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Hydrogen-bonded supramolecular motifs in 2-amino-4,6-dimethoxypyrimidinium 4-hydroxybenzoate monohydrate, 2-amino-4,6-dimethoxypyrimidinium 6-carboxypyridine-2-carboxylate monohydrate and 2-amino-4,6-dimethoxypyrimidinium hydrogen (2*R*,3*R*)-tartrate 2-amino-4,6-dimethoxypyrimidine

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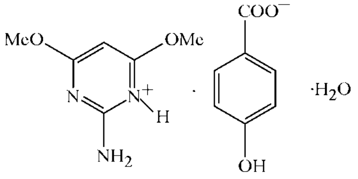
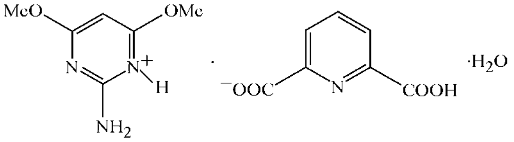
In the crystal structures of the title compounds, $C_6H_{10}N_3O_2^+\cdot C_7H_5O_3^-\cdot H_2O$, (I), $C_6H_{10}N_3O_2^+\cdot C_7H_4NO_4^-\cdot H_2O$, (II), and $C_6H_{10}N_3O_2^+\cdot C_4H_5O_6^-\cdot C_6H_9N_3O_2$, (III), the 2-amino-4,6-dimethoxypyrimidinium cation [abbreviated as $(MeO)_2$-Hampy$^+$] interacts with the carboxylate group of the corresponding anion through a pair of nearly parallel N—H···O hydrogen bonds to form $R_2^2(8)$ ring motifs. In (I), the $(MeO)_2$-Hampy$^+$ cation is centrosymmetrically paired through a pair of N—H···N hydrogen bonds involving the 2-amino group and a ring N atom forming an $R_2^2(8)$ motif. In (II), inversion-related $R_2^2(8)$ motifs (amino–pyrimidine–carboxylate motifs) are further bridged by N—H···O hydrogen bonds on either side forming a *DDAA* array of quadruple hydrogen bonds. This array is extended further on either side by O_{water}—H···$O_{methoxy}$ hydrogen bonds, resulting in an array of six hydrogen bonds (*ADDAAD*). The water molecule plays a pivotal role, and five hydrogen-bonded fused rings are formed around the water molecule. In (III), the carboxy group of the tartrate anion interacts with the ring N atom and 2-amino group of the neutral $(MeO)_2$-ampy molecule through N—H···O and O—H···N hydrogen bonds. There is also an intramolecular O—H···O hydrogen bond in the tartrate anion. In all three crystal structures, C—H···O hydrogen bonds are observed.

Comment

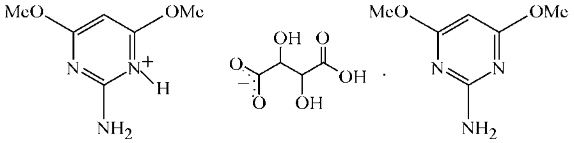
Pyrimidine and aminopyrimidine derivatives are biologically very important compounds as they occur in nature as components of nucleic acids. Some aminopyrimidine derivatives are used as antifolate drugs (Hunt *et al.*, 1980; Baker & Santi, 1965). Hydrogen bonding plays a key role in molecular recognition and crystal engineering research (Desiraju, 1989). 2-Aminopyrimidine forms 1:1 adducts with different mono- and dicarboxylic acids (Etter & Adsmond, 1990) rather than individual self-assembly compounds (Scheinbeim & Schempp, 1976). The adducts of carboxylic acids with 2-aminoheterocylic ring systems form a graph-set motif of $R_2^2(8)$ (Lynch & Jones, 2004). This motif is very robust in aminopyrimidine carboxylic acid/carboxylate systems. The crystal structures of aminopyrimidine derivatives (Schwalbe & Williams, 1982), aminopyrimidine carboxylates (Muthiah, Francis *et al.*, 2006) and cocrystals (Chinnakali *et al.*, 1999) have been reported. The crystal structure of 2-amino-4,6-dimethoxypyrimidine [abbreviated as $(MeO)_2$-ampy] has also been reported (Low *et al.*, 2002). The crystal structures of



(I)



(II)



(III)

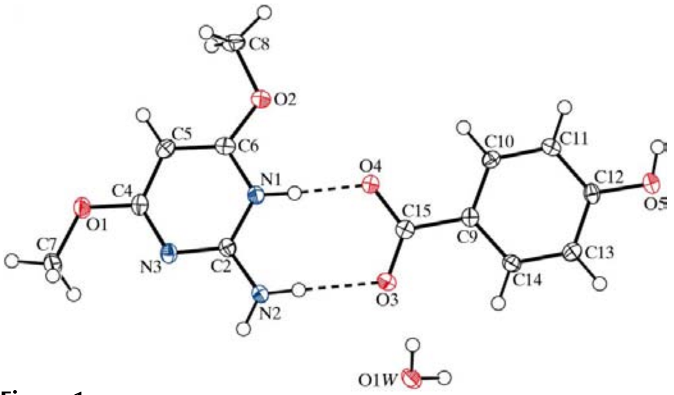


Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

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$(MeO)_2$-ampy–4-aminobenzoic acid (1/1) (Thanigaimani *et al.*, 2006), Me_2-Hampy bromide Me_2-ampy monohydrate (Me_2-Hampy is 2-amino-4,6-dimethylpyrimidinium; Panneerselvam *et al.*, 2004), Me_2-Hampy hydrogen sulfate (Hemamalini *et al.*, 2005), Me_2-ampy–cinnamic acid (1/2) (Balasubramani *et al.*, 2005), Me_2-Hampy picrate (Subashini *et al.*, 2006) and Me_2-Hampy salicylate (Muthiah, Balasubramani *et al.*, 2006) have been reported recently from our laboratory. We are interested in the network of hydrogen-bonding patterns in the carboxylate–aminopyrimidine interactions under a variety of molecular environments. In the present study, 4-hydroxybenzoic acid, dipicolinic acid (pyridine-2,6-dicarboxylic acid) and tartaric acid have been selected to form adducts with $(MeO)_2$-ampy. The crystal structures of 4-hydroxybenzoic acid monohydrate (Colapietro *et al.*, 1979; Fukuyama *et al.*, 1973), Me_2-ampy–4-hydroxybenzoic acid (1/1) (Balasubramani *et al.*, 2006), dipicolinic acid (Carranza Téllez *et al.*, 2002) and (+)-tartaric acid (Stern & Beevers, 1950) are also known.

ORTEP (Johnson, 1976) views of the title compounds, (I)–(III), are shown in Figs. 1–3, and selected geometric parameters are given in Tables 1, 3 and 5. In (I), the asymmetric unit contains an $(MeO)_2$-$Hampy^+$ cation, a 4-hydroxybenzoate anion and a water molecule. In (II), the asymmetric unit contains an $(MeO)_2$-$Hampy^+$ cation, a hydrogen dipicolinate anion and a water molecule. In (III), one $(MeO)_2$-$Hampy^+$ cation (*A*), a hydrogen (2*R*,3*R*)-tartrate anion and a neutral $(MeO)_2$-ampy molecule (*B*) constitute the asymmetric unit. In all three compounds, the pyrimidine rings are protonated at atom N1. Protonation of the pyrimidine base on the N1 site is reflected by an increase in bond angle at N1 [C2—N1—C6 = 120.01 (14)° in (I), 119.25 (15)° in (II) and 119.9 (2)° in cation *A* of (III)] when compared with that at the unprotonated atom N3 [C2—N3—C4 = 116.22 (14)° in (I), 115.98 (16)° in (II) and 116.8 (2)° in (III)]. In all three crystal structures, the carboxylate group of the respective anions [4-hydroxybenzoate, hydrogen dipicolinate and hydrogen (2*R*,3*R*)-tartrate] interacts with the aminopyrimidinium cation through a pair of N—H···O hydrogen bonds to form an eight-membered $R_2^2(8)$ ring motif (Etter, 1990; Bernstein *et al.*, 1995).

In (I), the $(MeO)_2$-$Hampy^+$ cations are centrosymmetrically paired through a pair of N2—H2*A*···N3($-x + 1$, $-y + 1$, $-z + 1$) hydrogen bonds (Table 2) to form an $R_2^2(8)$ ring motif (Fig. 4). Two inversion-related 4-hydroxybenzoate anions are connected by water molecules *via* O—H···O and C—H···O1*W* hydrogen bonds, forming an $R_4^4(16)$ ring motif. A similar type of C—H···O_{water} hydrogen bond has been

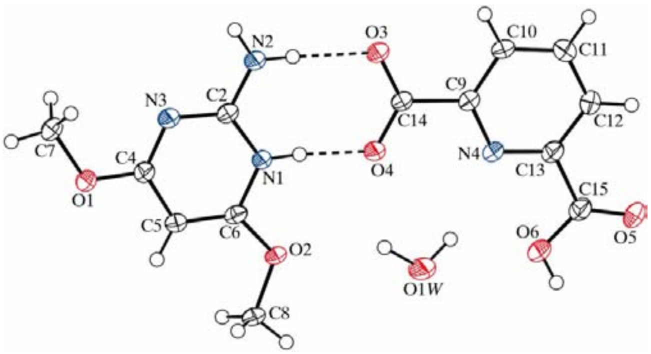

Figure 2
The asymmetric unit of (II), showing 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

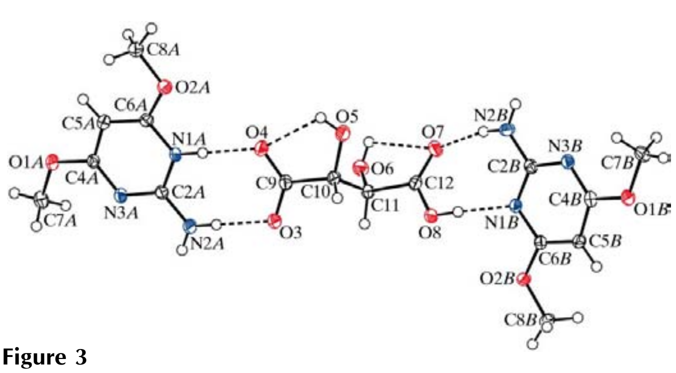

Figure 3
The asymmetric unit of (III), showing 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

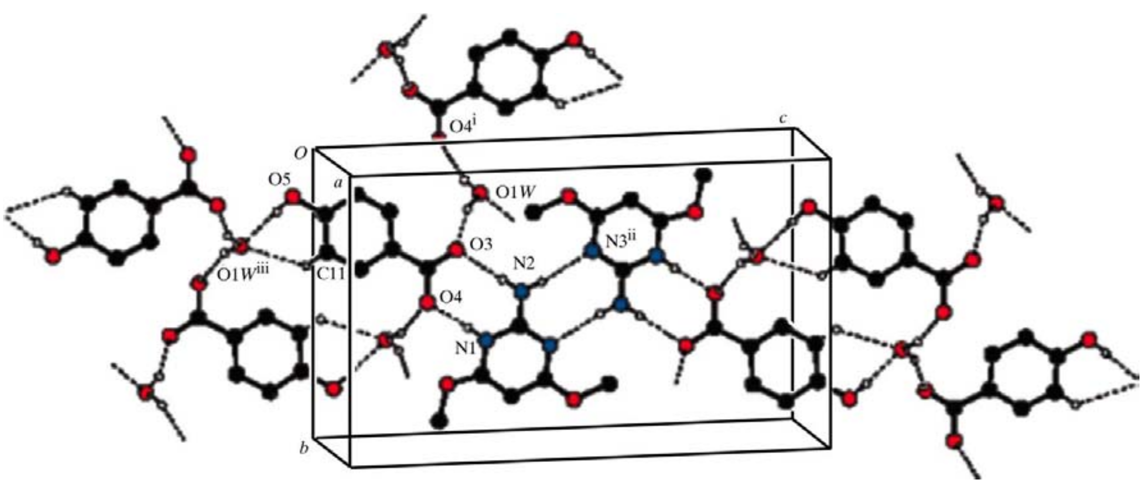

Figure 4
The crystal structure of (I). Dashed lines indicate hydrogen bonds [symmetry codes: (i) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $x, -y + \frac{1}{2}, z - \frac{1}{2}$].

o296 Thanigaimani et al. • $C_6H_{10}N_3O_2^+ \cdot C_7H_5O_3^- \cdot H_2O/C_7H_4NO_4^- \cdot H_2O/C_4H_5O_6^- \cdot C_6H_9N_3O_2$ Acta Cryst. (2007). C63, o295–o300

investigated on the basis of the structural data determined by neutron diffraction (Steiner & Saenger, 1993). The carboxylate groups are bridged by the intervening water molecules *via* O—H···O hydrogen bonds, resulting in a supramolecular chain along the *b* axis. The water molecules act as hydrogen-bond donors to the carboxylate group of the 4-hydroxybenzoate ion, and also act as hydrogen-bond acceptors to the hydroxy group of the 4-hydroxybenzoate ion, forming an O—H···O hydrogen-bonded sheet parallel to the (011) plane.

In (II), inversion-related $R_2^2(8)$ motifs (aminopyrimidine–carboxylate motifs) are further bridged by N—H···O hydrogen bonds (Table 4) on either side forming a *DDAA* array of quadruple hydrogen bonds (Fig. 5). This array is extended further on either side by O_{water}—H···$O_{methoxy}$ hydrogen bonds, resulting in an array of six hydrogen bonds (*ADDAAD*). The water molecule plays a pivotal role, and five hydrogen-bonded fused rings are formed around the water molecule. Two inversion-related water molecules are bridged by two inversion-related carboxyl OH groups, generating an $R_4^4(8)$ ring motif. Each H atom of the water molecule acts as a bifurcated donor and the O atom acts as a single acceptor. The water molecule–dipicolinate interaction *via* O—H···O and O—H···N hydrogen bonds leads to two hydrogen-bonded rings, *viz*. $R_1^2(5)$ and $R_2^2(7)$. Furthermore, these arrays are connected *via* a pair of C—H···O hydrogen bonds involving one of the O atoms of the carboxylate group and the methoxy group (C7 and C8) of the pyrimidinium cation, resulting in the formation of a 20-membered $R_4^2(20)$ ring.

In (III), the carboxyl group of the tartrate anion interacts with atom N1*B* and the 2-amino group of the neutral $(MeO)_2$-ampy molecule (*B*) through N—H···O and O—H···N hydrogen bonds (Table 6) to form an eight-membered ring [$R_2^2(8)$] (Fig. 6). The 2-amino group of the $(MeO)_2$-$Hampy^+$ cation (*A*) interacts with hydroxy group O5 through an N—H···O hydrogen bond, and the 2-amino group of molecule *B* interacts with one of the carboxylate atoms, O3, through an N—H···O hydrogen bond, forming a cyclic $R_4^3(12)$ hydrogen-bonded motif. These types of interactions are extended along the *c* axis to form a hydrogen-bonded supramolecular ribbon. In addition, both the carboxylate groups interact with adjacent hydroxy groups *via* intramolecular O—H···O hydrogen bonds, leading to a five-membered ring [*S*(5)]. Furthermore, these arrays are connected *via* C—H···O hydrogen bonds, resulting in a two-dimensional network.

In all three crystal structures, (I)–(III), π–π stacking interactions between aromatic rings are observed. In (I), the

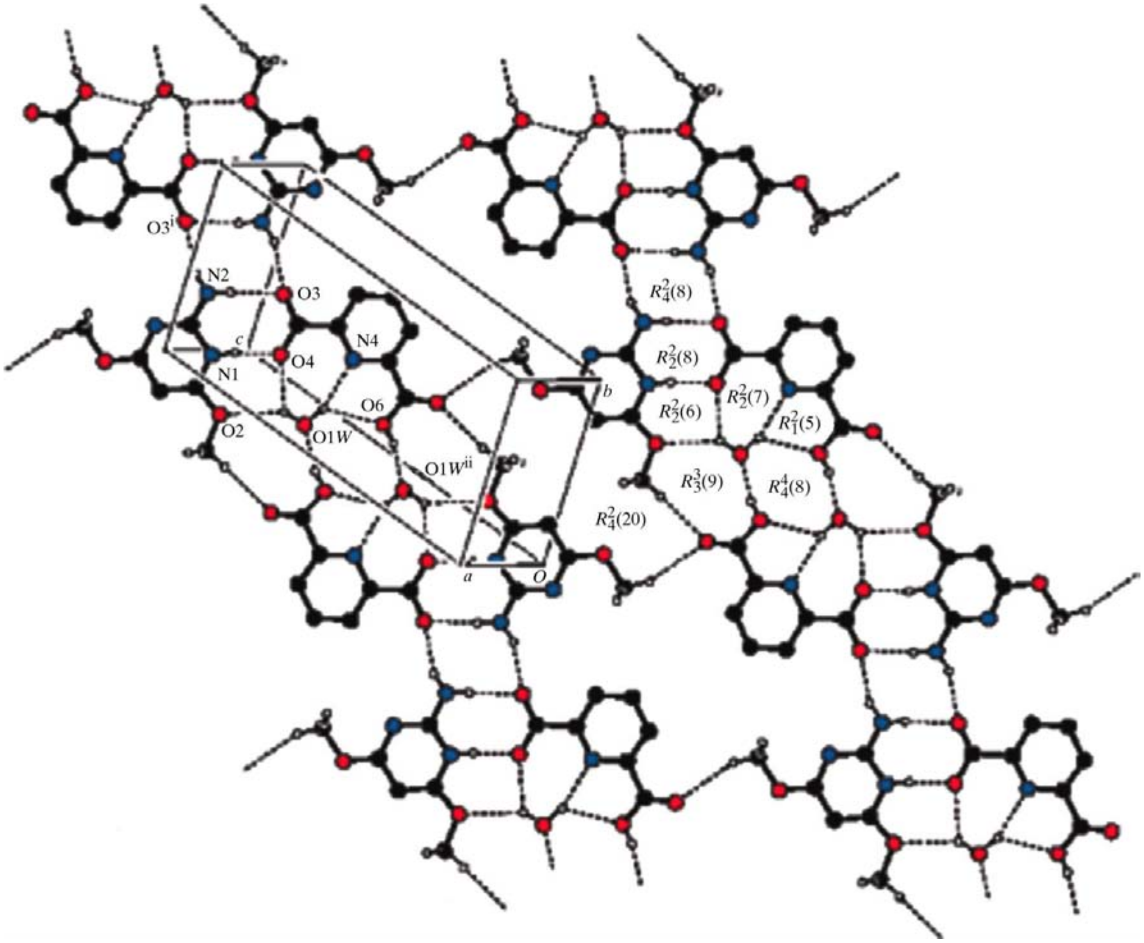

Figure 5
The crystal structure of (II). Dashed lines indicate hydrogen bonds [symmetry codes: (i) −*x* + 1, −*y* + 1, −*z* + 2; (ii) −*x* + 1, −*y*, −*z* + 1]. The graph-set notations for all the motifs are indicated.

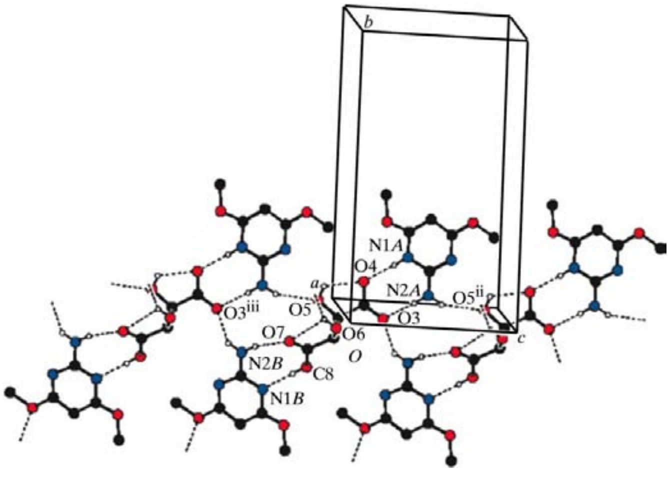

Figure 6
The crystal structure of (III). Dashed lines indicate hydrogen bonds [symmetry codes: (ii) $x, y, z + 1$; (iii) $x, y, z - 1$].

pyrimidine ring of the $(MeO)_2$-Hampy$^+$ cation stacks with the benzene ring of the 4-hydroxybenzoate anion, with interplanar and centroid-to-centroid distances of 3.317 and 3.554 Å, respectively, and a slip angle (angle between the centroid vector and the normal to the plane) of 18.9°. In (II), a π–π interaction is observed between two $(MeO)_2$-Hampy$^+$ cations related by an inversion centre. The centroid-to-centroid distance and interplanar distance are 3.310 and 3.253 Å, respectively, the slip angle being 10.7°. In (III), the pyrimidine rings of cation *A* form stacking interactions with molecule *B*; the centroid-to-centroid and interplanar distances are 3.625 and 3.335 Å, respectively, the slip angle being 21.2°. These are typical aromatic stacking values (Hunter, 1994).

Experimental

Compounds (I) and (II) were prepared by mixing a hot methanol solution (20 ml) of 2-amino-4,6-dimethoxypyrimidine (38 mg, Aldrich) with a hot aqueous solution of the corresponding acid [4-hydroxybenzoic acid (34 mg, Loba Chemie) or dipicolinic acid (41 mg, Loba Chemie)] in a 1:1 molar ratio, and warming for half an hour over a water bath. Each solution was cooled slowly and kept at room temperature. After a few days, colourless plate-like crystals were obtained [yields: 69 and 64% for (I) and (II), respectively]. Compound (III) was prepared by mixing a hot methanol solution (20 ml) of 2-amino-4,6-dimethoxypyrimidine (76 mg) and (2*R*,3*R*)-(+)-tartaric acid (37 mg, Loba Chemie) in a 2:1 molar ratio, and was crystallized as described above (yield 58%). Compound (III) was obtained even if the starting materials were in a 1:1 molar ratio.

Compound (I)

Crystal data

$C_6H_{10}N_3O_2^+ \cdot C_7H_5O_3^- \cdot H_2O$
$M_r = 311.30$
Monoclinic, $P2_1/c$
$a = 6.9710$ (2) Å
$b = 10.9014$ (3) Å
$c = 18.3749$ (6) Å
$\beta = 93.631$ (2)°
$V = 1393.57$ (7) Å^3
$Z = 4$
$D_x = 1.484$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.12$ mm^{-1}
$T = 120$ K
Plate, colourless
0.48 × 0.30 × 0.14 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
12896 measured reflections
3172 independent reflections
2415 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.6°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.140$
$S = 1.09$
3172 reflections
203 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0837P)^2 + 0.1403P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.65$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.053 (5)

Table 1
Selected geometric parameters (Å, °) for (I).

O3—C15	1.253 (2)	N1—C6	1.355 (2)
O4—C15	1.282 (2)	N2—C2	1.324 (2)
O5—C12	1.3592 (18)	N3—C4	1.330 (2)
N1—C2	1.353 (2)	N3—C2	1.340 (2)
C2—N1—C6	120.01 (14)	C2—N3—C4	116.22 (14)

Table 2
Hydrogen-bond geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4	0.86	1.75	2.6029 (17)	172
O1W—H1W···O4^{i}	0.94	2.00	2.9084 (16)	162
N2—H2A···N3^{ii}	0.86	2.26	3.1128 (19)	171
N2—H2B···O3	0.86	2.06	2.8832 (17)	161
O1W—H2W···O3	0.93	1.84	2.7284 (16)	160
O5—H5A···O1W^{iii}	0.82	1.87	2.6894 (16)	176
C11—H11···O1W^{iii}	0.93	2.57	3.241 (2)	130

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

Compound (II)

Crystal data

$C_6H_{10}N_3O_2^+ \cdot C_7H_4NO_4^- \cdot H_2O$
$M_r = 340.30$
Triclinic, $P\overline{1}$
$a = 6.8247$ (6) Å
$b = 7.9273$ (5) Å
$c = 14.4038$ (10) Å
$\alpha = 82.558$ (5)°
$\beta = 88.133$ (4)°
$\gamma = 75.075$ (5)°
$V = 746.63$ (10) Å^3
$Z = 2$
$D_x = 1.514$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.13$ mm^{-1}
$T = 120$ K
Plate, colourless
0.40 × 0.25 × 0.10 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
14555 measured reflections
3384 independent reflections
2397 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 27.6°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.064$
$wR(F^2) = 0.175$
$S = 1.07$
3384 reflections
221 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.108P)^2 + 0.0561P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.090 (13)

Table 3
Selected geometric parameters (Å, °) for (II).

O3—C14	1.244 (2)	N2—C2	1.321 (2)
O4—C14	1.266 (2)	N3—C2	1.335 (2)
O5—C15	1.207 (2)	N3—C4	1.326 (2)
O6—C15	1.324 (3)	N4—C13	1.339 (2)
N1—C6	1.349 (2)	N4—C9	1.341 (2)
N1—C2	1.359 (2)		
C2—N1—C6	119.25 (15)	C9—N4—C13	117.15 (17)
C2—N3—C4	115.98 (16)		

Table 4
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4	0.86	1.71	2.569 (2)	174
N2—H2*A*···O3^{i}	0.86	1.97	2.793 (2)	159
N2—H2*B*···O3	0.86	1.98	2.837 (2)	173
O1*W*—H1*W*···O2	0.96	2.44	3.275 (2)	146
O1*W*—H1*W*···O4	0.96	2.17	2.836 (2)	125
O1*W*—H2*W*···O6	0.91	2.34	2.946 (2)	124
O1*W*—H2*W*···N4	0.91	2.16	3.035 (2)	162
O6—H6···O1*W*^{ii}	0.82	1.77	2.577 (2)	165
C7—H7*B*···O5^{iii}	0.96	2.60	3.507 (3)	158
C8—H8*B*···O5^{ii}	0.96	2.41	3.365 (2)	175

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x+1, -y, -z+1$; (iii) $x+1, y-1, z+1$.

Compound (III)

Crystal data

$C_6H_{10}N_3O_2^+ \cdot C_4H_5O_6^- \cdot C_6H_9N_3O_2$
$M_r = 460.41$
Monoclinic, $P2_1$
$a = 7.3245\ (2)$ Å
$b = 15.8349\ (6)$ Å
$c = 8.9264\ (3)$ Å
$\beta = 105.251\ (2)°$
$V = 998.85\ (6)$ Å^3
$Z = 2$
$D_x = 1.531$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.13$ mm^{-1}
$T = 120$ K
Plate, colourless
$0.42 \times 0.28 \times 0.18$ mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
13297 measured reflections
2378 independent reflections
2122 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.035$
$\theta_{\rm max} = 27.6°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.110$
$S = 1.15$
2378 reflections
297 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.69$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.70$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.134 (10)

Table 5
Selected geometric parameters (Å, °) for (III).

O3—C9	1.255 (3)	N2*A*—C2*A*	1.320 (4)
O4—C9	1.254 (3)	N3*A*—C2*A*	1.340 (3)
O5—C10	1.418 (3)	N3*A*—C4*A*	1.324 (4)
O6—C11	1.407 (4)	N1*B*—C2*B*	1.345 (3)
O7—C12	1.218 (3)	N1*B*—C6*B*	1.347 (3)
O8—C12	1.307 (3)	N2*B*—C2*B*	1.338 (3)
N1*A*—C6*A*	1.355 (3)	N3*B*—C4*B*	1.321 (4)
N1*A*—C2*A*	1.371 (3)	N3*B*—C2*B*	1.347 (3)
C2*A*—N1*A*—C6*A*	119.9 (2)	C2*B*—N1*B*—C6*B*	116.9 (2)
C2*A*—N3*A*—C4*A*	116.8 (2)	C2*B*—N3*B*—C4*B*	115.4 (2)

Table 6
Hydrogen-bond geometry (Å, °) for (III).

D—H···A	D—H	H···A	D···A	D—H···A
N1*A*—H1*A*···O4	0.86	1.87	2.728 (3)	179
O5—H5···O4	0.82	2.13	2.629 (3)	119
O6—H6···O1*B*^{i}	0.82	2.20	2.860 (3)	138
O6—H6···O7	0.82	2.42	2.722 (3)	103
O8—H8···N1*B*	0.82	1.82	2.631 (3)	171
N2*A*—H21*A*···O5^{ii}	0.86	2.30	3.090 (3)	152
N2*A*—H22*A*···O3	0.86	1.96	2.814 (3)	176
N2*B*—H21*B*···O7	0.86	2.09	2.935 (3)	165
N2*B*—H22*B*···O3^{iii}	0.86	2.19	2.878 (3)	137
C8*A*—H81*A*···O7^{iv}	0.96	2.54	3.328 (4)	140
C8*B*—H82*B*···O6^{v}	0.96	2.37	3.308 (3)	166

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

The H atoms of the water molecules were located in difference Fourier maps and refined as riding in their as-found relative positions. The other H atoms were positioned geometrically and treated as riding, with N—H, O—H and C—H bond lengths of 0.86, 0.82 and 0.93–0.98 Å, respectively, and with $U_{\rm iso}$(H) values of $1.5U_{\rm eq}$(C,O) for OH groups in (I) and (II) and for all methyl groups, or $1.2U_{\rm eq}$(C,N,O) for other H atoms. For (III), Friedel pairs were averaged in the absence of significant anomalous scattering effects, and the absolute structure was assigned based on the known absolute configuration of (2*R*,3*R*)-(+)-tartaric acid (Bijvoet *et al.*, 1951; Hope & de la Camp, 1972).

For all compounds, data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: OB3031). Services for accessing these data are described at the back of the journal.

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