ApSimon (1984). (In the latter work a *trans* stereochemistry was tentatively assigned to the hydroxyl-bearing 7,8 linkage. This assignment is now shown to be incorrect.)

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Structure of Bis(1,2,3-triaminoguanidinium) Bis(5-aminotetrazolate) Monohydrate

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Abstract. $2CH_9N_6^+.2CH_2N_5^-.H_2O$, $M_r = 396{\cdot}4$, monoclinic, $C2/c$, $a = 10{\cdot}448\ (2)$, $b = 10{\cdot}387\ (1)$, $c = 15{\cdot}544\ (3)$ Å, $\beta = 93{\cdot}11\ (1)°$, $V = 1684{\cdot}4\ (5)$ Å^3, $Z = 4$, $D_x = 1{\cdot}56$ cm^{-3}, λ(Cu $K\alpha$) $= 1{\cdot}5418$ Å, $\mu = 10{\cdot}01$ cm^{-1}, $F(000) = 840$, $T = 296\ (1)$ K, final $R = 0{\cdot}041$ for 956 unique observed reflections. Ions and water molecules are packed in hydrogen-bonded helicoidal chains which are laterally hydrogen-bonded to form an infinite three-dimensional network. Close non-hydrogen-bonded N···N contacts are 3·043 (4) Å between unlike ions, 3·143 (4) Å between cations and 3·114 (4) Å between anions. Short hydrogen-bonded distances are 2·925 (4) Å (N–H···N) between cations, 2·899 (4) Å (N–H···N) between unlike ions, and 2·838 (3) Å (O–H···N) between the water molecule and the anion.

Experimental. Title compound $[(TAG5AT)_2.H_2O]$* recrystallized from water, pale-pink acicular crystal (0·05 × 0·05 × 0·20 mm) mounted on a glass fiber with its long axis approximately coaxial with the φ axis of the goniometer. Enraf–Nonius CAD-4 computer-controlled κ-axis diffractometer equipped with a graphite-crystal incident-beam monochromator. Lattice parameters obtained using 25 reflections in range $6 < \theta < 19°$. Intensity data* (upper limit 150° 2θ) collected with ω–θ scan technique on 1894 reflections (1733 unique, h 0→13, k −6→12, l −19→19). Systematic absences: hkl $h + k = 2n+1$; $h0l$ $l = 2n+1$. 3 standard reflections, 1% intensity variation. Data corrected for Lorentz and polarization effects, no correction for absorption. A secondary-extinction correction was applied (Zachariasen, 1963); final coefficient refined by least squares to $12{\cdot}5\ (6) \times 10^{-6}$ (absolute units). Structure solved by direct methods using 225 reflections (minimum E of 1·55) and 2374 relationships yielding 16 phase set having: absolute figure of merit = 1·32, residual = 0·18 and $\psi_0 = 1{\cdot}160$. Remaining atoms located in succeeding difference Fourier synthesis. Non-H atoms refined anisotropically and H atoms isotropically in full-matrix least squares. $\sum w(|F_o| - |F_c|)^2$ minimized; $w = 4F_o^2/\sigma^2(F_o^2)$. Scattering factors from Cromer & Waber (1974), anomalous dispersion included (Ibers & Hamilton, 1964) and f' and f'' values from Cromer (1974). Refinement of 172 variable parameters using 956

* Provided by John C. Gray, Rockwell International, Rocketdyne Division, Canoga Park, California.

* Lists of structure factors, anisotropic thermal parameters and interatomic hydrogen distances and angles, and hydrogen-bonding details have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42577 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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reflections ($I > 3\sigma$) converged with a largest parameter shift of 0·02 times its e.s.d.; $R = 0{\cdot}041$, $wR = 0{\cdot}052$, $S = 1{\cdot}24$. Max. and min. heights in final difference Fourier synthesis 0·25 (5) and −0·02 (5) e Å^{-3}. Atomic coordinates and isotropic thermal parameters are presented in Table 1; selected interatomic distances in Table 2. The TAG cation and 5AT anion are depicted in Fig. 1, and a stereoview of the unit-cell packing in Fig. 2.

Table 1. *Atomic coordinates and isotropic temperature factors and their e.s.d.'s*

	x	y	z	B_{eq}*/B(Å^2)
TAG cation				
C(1)	−0·0181 (3)	0·2008 (3)	0·0863 (2)	1·99 (5)
N(1)	0·0737 (2)	0·1902 (2)	0·1480 (1)	2·36 (5)
N(2)	0·1884 (2)	0·1260 (3)	0·1301 (2)	2·84 (5)
N(3)	−0·0021 (2)	0·1506 (2)	0·0093 (2)	2·39 (5)
N(4)	−0·1065 (2)	0·1558 (2)	−0·0529 (2)	2·55 (5)
N(5)	−0·1263 (2)	0·2619 (3)	0·1018 (9)	2·44 (5)
N(6)	−0·1443 (2)	0·3076 (3)	0·1851 (2)	2·76 (5)
H(2)	0·072 (3)	0·237 (4)	0·198 (2)	5·1 (8)
H(3)	0·243 (3)	0·188 (3)	0·114 (2)	4·1 (8)
H(4)	0·227 (3)	0·096 (3)	0·181 (2)	3·7 (8)
H(5)	0·077 (3)	0·119 (3)	−0·009 (2)	4·1 (8)
H(6)	−0·127 (3)	0·080 (3)	−0·065 (2)	4·1 (8)
H(7)	−0·075 (3)	0·185 (3)	−0·106 (2)	5·7 (9)
H(8)	−0·189 (3)	0·282 (4)	0·059 (2)	6·1 (10)
H(9)	−0·219 (3)	0·286 (3)	0·196 (2)	4·9 (9)
H(10)	−0·134 (3)	0·404 (3)	0·178 (2)	6·7 (10)
AT anion				
C(2)	0·6145 (3)	0·0206 (3)	0·1218 (2)	2·16 (6)
N(7)	0·4913 (2)	0·0694 (3)	0·1241 (2)	3·15 (6)
N(8)	0·6988 (2)	0·0227 (3)	0·1891 (2)	2·70 (5)
N(9)	0·8020 (2)	−0·0401 (3)	0·1598 (2)	2·91 (6)
N(10)	0·6580 (2)	−0·0377 (3)	0·0536 (2)	2·92 (6)
N(11)	0·7776 (2)	−0·0760 (3)	0·0805 (2)	3·16 (6)
H(11)	0·477 (3)	0·125 (3)	0·163 (2)	3·9 (8)
H(12)	0·441 (3)	0·062 (3)	0·072 (2)	5·3 (9)
Water of hydration				
O(1)	0·000	−0·1803 (3)	0·2500	4·62 (9)
H(1)	0·052 (3)	−0·133 (3)	0·277 (2)	5·9 (10)

* $B_{eq} = \frac{4}{3}\sum_i\sum_j \mathbf{a}_i.\mathbf{a}_j b_{ij}$.

Table 2. *Selected interatomic distances and angles and their e.s.d.'s*

TAG cation			
C(1)–N(1)	1·323 (3) Å	N(1)–C(1)–N(3)	120·0 (3)°
C(1)–N(3)	1·324 (3)	N(1)–C(1)–N(5)	119·9 (3)
C(1)–N(5)	1·330 (3)	N(3)–C(1)–N(5)	120·0 (3)
N(1)–N(2)	1·412 (3)	C(1)–N(1)–N(2)	119·1 (3)
N(3)–N(4)	1·419 (3)	C(1)–N(3)–N(4)	118·1 (2)
N(5)–N(6)	1·401 (3)	C(1)–N(5)–N(6)	119·1 (2)
AT anion			
C(2)–N(7)	1·386 (4) Å	N(7)–C(2)–N(8)	123·4 (3)°
C(2)–N(8)	1·331 (3)	N(7)–C(2)–N(10)	123·2 (3)
C(2)–N(10)	1·323 (3)	N(8)–C(2)–N(10)	113·3 (3)
N(8)–N(9)	1·360 (3)	C(2)–N(8)–N(9)	103·4 (2)
N(10)–N(11)	1·356 (3)	C(2)–N(10)–N(11)	103·8 (2)
N(9)–N(11)	1·299 (3)	N(8)–N(9)–N(11)	109·8 (2)
		N(9)–N(11)–N(10)	109·8 (2)

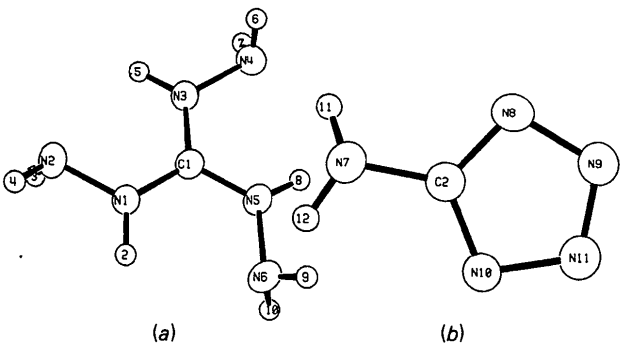

Fig. 1. (*a*) Triaminoguanidinium cation; (*b*) 5-aminotetrazolate anion.

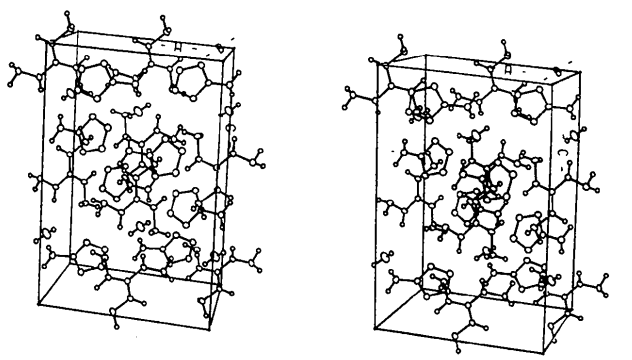

Fig. 2. Stereoscopic pair showing $(TAG5AT)_2$ monohydrate structure as viewed down the *c* axis.

Related literature. This compound is one of an extensive series of TAG salts currently being studied. Previous TAG salt investigations include the chloride (Okaya & Pepinsky, 1957; Bracuti, 1983) and the nitrate (Bracuti, 1979; Choi & Prince, 1979).

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