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Supramolecular architecture of bis(melaminium) L-tartrate 2.5-hydrate

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In the crystal structure of the title compound, $2C_3H_7N_6^+\cdot C_4H_4O_6^{2-}\cdot 2.5H_2O$, the melaminium ions form infinite tapes *via* N—H···N hydrogen bonds. The tartrate anions, lying on twofold rotation axes, are arranged in linear arrays. The crystal packing is stabilized by an extensive net of hydrogen bonds leading to a supramolecular architecture.

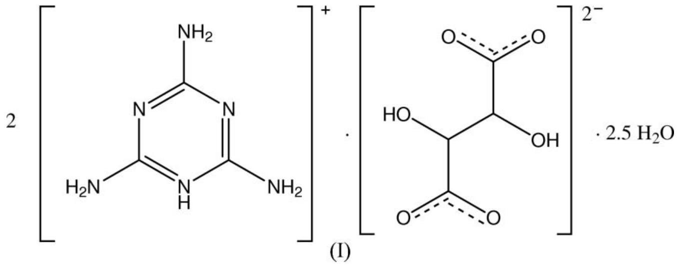
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
H-atom completeness 96%
R factor = 0.038
wR factor = 0.112
Data-to-parameter ratio = 5.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Melamine and its organic and inorganic counterparts can develop supramolecular assemblies *via* multiple hydrogen bonds through self-assembly of components which contain complementary arrays of hydrogen-bonding sites (Row, 1999; Krische & Lehn, 2000; Sherrington & Taskinen, 2001). The title compound, (I) (Figs. 1, 2 and 3), is being studied as a potential material for non-linear optics (NLO) since, like melaminium selenate (Marchewka *et al.*, 2003), it crystallizes in a non-centrosymmetric space group. The second harmonic generation (SHG) in (I) is 42% more efficient than that in urea.



(I)

In (I), the molecular geometries of the monoprotonated melaminium ions are comparable with those in melaminium benzoate dihydrate (Perpétuo & Janczak, 2005), melaminium

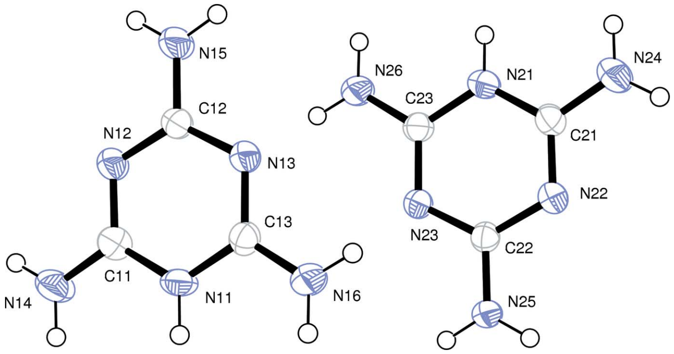


Figure 1
The melaminium cations in (I). Displacement ellipsoids are drawn at the 50% probability level.

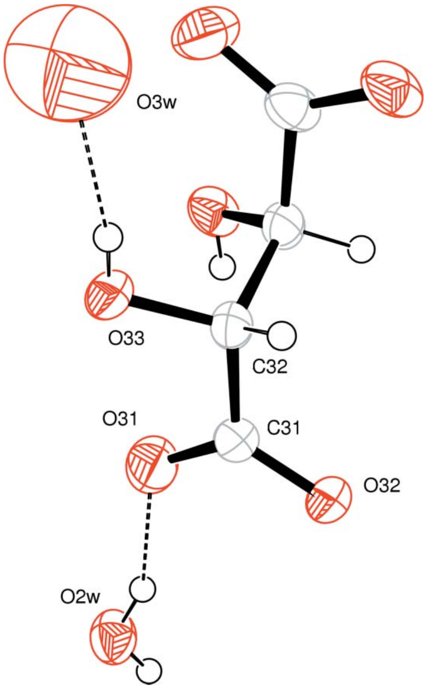


Figure 2
One tartrate anion of (I), showing water–tartrate–water interactions (dashed lines). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code for unlabelled atoms $(1 - x, y, 1 - z)$.]

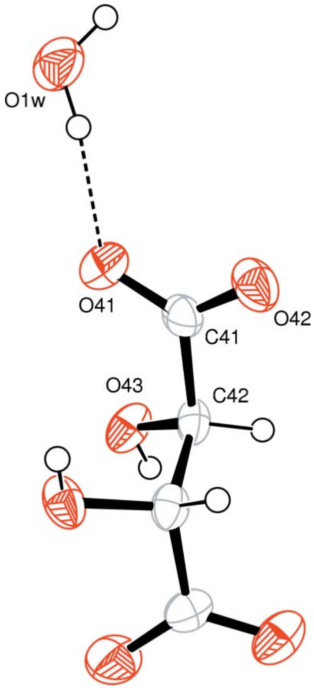


Figure 3
The second tartrate anion of (I), showing its water–tartrate interaction (dashed line). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code for unlabelled atoms $(1 - x, y, -z)$.]

glutarate monohydrate (Janczak & Perpétuo, 2002*a*), melaminium phosphate (Janczak & Perpétuo, 2002*b*) and melaminium acetate acetic acid monohydrate (Perpétuo & Janczak, 2002). The crystal structure of (I) (Fig. 4) is built from alternating layers of melaminium and tartrate ions. The tartrate anions and one water molecule lie on twofold rotation axes. The melaminium ions form infinite straight tapes *via* N—H···N hydrogen bonds (Table 1) and these tapes form one-dimensional stacks parallel to the (001) plane. Within one stack, the melaminium cations are separated by 3.3 Å, indicating the presence of π–π interactions. The tartrate ions are arranged, through O—H···O interactions (Table 1), in linear arrays along the *c* axis. The arrays form corrugated layers parallel to the *ac* plane (Fig. 5). It is interesting to note that the protonated amine group of one independent melaminium ion is involved in two weak hydrogen bonds with the carboxylate O41 and tartrate hydroxyl O43 atoms. In the second independent melaminium ion, weak hydrogen bonds are formed with the tartrate hydroxyl O33 atom and a water molecule (O3*W*), which occupies a special position (Table 1). The N atoms of the 2,4,6-triamine groups are involved in hydrogen-bonding interactions with tartrate anions from adjacent tartrate layers (Table 1). In addition, atoms N14 and N15 are involved in hydrogen-bonding interactions with water molecules O1*W* and O2*W*, respectively. Atoms N24 and N25 have hydrogen-bonding interactions with atoms O2*W* and O1*W*, respectively. Water-mediated interactions between one of the tartrate anions in one layer (O1*W*···O41 and O1*W*···O42) and other tartrate anions in another layer (O2*W*···O31 and O2···O32) also exist. The water molecules involved in these interactions form infinite hydrogen-bonded chains parallel to the *a* axis.

Experimental

Melamine and L-tartaric acid were dissolved in a 1:1 molar ratio in boiling water and the resulting solution allowed to cool to room temperature. After several days, colourless single crystals formed (m.p. 553–555 K).

Crystal data

$2C_3H_7N_6^+\cdot C_4H_4O_6^{2-}\cdot 2.5H_2O$
$M_r = 447.40$
Monoclinic, $C2$
$a = 7.5217$ (10) Å
$b = 22.186$ (3) Å
$c = 10.9869$ (18) Å
$\beta = 98.356$ (12)°
$V = 1814.0$ (4) Å^3
$Z = 4$

$D_x = 1.638$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 20$–$30°$
$\mu = 1.23$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.751$, $T_{\max} = 0.823$
1778 measured reflections
1692 independent reflections
1614 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.011$
$\theta_{\max} = 68.0°$
$h = -9 \rightarrow 8$
$k = 0 \rightarrow 26$
$l = 0 \rightarrow 13$
3 standard reflections
frequency: 120 min
intensity decay: none

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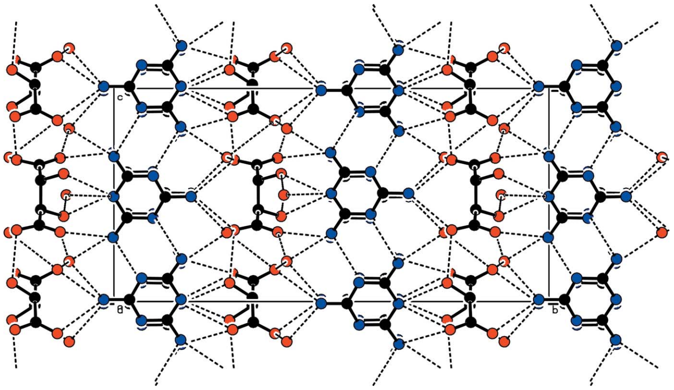

Figure 4
The crystal packing of (I), viewed along the *a* axis. Intermolecular hydrogen bonds are shown by dashed lines. H atoms have been omitted.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.112$
$S = 1.09$
1692 reflections
295 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0734P)^2 + 1.1012P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0010 (2)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N11—H11···O41	0.86	2.23	2.967 (5)	143
N11—H11···O43	0.86	2.09	2.807 (4)	140
N14—H141···N23^{i}	0.86	2.17	3.028 (4)	174
N14—H142···O1W^{i}	0.86	2.31	2.936 (5)	130
N15—H151···O42^{ii}	0.86	2.20	2.943 (5)	144
N15—H152···O2W^{iii}	0.86	1.99	2.839 (4)	167
N16—H161···N22^{iv}	0.86	2.21	3.070 (4)	174
N16—H162···O41	0.86	2.28	3.013 (4)	143
N21—H21···O33^{v}	0.86	2.21	2.944 (4)	143
N21—H21···O3W^{vi}	0.86	2.55	3.129 (10)	125
N24—H241···N13^{iv}	0.86	2.17	3.024 (4)	175
N24—H242···O2W^{vii}	0.86	2.18	2.808 (4)	130
N25—H252···O32^{iv}	0.86	2.15	2.923 (5)	150
N25—H251···O1W	0.86	1.97	2.812 (4)	165
N26—H261···N12^{i}	0.86	2.21	3.069 (4)	173
N26—H262···O31^{iii}	0.86	2.06	2.861 (4)	156
O33—H33···O3W	0.82	2.25	3.067 (2)	170
O43—H43···O32^{viii}	0.82	1.92	2.725 (4)	169
O1W—H2W···O32^{ix}	0.85 (5)	2.22 (5)	2.873 (4)	133 (5)
O1W—H1W···O41	0.84 (5)	1.90 (3)	2.720 (4)	166 (7)
O2W—H3W···O31	0.85 (5)	1.87 (2)	2.678 (4)	158 (4)
O2W—H4W···O42^{x}	0.86 (5)	2.00 (2)	2.834 (4)	166 (5)

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

All the H atoms, except water H atoms, were treated as riding with distances of C—H = 0.98 Å, N—H = 0.86 Å and O—H = 0.82 Å and with $U_{iso}(H) = 1.2U_{eq}$(C,N,O). The water H atoms were located in a difference Fourier map and were refined, subject to a bond length restraint of 0.85 (2) Å. The H atoms of the water molecule (O3W) in a special position were not located in the difference Fourier map. In the absence of significant anomalous scattering, Friedel pairs were merged before the final refinement and the absolute configuration of (I) was assigned to correspond to that of the known chiral centres in a precursor molecule, L-tartaric acid, which remained unchanged during the preparation of (I). The crystal structure of (I) exhibits a pesudo-centre of symmetry (*C*2/*c*). However, the structure of (I) is much better described in the non-centrosymmetric space group *C*2, in accordance with the presence of L-tartrate.

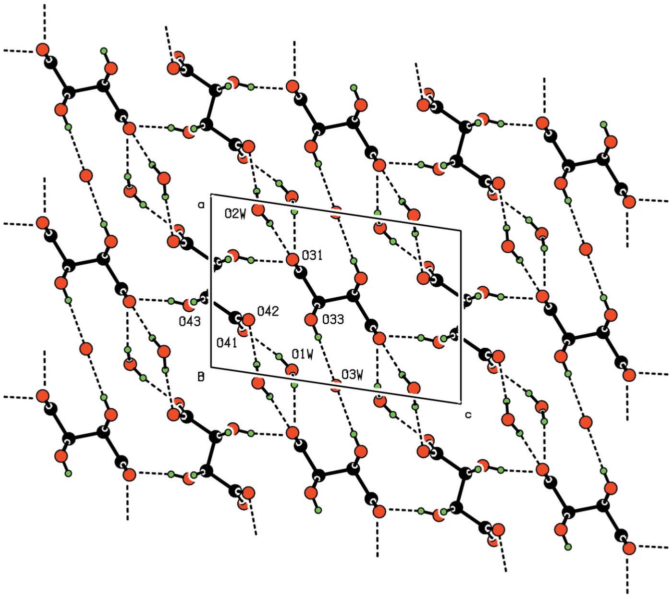

Figure 5
The arrangement of tartrate anions and water molecules in (I), viewed along the *b* axis. Intermolecular hydrogen bonds are shown by dashed lines.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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