

squares line of best fit  $(\text{Si}-\text{O})_{\text{est}} = 0.94(\text{Si}-\text{O})_{\text{obs}} + 0.09$  is statistically the same as the expected  $45^\circ$  line. We regard this as evidence of the correctness of the bonding model proposed for  $\text{Na}_2\text{ZnSi}_3\text{O}_8$ .<sup>\*</sup> Zn—O bonds may be predicted reasonably well by adding to the intercept the difference between the mean Zn—O and Si—O distances ( $1.945 - 1.623 = 0.322 \text{ \AA}$ ).

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### References

CRAIG, J. R., LOUISNATHAN, S. J. & GIBBS, G. V. (1973). *Trans. Amer. Geophys. Union*, **54**, 496.

<sup>\*</sup> A reviewer has pointed out that the equation  $\text{Si}-\text{O} = 1.623 - 0.055\Delta Z_{\text{Nbr}}$  estimates Si—O slightly better than the more general equation derived and used successfully by Phillips & Ribbe (1973) and Ribbe (1974) for the aluminosilicates. This indicates that  $\Delta Z_{\text{Nbr}}$  can be considered to be the preponderant factor in the analysis of bonding effects in  $\text{Na}_2\text{ZnSi}_3\text{O}_8$ , although this may not be the case in other framework structures. For example, in  $\text{Na}_2\text{ZnSiO}_4$  (Plakhov, Simonov, Egorov-Tismenko & Belov, 1976)  $[\text{ZnO}_4]$  and  $[\text{SiO}_4]$  tetrahedra alternate in the framework, and therefore  $\Delta Z_{\text{Nbr}}$  is zero for all Si—O bonds. Our model predicts Si—O bond lengths of 1.645, 1.636, 1.645, 1.634 Å corresponding to observed values 1.640, 1.625, 1.648, 1.626 Å. The longer Si—O bond lengths are those to O atoms coordinated by three Na atoms, the shorter to those coordinated by only two Na.

- GIBBS, G. V., HAMIL, M. M., LOUISNATHAN, S. J., BARTELL, L. S. & YOW, H. (1972). *Amer. Min.* **57**, 1578–1613.
- GRIFFEN, D. T., RIBBE, P. H. & GIBBS, G. V. (1977). *Amer. Min.* **62**. In the press.
- HAMILTON, D. L. & HENDERSON, C. M. B. (1968). *Miner. Mag.* **36**, 832–838.
- HESSE, K.-F. (1972). Dissertation, Univ. Kiel.
- HESSE, K.-F. & LIEBAU, F. (1974). *Fortschr. Miner.* **51**, Supp. 1, 75–76.
- HOWELLS, E. R., PHILLIPS, D. C. & ROGERS, D. (1950). *Acta Cryst.* **3**, 210–217.
- LIEBAU, F. (1972). In *Handbook of Geochemistry*, Vol. II/3, edited by K. H. WEDEPOHL. New York: Springer.
- LITVIN, B. N., MEL'NIKOV, O. K., ILYUKHIN, V. V. & NIKITIN, A. V. (1965). *Sov. Phys. Crystallogr.* **9**, 795–796.
- LOUISNATHAN, S. J. & GIBBS, G. V. (1972a). *Mater. Res. Bull.* **7**, 1281–1292.
- LOUISNATHAN, S. J. & GIBBS, G. V. (1972b). *Amer. Min.* **57**, 1614–1642.
- PHILLIPS, M. W. & RIBBE, P. H. (1973). *Contr. Miner. Petrol.* **39**, 327–339.
- PLAKHOV, G. F., SIMONOV, M. A. & BELOV, N. V. (1974). *Dokl. Akad. Nauk SSSR*, **215**, 1109–1112.
- PLAKHOV, G. F., SIMONOV, M. A., EGOROV-TISMENKO, YU. K. & BELOV, N. V. (1976). *Kristallografiya*, **21**, 73–75.
- RIBBE, P. H. (1974). *Amer. Min.* **59**, 341–344.
- ROSSI, G., TAZZOLI, V. & UNGARETTI, L. (1974). *Amer. Min.* **59**, 335–340.
- SMITH, J. V. (1953). *Acta Cryst.* **6**, 613–620.

*Acta Cryst.* (1977). **B33**, 1337–1341

## A Neutron Diffraction Study of Anhydrous Ethylenediamine D-Tartrate

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$\text{C}_6\text{H}_{14}\text{N}_2\text{O}_6$ , monoclinic,  $P2_1$ ,  $a = 8.974(5)$ ,  $b = 8.797(5)$ ,  $c = 5.984(4)$  Å,  $\beta = 105.40(10)^\circ$ ,  $Z = 2$ ,  $\rho_{\text{obs}} = 1.52(1)$ ,  $\rho_{\text{calc}} = 1.533(3)$  g cm<sup>-3</sup>. Neutron diffraction was used to locate precisely all the H atoms. The structure consists of diprotonated ethylenediamine cations and tartrate anions with extensive interionic hydrogen bonding and a weak intraionic hydrogen bond between a tartrate —OH and —COO<sup>-</sup> group [ $\text{O}-\text{H} = 0.956(6)$  Å and  $\text{H}\cdots\text{O} = 2.138(8)$  Å]. The shortest hydrogen bonds are from amine H atoms to carboxyl O atoms [ $\text{H}(21)\cdots\text{O}(2) = 1.74(1)$  and  $\text{H}(20)\cdots\text{O}(1) = 1.74(1)$  Å]. A comparison with D-tartaric acid is presented.

### Experimental

The crystal was provided by G. K. Johnson and was prepared by slow evaporation at room temperature of a one-to-one aqueous mixture of ethylenediamine and D-tartaric acid. Only the anhydrous form was obtained. The crystal used for this study was bounded by ten faces and had axial dimensions of

about  $0.30 \times 0.40 \times 0.15$  cm. The neutron data were collected on a Mitsubishi Diffractometer equipped with a full circle, designed and built by the Department of Physics, University of Missouri—Columbia, machine shop, and interfaced to a PDP-11 computer at the University of Missouri Research Reactor. The data were collected by the  $\theta$ - $2\theta$  step-scan technique. With 25 carefully centered reflections, for

most of which  $2\theta$  was between  $45$  and  $80^\circ$ , the neutron wavelength from the Be monochromator was determined to be  $1.109(3)$  Å, based on the reported cell dimensions (Pérez, Leger & Housty, 1973). Correction for background, integration, and  $L_p$  correction were accomplished with a local program. The data were corrected for absorption ( $\mu = 2.08$  cm $^{-1}$  and transmission factor =  $0.57$  to  $0.78$ ). The 1930 measured reflections were reduced to 1060 independent reflections of which the 997 with  $F_o^2 > 2.5\sigma(F_o^2)$  were used to refine the structure [ $\sigma^2(F_o^2) = \sigma^2(\text{counting}) + (0.03F_o^2)^2$ ]. The structure was then refined beginning with the reported coordinates (Pérez *et al.*, 1973). The final refinement, minimizing the function  $\Sigma \omega(F_o^2 - F_c^2)^2$ ,

allowed for anisotropic parameters of all 28 atoms as well as an isotropic extinction parameter [ $g = 3.26(8) \times 10^{-4}$ ] and resulted in a final conventional  $R$  value of 3.35%.\* Neutron scattering amplitudes were taken from Bacon (1972).

The coordinates of the atoms, along with those from the latest X-ray study (Pérez, 1976), are presented in Table 1, thermal parameters in Table 2, bond distances

\* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32211 (7 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Positional parameters* ( $\times 10^4$ )

Numbers in parentheses represent, throughout, the standard deviations. The X-ray coordinates (Pérez *et al.*, 1973) are on the second line for each atom, and those of Pérez (1976) are on the third.

	x	y	z		x	y	z
C(3)	8232 (2)	1284	6236 (3)	H(15)	5952 (6)	424 (9)	5774 (10)
	8234 (5)	1284 (6)	6236 (8)		6011 (67)	562 (69)	5845 (71)
	8238 (3)	1282 (6)	6247 (5)		6026 (43)	716 (43)	5829 (63)
C(4)	6514 (2)	1250 (4)	4898 (4)	H(16)	5882 (6)	3150 (8)	6219 (10)
	6513 (5)	1244 (6)	4895 (8)		5860 (82)	3292 (57)	6088 (82)
	6518 (3)	1247 (5)	4905 (5)		5884 (46)	3206 (46)	5945 (68)
C(6)	6376 (3)	698 (4)	2411 (4)	H(17)	6893 (7)	-457 (8)	2526 (11)
	6378 (5)	681 (6)	2421 (8)		6853 (75)	-338 (65)	2468 (66)
	6379 (4)	693 (5)	2416 (6)		6837 (39)	-380 (39)	2438 (56)
C(8)	4673 (3)	577 (4)	1075 (4)	H(18)	6475 (7)	2406 (10)	427 (10)
	4672 (5)	578 (7)	1058 (8)		6709 (51)	2407 (74)	177 (79)
	4676 (4)	570 (5)	1079 (6)		6610 (50)	2457 (53)	402 (71)
C(12)	983 (3)	1283 (4)	2211 (4)	H(19)	2398 (6)	2280 (7)	373 (9)
	990 (5)	1269 (7)	2202 (9)		2253 (69)	2356 (82)	278 (90)
	985 (4)	1260 (6)	2223 (6)		2370 (72)	2180 (73)	215 (109)
C(13)	2053 (2)	1422 (4)	4643 (4)	H(20)	1383 (7)	3533 (8)	1535 (10)
	2056 (5)	1417 (7)	4650 (9)		1412 (70)	3345 (70)	1515 (98)
	2051 (4)	1420 (5)	4644 (6)		1460 (55)	3525 (56)	1390 (82)
N(11)	1351 (2)	2486 (4)	716 (3)	H(21)	479 (6)	2531 (8)	-846 (9)
	1355 (5)	2485 (6)	728 (7)		680 (77)	2633 (92)	-623 (99)
	1350 (3)	2479 (4)	762 (5)		582 (60)	2959 (64)	-826 (90)
N(14)	1888 (2)	101 (4)	6086 (3)	H(22)	1175 (9)	193 (9)	1465 (10)
	1888 (5)	109 (5)	6079 (8)		1189 (85)	333 (88)	1617 (63)
	1875 (3)	92 (4)	6078 (5)		1108 (44)	274 (48)	1632 (64)
O(1)	8896 (3)	23 (5)	6702 (5)	H(23)	-220 (6)	1379 (11)	2201 (11)
	8896 (4)	19 (5)	6694 (7)		-60 (91)	1284 (91)	2207 (78)
	8897 (3)	7 (3)	6704 (4)		-47 (55)	1405 (61)	2226 (75)
O(2)	8893 (3)	2531 (5)	6738 (5)	H(24)	3240 (6)	1509 (11)	4588 (11)
	8890 (4)	2534 (5)	6748 (7)		3148 (63)	1571 (78)	4406 (86)
	8889 (3)	2528 (3)	6742 (4)		3131 (48)	1531 (51)	4550 (67)
O(5)	5800 (3)	2685 (5)	4711 (5)	H(25)	1790 (10)	2449 (8)	5485 (10)
	5797 (4)	2680 (5)	4716 (7)		1821 (72)	2258 (64)	5629 (89)
	5796 (3)	2671 (3)	4721 (4)		1782 (47)	2246 (47)	5376 (66)
O(7)	7185 (4)	1668 (6)	1271 (6)	H(26)	2031 (10)	-898 (9)	5279 (12)
	7195 (4)	1683 (6)	1300 (7)		2001 (75)	-724 (82)	5534 (86)
	7188 (3)	1671 (4)	1289 (4)		1982 (57)	-913 (62)	5579 (81)
O(9)	3893 (4)	-506 (5)	1483 (6)	H(27)	2686 (7)	-217 (9)	7652 (10)
	3890 (4)	-512 (5)	1491 (8)		2565 (81)	-479 (100)	7625 (120)
	3896 (3)	-513 (4)	1467 (5)		2660 (67)	306 (68)	7619 (92)
O(10)	4143 (3)	1610 (5)	-362 (5)	H(28)	801 (6)	64 (7)	6373 (9)
	4148 (4)	1602 (6)	-351 (7)		854 (115)	-195 (154)	6511 (199)
	4148 (3)	1610 (4)	-342 (4)		834 (69)	50 (77)	6539 (96)

Table 2. *Final thermal parameters* ( $\times 10^4$ )

Anisotropic temperature factors are of the form:  
 $\exp[-2\pi^2(h^2U_{11}a^{*2} + k^2U_{22}b^{*2} + l^2U_{33}c^{*2} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23})]$ .

	$U_{11}$	$U_{22}$	$U_{33}$	$U_{12}$	$U_{13}$	$U_{23}$
C(3)	142 (9)	232 (10)	201 (9)	-5 (9)	-5 (7)	37 (9)
C(4)	131 (9)	281 (11)	200 (9)	6 (9)	6 (8)	13 (9)
C(6)	146 (9)	310 (12)	230 (10)	15 (9)	15 (8)	-14 (9)
C(8)	158 (9)	331 (12)	218 (10)	-15 (9)	7 (8)	-33 (9)
C(12)	172 (10)	336 (12)	275 (11)	-26 (10)	8 (8)	-51 (11)
C(13)	193 (12)	328 (12)	242 (10)	-55 (10)	24 (8)	-70 (11)
N(11)	234 (9)	322 (10)	288 (9)	20 (7)	23 (7)	-54 (8)
N(14)	231 (9)	210 (9)	280 (9)	12 (7)	16 (7)	-65 (8)
O(1)	185 (11)	235 (12)	384 (15)	45 (10)	17 (10)	78 (11)
O(2)	228 (12)	228 (12)	332 (13)	-39 (11)	-64 (11)	43 (12)
O(5)	250 (13)	358 (15)	276 (14)	115 (12)	15 (10)	-15 (13)
O(7)	172 (12)	612 (24)	281 (13)	-46 (15)	55 (11)	73 (15)
O(9)	273 (14)	359 (15)	443 (17)	-75 (12)	46 (13)	-19 (13)
O(10)	224 (13)	551 (23)	287 (13)	-9 (13)	-44 (11)	119 (14)
H(15)	290 (22)	643 (38)	356 (23)	-64 (23)	89 (19)	86 (24)
H(16)	398 (28)	427 (26)	394 (28)	85 (23)	106 (21)	-85 (23)
H(17)	367 (26)	452 (29)	524 (32)	132 (24)	77 (23)	-73 (24)
H(18)	359 (28)	654 (37)	375 (24)	-14 (30)	99 (22)	72 (30)
H(19)	295 (25)	482 (31)	209 (24)	6 (23)	121 (21)	-19 (22)
H(20)	455 (29)	441 (34)	397 (27)	23 (25)	50 (22)	-88 (25)
H(21)	328 (25)	483 (28)	375 (25)	50 (24)	18 (23)	-20 (25)
H(22)	735 (42)	448 (34)	350 (27)	-68 (32)	21 (28)	-110 (25)
H(23)	257 (25)	787 (43)	593 (34)	-49 (30)	72 (22)	62 (39)
H(24)	219 (24)	810 (49)	572 (33)	-143 (28)	89 (21)	24 (34)
H(25)	779 (45)	374 (29)	423 (28)	-2 (31)	138 (29)	-116 (27)
H(26)	759 (45)	427 (35)	484 (32)	140 (31)	194 (32)	-37 (27)
H(27)	352 (25)	690 (42)	396 (30)	50 (28)	-17 (24)	-49 (28)
H(28)	310 (24)	395 (24)	436 (26)	-35 (23)	86 (20)	-7 (22)

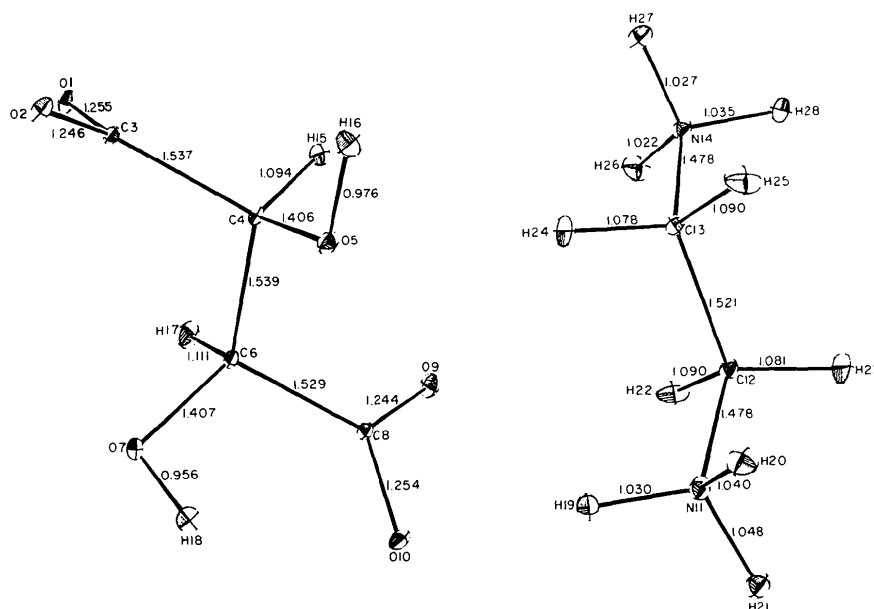


Fig. 1. Bond distances (Å) [numbering system after Pérez *et al.* (1973)]. The standard deviations are: C-N and C-C 0.003; C-O 0.004; C-H 0.006-0.007; N-H 0.005-0.006; and O-H 0.006-0.009 Å.

Table 3. *Hydrogen bonds* ( $X-H \cdots Y$ )

	$X \cdots Y$ (Å)	$X-H$ (Å)	$H \cdots Y$ (Å)	$X-H \cdots Y$ (°)
O(7)—H(18) $\cdots$ O(10)*	2.645 (4)	0.957 (9)	2.138 (7)	111.7 (6)
O(7)—H(18) $\cdots$ O(9)†	2.999 (4)	0.957 (9)	2.142 (8)	148.5 (5)
O(5)—H(16) $\cdots$ O(9)	2.732 (4)	0.976 (6)	1.783 (7)	163.0 (6)
N(11)—H(19) $\cdots$ O(10)	2.854 (4)	1.030 (5)	1.833 (6)	170.9 (5)
N(11)—H(20) $\cdots$ O(1)	2.757 (4)	1.040 (6)	1.742 (7)	164.0 (6)
N(11)—H(21) $\cdots$ O(2)†	2.783 (4)	1.048 (5)	1.739 (6)	173.5 (5)
N(14)—H(26) $\cdots$ O(2)	2.798 (4)	1.022 (6)	1.877 (8)	147.5 (7)
N(14)—H(26) $\cdots$ O(5)*	3.095 (5)	1.022 (6)	2.311 (8)	132.1 (6)
N(14)—H(27) $\cdots$ O(10)	2.844 (4)	1.027 (7)	1.948 (8)	144.6 (6)
N(14)—H(28) $\cdots$ O(2)	2.798 (4)	1.035 (5)	1.772 (6)	176.9 (5)

\* Not included in the hydrogen-bond tables of Pérez *et al.* (1973) or Pérez (1976).

† Not included in the hydrogen-bond table of Pérez *et al.* (1973).

Table 4. *Bond angles* (°)

O(1)—C(3)—C(4)	116.7 (2)	C(12)—N(11)—H(21)	109.5 (4)
O(1)—C(3)—O(2)	123.8 (2)	H(19)—N(11)—H(20)	109.7 (5)
O(2)—C(3)—C(4)	119.4 (2)	H(19)—N(11)—H(21)	109.4 (5)
C(3)—C(4)—O(5)	113.4 (2)	H(20)—N(11)—H(21)	107.9 (5)
C(3)—C(4)—C(6)	108.8 (2)	N(11)—C(12)—C(13)	109.6 (2)
C(3)—C(4)—H(15)	106.8 (3)	N(11)—C(12)—H(22)	107.3 (4)
O(5)—C(4)—C(6)	106.8 (2)	N(11)—C(12)—H(23)	108.9 (5)
O(5)—C(4)—H(15)	112.1 (4)	C(13)—C(12)—H(22)	109.5 (4)
C(6)—C(4)—H(15)	108.9 (4)	C(13)—C(12)—H(23)	112.0 (4)
C(4)—C(6)—O(7)	110.9 (2)	H(22)—C(12)—H(23)	109.4 (7)
C(4)—C(6)—C(8)	109.9 (2)	C(12)—C(13)—N(14)	111.1 (2)
C(4)—C(6)—H(17)	107.7 (4)	C(12)—C(13)—H(24)	110.8 (4)
O(7)—C(6)—C(8)	111.2 (2)	C(12)—C(13)—H(25)	110.5 (4)
O(7)—C(6)—H(17)	108.9 (4)	N(14)—C(13)—H(24)	109.1 (5)
C(8)—C(6)—H(17)	108.2 (4)	N(14)—C(13)—H(25)	108.3 (4)
C(6)—C(8)—O(9)	119.1 (3)	H(24)—C(13)—H(25)	107.0 (7)
C(6)—C(8)—O(10)	116.9 (2)	C(13)—N(14)—H(26)	110.7 (5)
O(9)—C(8)—O(10)	123.9 (3)	C(13)—N(14)—H(27)	107.6 (5)
C(4)—O(5)—H(16)	112.5 (4)	C(13)—N(14)—H(28)	111.5 (4)
C(6)—O(7)—H(18)	108.2 (4)	H(26)—N(14)—H(27)	107.0 (6)
C(12)—N(11)—H(19)	110.9 (4)	H(26)—N(14)—H(28)	107.0 (6)
C(12)—N(11)—H(20)	109.4 (4)	H(27)—N(14)—H(28)	108.3 (5)

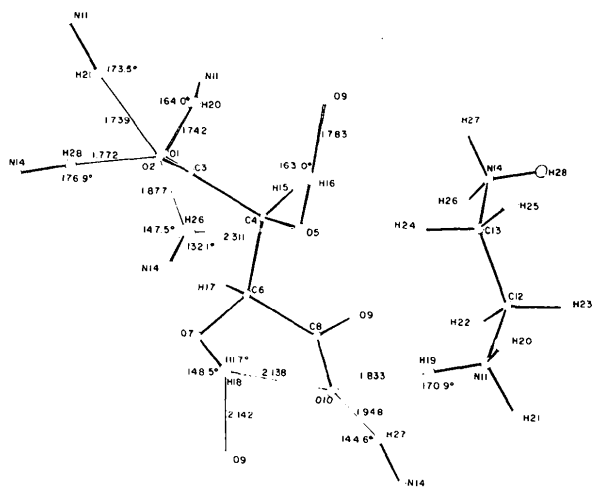


Fig. 2. Hydrogen-bond distances (Å) and angles (°). The standard deviations in the distances are 0.006–0.008 Å and in the angles 0.5–0.7°. The narrow lines indicate hydrogen bonds.

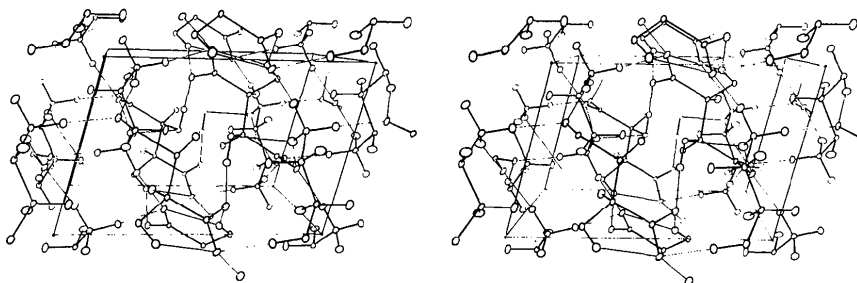


Fig. 3. Stereoscopic view of unit-cell contents and the associated hydrogen bonds (narrow lines). The view is nearly down the  $b$  axis as in Fig. 2. This figure can be compared with Fig. 3 of Pérez (1976).

in Fig. 1, and hydrogen-bond angles and distances in Fig. 2 and Table 3. Fig. 3 presents a stereo view of the crystal packing. The bond angles are given in Table 4.

### Discussion

The primary interest in this structure was the nature of the hydrogen-bond interactions in comparison with those in D-tartaric acid. Although the earlier X-ray studies (Pérez *et al.*, 1973; Pérez, 1976) reported H atom positions, those positions were not of high accuracy nor was the hydrogen bonding completely described.

Because of the presence of the ethylenediammonium ion, the hydrogen bonding in this salt is considerably different from that in tartaric acid (Okaya, Stemple & Kay, 1966). In the present compound the shortest hydrogen bonds ( $H \cdots Y$ ) (Table 3) are between H atoms on the ethylenediamine N atoms and carboxyl O atoms, two of length 1.74 (1) Å, but the shortest  $X \cdots Y$  distance (2.732 Å) is from the hydroxyl O(5) to the carboxyl O(9) on an adjacent ion. These distances can be compared with the shortest  $O \cdots O$  distances (2.63 and 2.71 Å) and the shortest

$H \cdots O$  distances of 1.64 and 1.71 Å in tartaric acid. As in tartaric acid each half of the tartrate ion ( $O_2C-CO$ ) is nearly planar (Table 5). The dihedral angle between the two planes is 33° compared with the 55° angle observed for tartaric acid. The half containing O(7) and O(10), which are associated by an intraionic hydrogen bond  $H(18) \cdots O(10)$  (2.138 Å), deviates most from planarity. That hydroxyl group is involved in a nearly symmetrically bifurcated hydrogen bond in that the interionic  $H(18) \cdots O(9)$  distance of 2.142 Å is almost identical with the intraionic  $H \cdots O$  distance (Figs. 2 and 3).

The nonhydrogen bond distances are all within one X-ray standard deviation ( $\pm 0.005-0.007$  Å) of those reported by Pérez *et al.* (1973) except C(6)-O(7), which is 0.016 Å shorter in this study, and C(13)-N(4), which is 0.013 Å longer. These two distances in the present study are in remarkable agreement with their chemically equivalent counterparts in the other half of the ion. Interestingly the refinement reported by Pérez (1976) gives coordinates (Table 1) and bond distances which are in somewhat poorer agreement with the present study. No unusual features are observed in either the bond distances or bond angles.

Correction of the distances involving H atoms for riding on C, N, or O gave a somewhat smaller range of distances C-H (1.115-1.138), N-H (1.044-1.062), and O-H (0.969-0.990 Å). The actual distances are probably intermediate between these corrected distances and those shown in Fig. 1.

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### References

- BACON, G. E. (1972). *Acta Cryst.* **A28**, 357-358.  
 OKAYA, Y., STEMPLE, N. R. & KAY, M. I. (1966). *Acta Cryst.* **21**, 237-243.  
 PÉREZ, S. (1976). *Acta Cryst.* **B32**, 2064-2070.  
 PÉREZ, S., LEGER, J. M. & HOUSTY, J. (1973). *Cryst. Struct. Commun.* **2**, 303-306.

Table 5. *Least-squares planes and atomic deviations (Å)*

O(9), O(10), C(6), C(8), O(7) plane

$$3.48(5)X - 5.36(7)Y - 4.61(6)Z - 0.83(1) = 0$$

O(9)	0.112 (4)	O(7)	0.186 (4)
O(10)	-0.086 (4)	H(18)	-0.063
C(6)	-0.098 (3)	H(17)	0.650
C(8)	-0.010 (3)	C(4)	-1.491

O(1), O(2), C(3), C(4), O(5) plane

$$4.23(11)X + 0.53(2)Y - 5.82(15)Z + 0.07(1) = 0$$

O(1)	-0.063 (3)	O(5)	-0.073 (3)
O(2)	0.048 (3)	H(16)	-0.894
C(3)	-0.006 (2)	H(15)	-0.751
C(4)	0.044 (2)	C(6)	1.401