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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.036  
 $wR$  factor = 0.094  
Data-to-parameter ratio = 26.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## Propane-1,3-diaminium bis(dihydrogenarsenate)

The title compound,  $(\text{C}_3\text{H}_{12}\text{N}_2)[\text{H}_2\text{AsO}_4]_2$ , contains a network of propane-1,3-diaminium cations and dihydrogenarsenate anions [mean  $\text{As}-\text{O} = 1.682(2)$  Å]. The crystal packing involves anion-to-anion  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, resulting in double chains of dihydrogenarsenate tetrahedra. Cation-to-anion  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds generate a three-dimensional overall structure. One C atom occupies a special position with twofold symmetry.

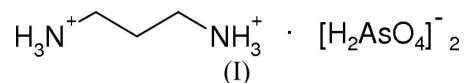
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## Comment

The title compound,  $\text{C}_3\text{H}_{12}\text{N}_2^{2+}\cdot 2[\text{H}_2\text{AsO}_4]^-$ , (I), (Fig. 1), was prepared as part of our ongoing structural studies of hydrogen-bonding interactions in protonated-amine (di)hydrogen arsenates (Lee & Harrison, 2003*a,b,c*; Wilkinson & Harrison, 2004; Todd & Harrison, 2005*a*).



The  $[\text{H}_2\text{AsO}_4]^-$  dihydrogenarsenate group in (I) has normal tetrahedral geometry [mean  $\text{As}-\text{O} = 1.682(2)$  Å], with the protonated  $\text{As1}-\text{O1}$  and  $\text{As1}-\text{O2}$  vertices showing their expected lengthening relative to the unprotonated  $\text{As1}-\text{O3}$  and  $\text{As1}-\text{O4}$  bonds, which have formal partial double-bond character (Table 1). The propane-1,3-diaminium cation, which is generated by twofold symmetry from the atoms of the asymmetric unit (C2 occupies a special position with site symmetry 2), shows no unusual geometrical features.

As well as electrostatic attractions, the component species in (I) interact by means of a network of cation-to-anion  $\text{N}-\text{H}\cdots\text{O}$  and anion-to-anion  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2). The  $[\text{H}_2\text{AsO}_4]^-$  units are linked into polymeric

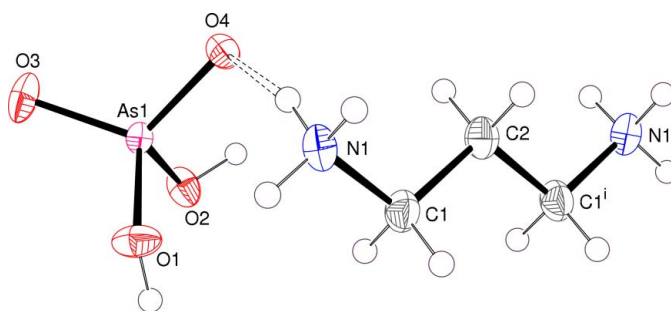
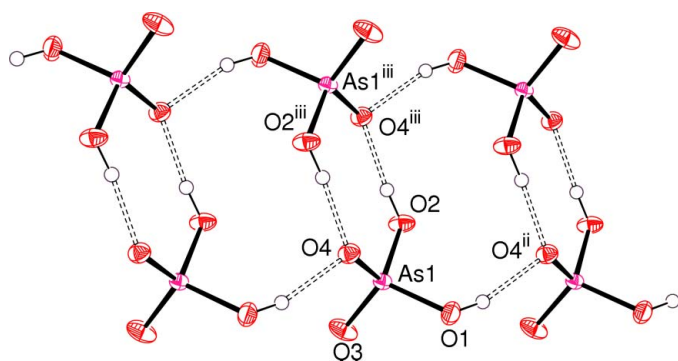
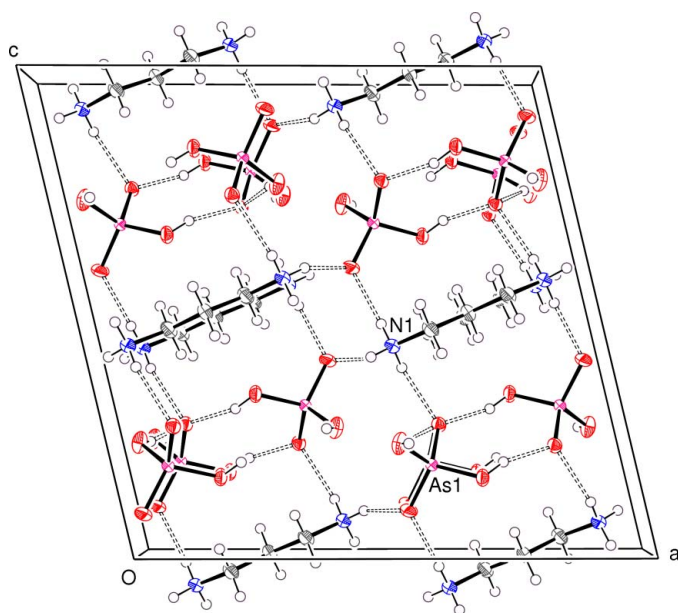


Figure 1

View of (I), showing 50% probability displacement ellipsoids (H atoms are drawn as spheres of arbitrary radii and the hydrogen bond is indicated by dashed lines). Symmetry code as in Table 1.



**Figure 2**  
Detail of a hydrogen-bonded (dashed lines) dihydrogenarsenate double chain in (I). Symmetry codes as in Table 2.



**Figure 3**  
Projection of the unit cell contents of (I) on to (010). Dashed lines indicate hydrogen bonds.

double chains (Fig. 2) propagating along [010] by way of inversion-symmetry-generated pairs of  $O2-H2 \cdots O4^{iii}$  and  $O1-H1 \cdots O4^{ii}$  bonds (see Table 2 for symmetry codes). The first of these bonds results in 'dimers' of dihydrogenarsenate tetrahedra, which in turn are linked into double chains by the second hydrogen bond. In graph-set notation (Bernstein *et al.*, 1995), these bonding patterns correspond to  $R_2^2(8)$  and  $R_4^4(12)$  loops, respectively. This scheme results in every  $[H_2AsO_4]^-$  group in the chain forming two hydrogen bonds to its neighbours and accepting two hydrogen bonds from its neighbours. The  $As \cdots As^{iii}$  (via  $O2-H2 \cdots O4^{iii}$ ) and  $As \cdots As^{ii}$  (via  $O1-H1 \cdots O4^{ii}$ ) separations are 4.5325 (4) and 4.6549 (4) Å, respectively (symmetry codes as in Table 2).

The organic species interacts with the dihydrogenarsenate anions by way of three  $N-H \cdots O$  hydrogen bonds [mean  $H \cdots O = 2.00$  Å, mean  $N-H \cdots O = 158^\circ$  and mean  $N \cdots O = 2.892$  (3) Å], such that the [010] dihydrogenarsenate double chains are crosslinked in the *a* and *c* directions to result in a

three-dimensional network (Fig. 3). A *PLATON* (Spek, 2003) analysis of (I) indicated the presence of two short  $C-H \cdots O$  contacts (Table 2) although their structural significance is not clear.

The hydrogen-bonded tetrahedral double chains in (I) are different from the motifs seen in related structures. In bis(cycloheptylammonium) hydrogenarsenate monohydrate (Todd & Harrison, 2005a) and bis(benzylammonium) hydrogenarsenate monohydrate (Lee & Harrison, 2003c), hydrogen-bonded dimers of  $[HAsO_4]^{2-}$  units occur, with the dimers bridged into double chains by intervening water molecules. In piperidinium dihydrogenarsenate (Lee & Harrison, 2003b) and *t*-butylammonium dihydrogenarsenate (Wilkinson & Harrison, 2004), single chains of  $[H_2AsO_4]^-$  anions occur with each adjacent dihydrogenarsenate pair linked by a pair of hydrogen bonds. In propane-1,3-diaminium hydrogenarsenate monohydrate (Todd & Harrison, 2005b), containing the same cation as (I) but prepared at higher pH, yet another hydrogen-bonded chain motif occurs.

## Experimental

0.5 M aqueous propane-1,3-diamine solution (10 ml) was added to 0.5 M aqueous  $H_3AsO_4$  solution (10 ml) to result in a clear solution. A mass of plate- and slab-like crystals of (I) grew as the water evaporated over the course of a few days.

### Crystal data

$(C_3H_{12}N_2)[AsH_2O_4]_2$   
 $M_r = 358.02$   
 Monoclinic,  $I2/a$   
 $a = 15.5563$  (8) Å  
 $b = 4.6549$  (2) Å  
 $c = 15.0454$  (7) Å  
 $\beta = 103.399$  (1)°  
 $V = 1059.83$  (9) Å<sup>3</sup>  
 $Z = 4$

$D_x = 2.244$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 3458 reflections  
 $\theta = 2.7-32.5^\circ$   
 $\mu = 6.33$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
 Plate, colourless  
 $0.50 \times 0.19 \times 0.03$  mm

### Data collection

Bruker SMART 1000 CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (*SADABS*; Bruker, 1999)  
 $T_{min} = 0.144$ ,  $T_{max} = 0.833$   
 5128 measured reflections

1899 independent reflections  
 1667 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.044$   
 $\theta_{max} = 32.5^\circ$   
 $h = -23 \rightarrow 23$   
 $k = -7 \rightarrow 5$   
 $l = -22 \rightarrow 17$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.094$   
 $S = 1.02$   
 1899 reflections  
 71 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0677P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.002$   
 $\Delta\rho_{max} = 1.07$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -1.49$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.0037 (6)

**Table 1**  
Selected geometric parameters (Å, °).

As1—O3	1.6375 (17)	As1—O1	1.7071 (17)
As1—O4	1.6669 (16)	As1—O2	1.7180 (18)
N1—C1—C2—C1 <sup>†</sup>	179.5 (3)		

Symmetry code: (i)  $-x + \frac{1}{2}, y, -z + 1$ .

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 $\cdots$ O4 <sup>ii</sup>	0.83	1.82	2.608 (3)	159
O2—H2 $\cdots$ O4 <sup>iii</sup>	0.90	1.74	2.603 (3)	161
N1—H3 $\cdots$ O3 <sup>iv</sup>	0.89	1.89	2.740 (3)	160
N1—H4 $\cdots$ O4	0.89	2.13	2.967 (3)	156
N1—H5 $\cdots$ O3 <sup>v</sup>	0.89	1.97	2.818 (3)	158
C1—H7 $\cdots$ O2 <sup>vi</sup>	0.97	2.48	3.389 (3)	156
C2—H8 $\cdots$ O2 <sup>v</sup>	0.97	2.52	3.482 (3)	174

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

The *I*-centred unit cell was chosen in preference to the *C*-centred setting (space group *C2/c*) to avoid a very obtuse  $\beta$  angle of 127° (Mighell, 2003). The O-bound H atoms were found in difference maps and refined as riding on their carrier O atoms in their as-found relative positions. H atoms bonded to C and N atoms were placed in idealized positions ( $C-H = 0.97$  Å and  $N-H = 0.89$  Å) and refined as riding, allowing for free rotation of the  $-NH_3$  group. The constraint  $U_{iso}(H) = 1.2U_{eq}(\text{carrier})$  was applied in all cases. The highest difference peak is 0.95 Å from O3 and the deepest difference hole is 1.20 Å from As1.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); 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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