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Propane-1,2-diammonium hydrogenarsenate monohydrate

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The title compound, $[H_3NCH_2CH(NH_3)CH_3][HAsO_4]\cdot H_2O$, contains a network of doubly protonated propane-1,2-diammonium cations, hydrogenarsenate anions [d_{av}(As—O) = 1.682 (1) Å] and water molecules. Crystal symmetry generates a racemic mixture of the two enantiomers of the organic species. The crystal packing is controlled by N—H···O [d_{av}(H···O) = 1.89 Å, θ_{av}(N—H···O) = 167° and d_{av}(N···O) = 2.760 (1) Å] and O—H···O [d_{av}(H···O) = 1.86 Å, θ_{av}(O—H···O) = 175° and d_{av}(O···O) = 2.712 (1) Å] hydrogen bonds. It is isostructural with its hydrogenphosphate congener.

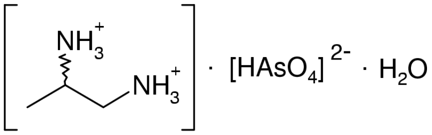
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.023
wR factor = 0.051
Data-to-parameter ratio = 31.3

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

Comment

The title compound, (I) (Fig. 1), complements recently reported (protonated) amine phosphates, such as triethanolammonium dihydrogenphosphate, $NH(CH_2CH_2OH)_3\cdot H_2PO_4$ (Demir *et al.*, 2003). It is isostructural with its hydrogenphosphate congener, $[H_3NCH_2CH(NH_3)CH_3](HPO_4)\cdot H_2O$ (Baouab & Jouini, 1998). One interesting use of $[H_3NCH_2CH(NH_3)CH_3]^{2+}$ is as a template in the synthesis of new open-framework materials (Natarajan, 1999).



(I)

The structure of (I) contains propane-1,2-diammonium cations, hydrogenarsenate $(HAsO_4)^{2-}$ anions and water molecules. Each $[H_3NCH_2CH(NH_3)CH_3]^{2+}$ molecule is chiral (in the asymmetric unit shown in Fig. 1, atom C2 has an *R* configuration), with crystal symmetry generating a 50:50 mixture of the two enantiomers, which is consistent with the racemic starting material. Its geometrical parameters [d_{av}(C—N) = 1.495 (2) Å and d_{av}(C—C) = 1.516 (2) Å] are similar to those of the same cation in $[H_3NCH_2CH(NH_3)CH_3](BF_4)$ (Gerrard & Weller, 2002). The $(HAsO_4)^{2-}$ hydrogenarsenate group shows its standard tetrahedral geometry [d_{av}(As—O) = 1.682 (1) Å and θ_{av}(O—As—O) = 109.4 (1)°], with the protonated As—O4 vertex showing its expected lengthening relative to the other As—O bonds.

As well as electrostatic attractions, the component species in (I) interact by means of a network of N—H···O and O—H···O links (Table 2). The $(HAsO_4)^{2-}$ units and the water molecule (atom O5) are linked into a polymeric chain in the

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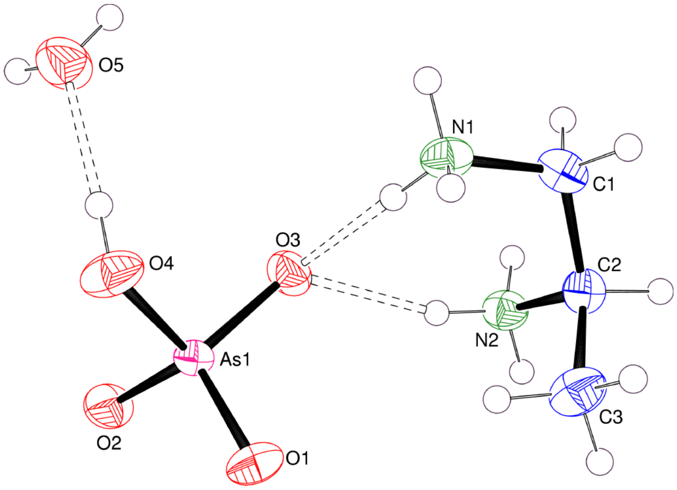

Figure 1
The asymmetric unit of (I) (50% displacement ellipsoids). H atoms are drawn as small spheres of arbitrary radius and hydrogen bonds are indicated by dashed lines.

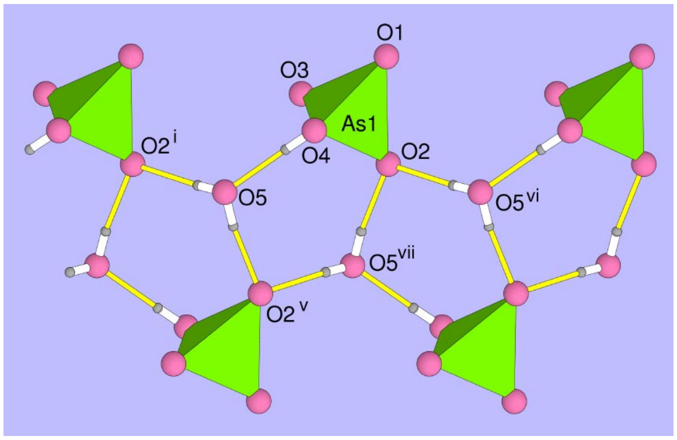

Figure 2
Detail of a hydrogen-bonded hydrogenarsenate/water chain in (I) Colour key: $[HAsO_4]^{2-}$ tetrahedra green, O atoms rose and H atoms grey. The H$\cdots$O portions of the hydrogen bonds are highlighted in yellow. Symmetry codes as in Table 2; additionally (vi) x, $1 - y$, z; (vii) $-\frac{1}{2} - x$, $y - \frac{1}{2}$, $\frac{1}{2} - z$.

[010] direction by hydrogen bonds mediated by the water molecules (Fig. 2); each hydrogenarsenate tetrahedron is associated with three water neighbouring water molecules. There are no direct inter-tetrahedral As—OH$\cdots$O—As bonds, contrary to the commonly seen P—OH$\cdots$O—P bonds in amine phosphates (Demir *et al.*, 2003).

The organic species crosslink the chains in the [100] and [010] directions by way of N—H$\cdots$O—As hydrogen bonds (Table 2). All six of the $—NH_3^+$ H atoms are involved in these links [d_{av}(H$\cdots$O) = 1.89 Å, θ_{av}(N—H$\cdots$O) = 167° and d_{av}(N$\cdots$O) = 2.760 (1) Å]. This results in (001) pseudo-layers of alternating hydrogenarsenate/water and organic moieties (Fig. 3).

A short C1—H8$\cdots$O4^{ii} (symmetry code as in Table 2) intermolecular contact [d(C—H) = 0.97 Å, d(H$\cdots$O) = 2.51 Å, θ(C—H$\cdots$O) = 138° and d(C$\cdots$O) = 3.2929 (19) Å] was identified in a *PLATON* (Spek, 2003) analysis of the structure. If it is not merely a packing artefact, it may provide some additional coherence between the (001) pseudo-layers.

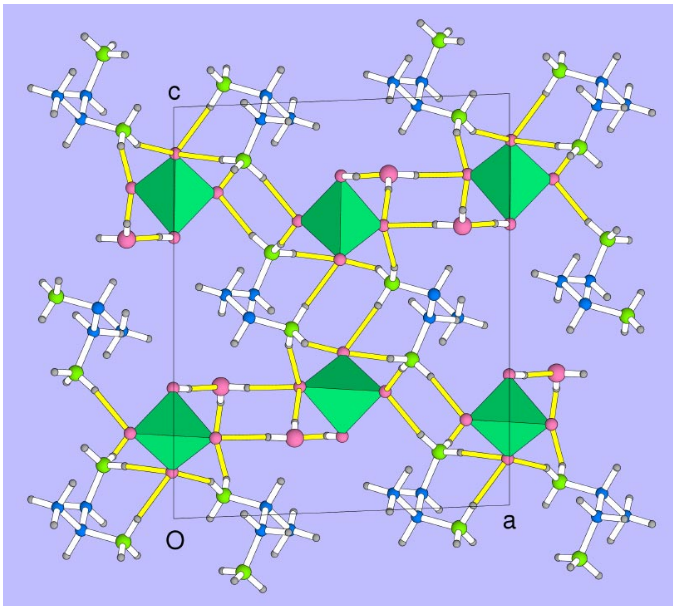

Figure 3
[010] projection of (I). Colour key as in Fig. 2; additionally C atoms blue, N atoms green. The H$\cdots$O portions of the hydrogen bonds are highlighted in yellow.

Experimental

Racemic propane-1,2-diamine (1 ml) was added to 8 ml of 0.5 *M* H_3AsO_4, giving a clear solution. Chunky, faceted crystals of (I) grew as the water evaporated over the course of a few days.

Crystal data

$(C_3H_{12}N_2)[HAsO_4]\cdot H_2O$
$M_r = 234.09$
Monoclinic, $P2_1/n$
$a = 10.9115$ (5) Å
$b = 6.1530$ (3) Å
$c = 13.3653$ (6) Å
$\beta = 92.315$ (1)°
$V = 896.59$ (7) Å^3
$Z = 4$

$D_x = 1.734$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3887 reflections
$\theta = 2.4$–32.2°
$\mu = 3.78$ mm^{-1}
$T = 293$ (2) K
Chunk, colourless
0.23 × 0.21 × 0.19 mm

Data collection

Bruker SMART1000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min} = 0.431$, $T_{max} = 0.488$
8758 measured reflections

3224 independent reflections
2519 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 32.5°$
$h = -16 \rightarrow 15$
$k = -9 \rightarrow 5$
$l = -19 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.051$
$S = 0.92$
3224 reflections
103 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0251P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

As1—O1	1.6583 (10)	N1—C1	1.490 (2)
As1—O2	1.6671 (11)	N2—C2	1.500 (2)
As1—O3	1.6730 (11)	C1—C2	1.517 (2)
As1—O4	1.7302 (11)	C2—C3	1.514 (2)
N1—C1—C2—C3	−54.09 (18)	N1—C1—C2—N2	70.26 (16)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H1···O5	0.85	1.81	2.6534 (17)	177
N1—H2···O1^{i}	0.89	1.80	2.6904 (17)	174
N1—H3···O1^{ii}	0.89	1.86	2.7412 (17)	169
N1—H4···O3	0.89	1.96	2.8436 (18)	176
N2—H5···O3^{iii}	0.89	1.90	2.7449 (17)	158
N2—H6···O3	0.89	1.90	2.7596 (17)	163
N2—H7···O2^{iv}	0.89	1.92	2.7782 (17)	161
O5—H14···O2^{v}	0.90	1.82	2.7056 (17)	172
O5—H15···O2^{i}	0.82	1.96	2.7782 (17)	176

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

O—H H atoms were found in difference maps and were refined as riding, starting in their as-found positions. H atoms bonded to carbon and nitrogen were placed in calculated positions [d(C—H) = 0.96–0.98 Å and d(N—H) = 0.89 Å] and refined as riding [free rotation of the rigid R—NH$_3$ and R—CH$_3$ groups about the R—N and R—C bonds, respectively, was allowed.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97; molecular graphics: *ORTEP*-3 (Farrugia, 1997) and *ATOMS* (Shape Software, 1999); software used to prepare material for publication: *SHELXL*97.

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