

Hydrogen-bonded supramolecular motifs in the 1:1 monohydrated molecular adduct of acetoguanaminium chloride with acetoguanamine and in 2,4,6-triaminopyrimidinediium dichloride dihydrate

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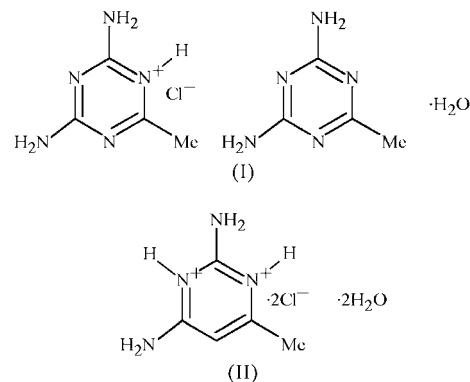
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In the 1:1 monohydrated molecular adduct 2,4-diamino-6-methyl-1,3,5-triazin-1-ium chloride 2,4-diamino-6-methyl-1,3,5-triazine monohydrate, $C_4H_8N_5^+ \cdot Cl^- \cdot C_4H_7N_5 \cdot H_2O$, formed between 2,4-diamino-6-methyl-1,3,5-triazin-1-ium chloride (acetoguanaminium chloride) and 2,4-diamino-6-methyl-1,3,5-triazine (acetoguanamine), and in triaminopyrimidinediium dichloride dihydrate, $C_4H_9N_5^{2+} \cdot 2Cl^- \cdot 2H_2O$, whose cationic component lies across a twofold rotation axis, the protonation occurs at the ring N atoms and the bond distances in the protonated molecules indicate significant bond alterations, consistent with charge-separated polar forms. The supramolecular structures of both compounds are stabilized by systems of hydrogen bonds forming complex sheets, interlinked by sets of hydrogen bonds involving the solvent water molecules and the chloride anions.

Comment

We report here the structures of the 1:1 monohydrated molecular adduct, (I), formed between 2,4-diamino-6-methyl-1,3,5-triazin-1-ium chloride [acetoguanaminium (AceguH⁺) chloride] and 2,4-diamino-6-methyl-1,3,5-triazine (acetoguanamine, Acegu), which we compare with the structure of 2,4,6-triaminopyrimidinediium (TripidH₂²⁺) dichloride dihydrate, (II). The heterocyclic system in (I) differs from that in (II) only in the replacement of one amino substituent on the triazine ring by a methyl substituent and by the substitution of an N atom for a C atom in the triazine ring, and this provides an opportunity to observe the effects that simple changes of substituent and in the heterocyclic skeleton exert upon the site of protonation and the supramolecular aggregation. This work is a continuation of our studies on crystal adducts of DNA/RNA pyrimidine bases coupled with amino derivatives of

aromatic N-heterocycles *via* multiple hydrogen bonds to mimic the base-pairing of nucleic acids (Portalone *et al.*, 1999, 2002; Brunetti *et al.*, 2000, 2002; Portalone & Colapietro, 2004*a,b*, 2006, 2007*a,b,c,d*; Portalone, 2007). In this context, our attention has been focused on the protonated form of the two previously mentioned aromatic N-heterocycles, as polyaminopyrimidine and polyamino-1,3,5-triazine are capable of interacting with RNA through Watson–Crick pairing (Gilbert *et al.*, 2006), and the relevance of proton transfer in DNA/RNA systems was demonstrated many years ago (Steenken, 1989, 1997).



The asymmetric unit of (I) consists of one protonated (AceguH⁺) and one neutral (Acegu) acetoguanamine molecule, a chloride anion and a water molecule of crystallization (Fig. 1). Of the different sites available in the acetoguanamine molecule, protonation occurs at one of the two ring N atoms

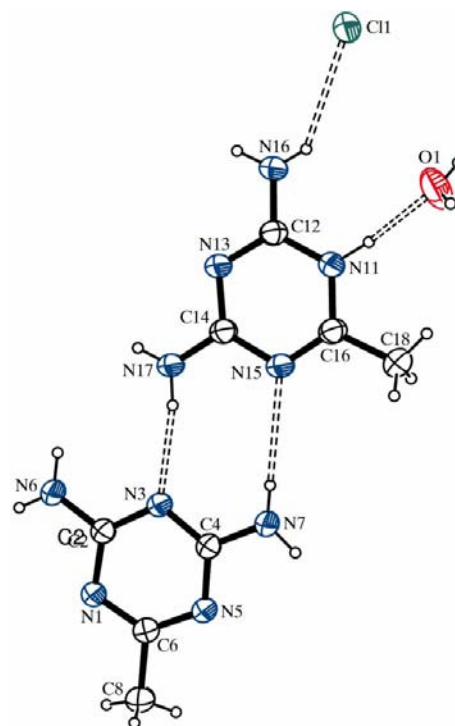
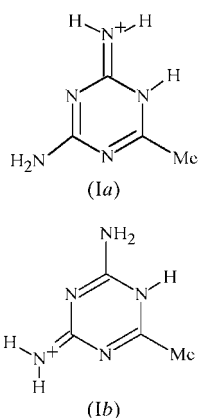


Figure 1

The asymmetric unit in (I), showing the atom-labelling scheme and hydrogen bonding (dashed lines). Displacement ellipsoids are drawn at the 50% probability level.

ortho to the C atom bearing the methyl group. Comparison of the molecular geometry of the planar heterocyclic ring of Acegu with that reported for guanamine (Portalone, 2007) shows that the corresponding bond lengths and angles are equal within experimental error and conform to C_s symmetry (Table 3). The effects of protonation can be appreciated by comparing the molecular geometry of the AceguH⁺ cation with that of the free base (Table 3), and can be summarized as follows: (i) an increase of the N11–C12 and N11–C16 bond distances by 0.007 (2) and 0.018 (2) Å, respectively; (ii) a decrease of the N13–C12, N15–C16, N16–C12 and N17–C14 bond distances by 0.014 (2)–0.026 (2) Å; (iii) an increase of the C12–N11–C16 bond angle by 5.6 (1)°; (iv) a decrease of the N11–C12–N13 and N11–C16–N15 bond angles by 4.1 (1) and 4.0 (1)°, respectively.

Protonation of atom N11 causes a redistribution of π -electron density so that the resulting distortions in the molecular geometry of the cation, which have been observed in the only two previously reported crystal structures containing the 2,4-diamino-6-methyl-1,3,5-triazin-1-ium unit (Wijaya *et al.*, 2004; Perpétuo & Janczak, 2007), point to the importance of the charge-separated quinoid forms (Ia) and (Ib) as significant contributors.



As previously mentioned, compound (I) crystallizes as a 1:1 monohydrated molecular adduct. In the crystal structure, the hydrogen-bonding scheme is rather complex and involves all available hydrogen-bond donor/acceptor sites, except for O1, which participates as a hydrogen-bond donor in two intermolecular interactions but in only one as an acceptor. In total, the supramolecular structure of (I) is characterized by 11 two-centre hydrogen bonds, namely nine N–H···X (X = N, O and Cl[−]) and two O–H···Y bonds (Y = N and Cl[−]) (Table 1), and is dominated by two main motifs. Firstly, an $R_2^2(8)$ ring (Etter *et al.*, 1990; Bernstein *et al.*, 1995; Motherwell *et al.*, 1999) forms from N–H···N double intermolecular hydrogen bonds between centrosymmetric coplanar Acegu pairs. These pairs further self-organize through $R_2^2(8)$ N–H···N double intermolecular hydrogen bonds with centrosymmetric coplanar $R_2^2(8)$ AceguH⁺ pairs to generate infinite chains of rings running approximately parallel to the [010] direction (Fig. 2). In other words, this hydrogen-bonding scheme corresponds to an alternating double repetition of AceguH⁺ and Acegu molecules. These infinite chains are then crosslinked by one

N⁺–H···O, one O–H···N and four N–H···Cl[−] intermolecular hydrogen bonds between pairs of Acegu and AceguH⁺ molecules, forming a sheet-like structure *via* four adjoining hydrogen-bonded rings [$R_3^2(8)$, $R_3^2(8)$, $R_4^2(8)$ and $R_4^2(12)$], and form the second major motif, also shown in Fig. 2. The hydrogen bonds so far discussed in the two-dimensional arrays in the *bc* plane are bridged by water molecules *via* O–H···Cl[−] interactions. It is noteworthy that in AceguH⁺, where the charge-separated forms (Ia) and (Ib) are significant, the intermolecular N–H···Cl[−] and N–H···N hydrogen bonds are characterized by shorter N···Cl[−] and N···N distances (Table 1) than those in Acegu where the development of comparable charge-separated forms is not possible.

The asymmetric unit of compound (II) comprises a planar half-molecule of 2,4,6-triaminopyrimidine disposed about a twofold axis along the line joining atoms N6, C2 and C5, and protonated at the ring N atom (TripidH⁺), a chloride anion and a water molecule of crystallization (Fig. 3). Comparison of the molecular geometry of TripidH⁺ with that reported for the free base (Schwalbe & Williams, 1982) was not possible because of the low accuracy of the latter structure determination (twinned crystals, $R = 0.104$ with a data-to-parameter ratio of 4.9 and standard deviations of 0.01 Å in bond lengths and 0.8° in bond angles for the two molecules in the asymmetric unit). Consequently, the effects of protonation can be appreciated by matching the molecular geometry of the TripidH⁺ cation with that of Acegu (Table 3). As for (I), the observed geometrical distortions suggest that the charge-separated quinoid forms (IIa), (IIb) and (IIc) are significant contributors to the overall molecular–electronic structure.

The crystal packing of (II) involves all available hydrogen-bond donor/acceptor sites, and is stabilized by seven hydrogen bonds, namely five N–H···X (X = O and Cl[−]) and two O–H···Cl[−] bonds (Table 2). The supramolecular structure takes

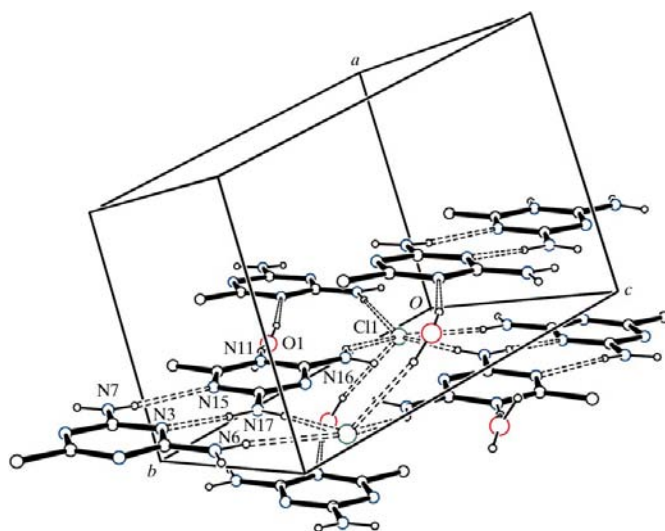
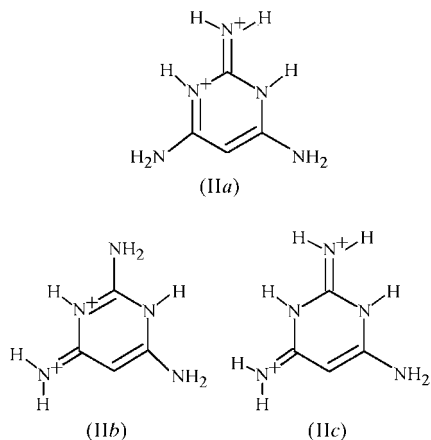


Figure 2
A perspective view of the crystal packing for (I) approximately along the *c*-axis direction. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonding is indicated by dashed lines.

the form of sheets generated by a combination of $\text{N}-\text{H}\cdots\text{Cl}^-$, $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{Cl}^-$ hydrogen bonds (Fig. 4); this may be contrasted with (I), where $\text{N}-\text{H}\cdots\text{N}$ and $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds are present. Moreover, at variance with the previously observed supramolecular organization of (I), in the



two-dimensional arrays in (II), water molecules and Cl^- anions act as bridges between TripidH_2^{2+} cations, forming three different types of hydrogen-bonded rings, *viz.* one of $R_2^2(8)$ type, one of $R_2^1(6)$ type and one of $R_4^3(8)$ type. The (010)-nets thus formed are themselves linked into a three-dimensional network by pairs of $\text{O1}-\text{H1}\cdots\text{Cl1}^{\text{iii}}$ [symmetry code: (iii) $-x + \frac{3}{2}, -y - \frac{1}{2}, -z + \frac{1}{2}$] hydrogen bonds, so forming centrosymmetric hydrogen-bonded rings of $R_4^2(8)$ motif and approximately in the [001] direction (Fig. 4). In one of the three $\text{N}-\text{H}\cdots\text{Cl}^-$ interactions, where atom N7 acts as a hydrogen-bond donor *via* atom H71, there is some uncertainty as to whether this is a hydrogen bond or not. However, as is very frequently found for bifurcated hydrogen bonds, the sum of the inter-bond angles at the H atom is close to 360° and the $\text{H}\cdots\text{Cl}^-$ distance can be greater than the van der Waals separation (Jeffrey & Saenger, 1991; Desiraju & Steiner, 1999; Steiner, 2002).

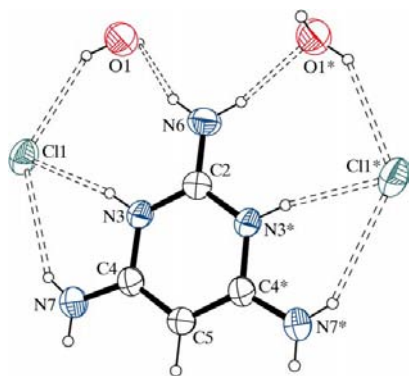


Figure 3

The molecular components in (II), showing the TripidH_2^{2+} cation lying across a twofold axis, the two water molecules of crystallization and the chloride counter-ions. The atom-labelling scheme and hydrogen bonding (dashed lines) are shown; atoms marked with an asterisk (*) are at the symmetry position $(-x + \frac{3}{2}, y, -z + 1)$. Displacement ellipsoids are drawn at the 50% probability level.

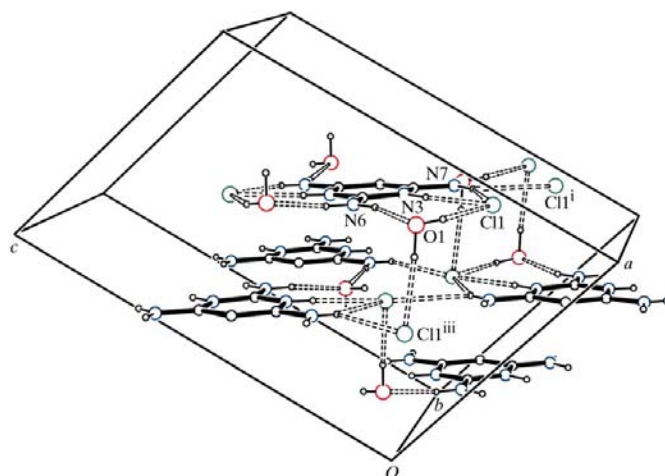


Figure 4

A perspective view of the crystal packing for (II) approximately along the *b*-axis direction. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonding is indicated by dashed lines. Selected atoms are labelled. [Symmetry code: (iii) $-x + \frac{3}{2}, -y - \frac{1}{2}, -z + \frac{1}{2}$]

Experimental

Compounds (I) and (II) (0.5 mmol, Aldrich, 98% purity) were dissolved without further purification in 8 ml of hot dimethylformamide and in 10 ml of methanol/chloroform (3:1), respectively. While stirring, HCl (6 mol l^{-1}) was added dropwise until the pH reached 2. After several days, colourless single crystals suitable for X-ray experiments were obtained by slow evaporation of the solvents.

Compound (I)

Crystal data

$\text{C}_4\text{H}_8\text{N}_5^+\cdot\text{Cl}^-\cdot\text{C}_4\text{H}_7\text{N}_5\cdot\text{H}_2\text{O}$
 $M_r = 304.77$
 Triclinic, $P\bar{1}$
 $a = 7.3808$ (9) Å
 $b = 9.4538$ (10) Å
 $c = 10.3942$ (9) Å
 $\alpha = 90.971$ (12)°
 $\beta = 101.554$ (14)°

$\gamma = 104.252$ (16)°
 $V = 687.03$ (13) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.29 \text{ mm}^{-1}$
 $T = 298$ (2) K
 $0.20 \times 0.20 \times 0.10 \text{ mm}$

Data collection

Huber CS four-circle diffractometer
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\text{min}} = 0.940$, $T_{\text{max}} = 0.971$
 2758 measured reflections
 2324 independent reflections

2246 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$
 3 standard reflections
 every 97 reflections
 intensity decay: 2%

Table 1

Hydrogen-bond geometry (Å, °) for (I).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N6}-\text{H61}\cdots\text{Cl1}^{\text{i}}$	0.80 (2)	2.54 (2)	3.3044 (16)	160.4 (19)
$\text{N6}-\text{H62}\cdots\text{Cl1}^{\text{ii}}$	0.85 (2)	2.63 (2)	3.4265 (16)	157 (2)
$\text{N7}-\text{H71}\cdots\text{N5}^{\text{iii}}$	0.84 (2)	2.25 (2)	3.082 (2)	174.8 (17)
$\text{N7}-\text{H72}\cdots\text{N15}$	0.82 (2)	2.47 (2)	3.287 (2)	172.5 (18)
$\text{N11}-\text{H11}\cdots\text{O1}$	0.83 (2)	1.85 (2)	2.6753 (19)	170.8 (19)
$\text{N16}-\text{H161}\cdots\text{Cl1}$	0.78 (2)	2.60 (2)	3.2315 (16)	139.6 (19)
$\text{N16}-\text{H162}\cdots\text{N13}^{\text{ii}}$	0.83 (2)	2.15 (2)	2.983 (2)	176.3 (18)
$\text{N17}-\text{H171}\cdots\text{N3}$	0.83 (2)	2.12 (2)	2.9368 (19)	169 (2)
$\text{N17}-\text{H172}\cdots\text{Cl1}^{\text{iv}}$	0.78 (2)	2.49 (2)	3.2328 (16)	160 (2)
$\text{O1}-\text{H1}\cdots\text{N1}^{\text{iv}}$	0.73 (3)	2.25 (3)	2.9182 (19)	153 (3)
$\text{O1}-\text{H2}\cdots\text{Cl1}^{\text{v}}$	0.91 (3)	2.40 (3)	3.2881 (19)	165 (2)

Symmetry codes: (i) $x, y + 1, z + 1$; (ii) $-x, -y + 1, -z + 1$; (iii) $-x + 1, -y + 3, -z + 1$; (iv) $x, y - 1, z - 1$; (v) $-x, -y + 1, -z$.

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.092$
 $S = 1.09$
 2324 reflections
 227 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.23 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

Compound (II)

Crystal data

$\text{C}_4\text{H}_9\text{N}_5^{2+} \cdot 2\text{Cl}^- \cdot 2\text{H}_2\text{O}$
 $M_r = 234.09$
 Monoclinic, $I2/a$
 $a = 9.4045 (10) \text{ \AA}$
 $b = 8.6089 (9) \text{ \AA}$
 $c = 13.7420 (12) \text{ \AA}$
 $\beta = 107.742 (10)^\circ$

$V = 1059.67 (18) \text{ \AA}^3$
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.59 \text{ mm}^{-1}$
 $T = 298 (2) \text{ K}$
 $0.20 \times 0.15 \times 0.10 \text{ mm}$

Data collection

Huber CS four-circle diffractometer
 Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.891$, $T_{\max} = 0.943$
 1788 measured reflections
 1106 independent reflections

1066 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.020$
 3 standard reflections every 97 reflections
 intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.070$
 $S = 1.10$
 1106 reflections

87 parameters
 All H-atom parameters refined
 $\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.14 \text{ e } \text{\AA}^{-3}$

Table 2

Hydrogen-bond geometry (\AA , $^\circ$) for (II).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N3}-\text{H3} \cdots \text{Cl1}$	0.850 (18)	2.230 (18)	3.0686 (11)	169.0 (16)
$\text{N6}-\text{H61} \cdots \text{O1}$	0.867 (16)	1.979 (16)	2.8301 (14)	166.8 (16)
$\text{N7}-\text{H71} \cdots \text{Cl1}$	0.81 (2)	2.70 (2)	3.4074 (14)	147.0 (17)
$\text{N7}-\text{H71} \cdots \text{Cl1}^{\text{ii}}$	0.81 (2)	2.967 (19)	3.2983 (12)	107.2 (15)
$\text{N7}-\text{H72} \cdots \text{O1}^{\text{ii}}$	0.80 (2)	2.16 (2)	2.9521 (18)	170.4 (18)
$\text{O1}-\text{H1} \cdots \text{Cl1}^{\text{iii}}$	0.91 (2)	2.21 (2)	3.1143 (13)	175 (2)
$\text{O1}-\text{H2} \cdots \text{Cl1}$	0.83 (3)	2.53 (3)	3.2599 (12)	146 (2)

Symmetry codes: (i) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $x, y + 1, z$; (iii) $-x + \frac{3}{2}, -y - \frac{1}{2}, -z + \frac{1}{2}$.

Table 3

Selected geometric parameters (\AA) for Guan^a, (I) and (II).

	Guan ^a	$n = \text{nil}^b$	$n = 1^b$	$n = \text{nil}^c$	Δ^d	Δ^e
$\text{Nn1}-\text{Cn2}$	1.360 (1)	1.356 (2)	1.363 (2)	–	0.007 (2)	–
$\text{Nn5}-\text{Cn4}$	1.360 (1)	1.354 (2)	1.375 (2)	–	0.021 (2)	–
$\text{Nn1}-\text{Cn6}$	1.328 (1)	1.337 (2)	1.355 (2)	–	0.018 (2)	–
$\text{Nn5}-\text{Cn6}$	1.325 (1)	1.327 (2)	1.301 (2)	–	-0.026 (2)	–
$\text{Nn3}-\text{Cn2}$	1.340 (1)	1.344 (2)	1.330 (2)	1.337 (1)	-0.014 (2)	-0.007 (2)
$\text{Nn3}-\text{Cn4}$	1.338 (1)	1.338 (2)	1.346 (2)	1.376 (2)	0.008 (2)	0.038 (2)
$\text{Nn6}-\text{Cn2}$	1.333 (1)	1.333 (2)	1.313 (2)	1.310 (2)	-0.020 (2)	-0.023 (2)
$\text{Nn7}-\text{Cn4}$	1.331 (1)	1.336 (2)	1.309 (2)	1.318 (2)	-0.027 (2)	-0.018 (2)

Notes: (a) Portalone (2007); (b) this work, compound (I); (c) this work, compound (II); (d) Δ is defined as the difference (\AA) between corresponding $\text{Nn}-\text{Cn}$ bond distances ($n = 1$ for AceguH⁺ and $n = \text{nil}$ for Acegu) in (I); (e) Δ is defined as the difference (\AA) between corresponding $\text{Nn}-\text{Cn}$ bond distances ($n = 1$ for TripidH⁺ and $n = \text{nil}$ for Acegu) in (II) and (I).

All H atoms of both compounds were found in difference maps. In (I), the positional and isotropic displacement parameters of the H atoms of the amino groups and of the triazine ring, as well as the positional parameters of the H atoms of the water molecule, for which $U_{\text{iso}}(\text{H})$ values were set equal to $1.5U_{\text{eq}}(\text{O1})$, were refined. Methyl H atoms were positioned with idealized geometry and refined isotropically using a riding model [$\text{C}-\text{H} = 0.88-0.91 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$]. In (II), positional and isotropic displacement parameters were refined for all H atoms.

For both compounds, data collection: XCS (Colapietro *et al.*, 1992); cell refinement: XCS; data reduction: XCS; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: GZ3095). Services for accessing these data are described at the back of the journal.

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