2—O2	111.9 (1)	C4—C3—O3	113.6 (1)
C3—C2—O2	109.8 (1)	C2—C3—O3	109.7 (1)
O11—C1—C2—C3	61.2 (1)	C2—C3—C4—O41	54.2 (2)
O11—C1—C2—O2	−175.9 (1)	O3—C3—C4—O41	176.8 (2)
O12—C1—C2—C3	−120.4 (1)	C2—C3—C4—O42	−127.8 (2)
O12—C1—C2—O2	2.4 (2)	O3—C3—C4—O42	−5.1 (2)
C1—C2—C3—O3	60.4 (2)	O2—C2—C3—C4	61.2 (2)
C1—C2—C3—C4	−174.7 (1)	O2—C2—C3—O3	−63.7 (2)

TALCHO

C1—C7	1.517 (2)	C2—C8	1.517 (2)
C7—O71	1.266 (2)	C8—O81	1.245 (2)
C7—O72	1.249 (2)	C8—O82	1.268 (2)
C1—C6	1.398 (2)	C2—C3	1.405 (2)
C6—C5	1.386 (2)	C3—C4	1.383 (2)
C1—C2	1.401 (2)	C4—C5	1.389 (2)
C2—C1—C6	119.4 (1)	C1—C2—C3	118.6 (1)
C6—C1—C7	119.1 (1)	C3—C2—C8	119.1 (1)
C2—C1—C7	121.2 (1)	C1—C2—C8	122.3 (1)
C1—C7—O71	117.4 (1)	C2—C8—O81	118.5 (1)
C1—C7—O72	117.2 (1)	C2—C8—O82	116.1 (1)
O71—C7—O72	125.5 (1)	O81—C8—O82	125.4 (1)
C1—C6—C5	121.3 (1)	C2—C3—C4	121.2 (1)
C6—C5—C4	119.3 (2)	C3—C4—C5	120.2 (1)
C7—C1—C2—C3	−172.4 (1)	C8—C2—C1—C6	−178.2 (1)
C7—C1—C6—C5	172.5 (2)	C8—C2—C3—C4	179.0 (1)
O71—C7—C1—C2	−151.7 (1)	O81—C8—C2—C1	63.6 (2)
O71—C7—C1—C6	34.3 (2)	O81—C8—C2—C3	−116.1 (2)
O72—C7—C1—C2	30.7 (2)	O82—C8—C2—C1	−119.2 (2)
O72—C7—C1—C6	−143.2 (2)	O82—C8—C2—C3	61.1 (2)
C2—C1—C6—C5	−1.6 (2)	C1—C2—C3—C4	−0.7 (2)
C1—C6—C5—C4	0.8 (3)	C2—C3—C4—C5	−0.1 (3)
C3—C4—C5—C6	0.0 (3)	C8—C2—C1—C7	7.9 (2)
C6—C1—C2—C3	1.5 (2)		

Table 3. *Hydrogen-bonding geometry* (Å, °) *for the four title structures*

D—H···*A*	H···*A*	*D*···*A*	*D*—H···*A*
SERCHO			
O24—H24···O12^{i}	1.86 (2)	2.661 (1)	165 (2)
O3—H3···O11^{ii}	1.91 (2)	2.704 (1)	173 (2)
N4—H4···O12^{ii}	2.08 (2)	2.883 (2)	172 (2)
BITART			
O24—H24···O41^{iii}	1.95 (5)	2.695 (2)	169 (6)
O3—H3···O24	2.21 (4)	2.891 (2)	142 (5)
O11—H11···O42^{iv}	1.60 (5)	2.514 (2)	171 (6)
PHECHO			
O24—H24···O12	1.80 (3)	2.593 (3)	173 (3)
N4—H4···O11^{v}	1.88	2.858 (3)	174
TALCHO			
O14—H14···O71^{vi}	1.87 (2)	2.675 (2)	167 (2)
O24—H24···O82^{vi}	1.87 (2)	2.619 (2)	168 (2)

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

Friedal pairs were not averaged for SERCHO, BITART and TALCHO, as two of the compounds and all three space groups are chiral. The structures were solved by direct methods (*MULTAN*80; Main *et al.*, 1980) and refined by full-matrix least-squares minimizations. The positions of the H atoms in SERCHO, BITART and TALCHO were determined from successive difference Fourier maps. Only the position of the hydroxy H atom in PHECHO could be determined (room-temperature study as the crystals were destroyed by cooling); the remaining H atoms were calculated and fixed completely. The non-H atoms of all four structures were refined anisotropically. *SDP* (B. A. Frenz & Associates, Inc., 1982) was used for all calculations.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and geometry, and refcodes from the Cambridge Structural Database for the compounds used in Fig. 2, have been deposited with the British Library Document Supply Centre as Supp'lementary Publication No. SUP 71601 (105 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AB0303]

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