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Key indicators

 Single-crystal X-ray study
 $T = 293$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.022
 wR factor = 0.057
 Data-to-parameter ratio = 31.9

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

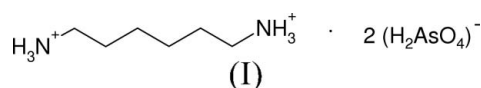
Hexane-1,6-diammonium bis(dihydrogenarsenate): infinite anionic layers containing $R_6^6(24)$ loops

 Received 13 February 2007
 Accepted 14 February 2007

The title compound, $\text{C}_6\text{H}_{18}\text{N}_2^{2+} \cdot 2\text{H}_2\text{AsO}_4^-$, contains a network of doubly protonated centrosymmetric hexane-1,6-diammonium cations and dihydrogenarsenate anions. These species interact by way of cation-to-anion $\text{N}-\text{H} \cdots \text{O}$ and anion-to-anion $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, the latter leading to infinite sheets of the H_2AsO_4^- anions.

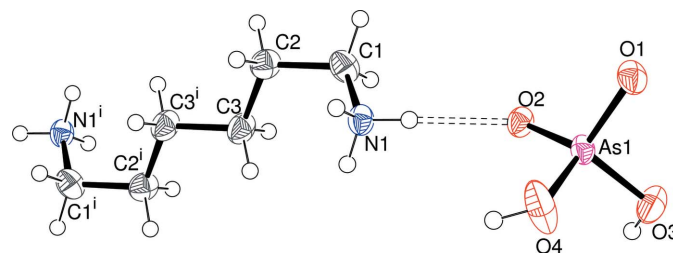
Comment

The title compound, (I) (Fig. 1), was prepared as part of our ongoing studies of hydrogen-bonding interactions in the molecular salts of oxo-anions (Wilkinson & Harrison, 2005).



The tetrahedral H_2AsO_4^- anion in (I) [mean $\text{As}-\text{O} = 1.683$ (2) Å] shows the usual distinction (Table 1) between the protonated and unprotonated $\text{As}-\text{O}$ bond lengths. The complete hexane-1,6-diammonium dication has a centre of symmetry at the mid-point of the $\text{C}3-\text{C}3^i$ bond [symmetry code: (i) $-x, -y, -z$]. The $\text{N}1-\text{C}1-\text{C}2-\text{C}3$ torsion angle of -72.87 (18) $^\circ$ indicates a *gauche* conformation for these four atoms within the dication, whereas $\text{C}1-\text{C}2-\text{C}3-\text{C}3^i$ are *anti* [torsion angle = 179.17 (19) $^\circ$]

As well as Coulombic forces, the component species in (I) interact by way of a network of $\text{O}-\text{H} \cdots \text{O}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds (Table 2). The H_2AsO_4^- units are linked into infinite sheets (Fig. 2) by way of the $\text{O}-\text{H} \cdots \text{O}$ bonds. The $\text{O}3-\text{H}1 \cdots \text{O}2^{\text{ii}}$ bond (see Table 2 for symmetry code) results in inversion-generated dimeric pairs of H_2AsO_4^- tetrahedra linked by a double (*i.e.* $\text{O}-\text{H} \cdots \text{O} + \text{O} \cdots \text{H}-\text{O}$) hydrogen bond. The $\text{O}4-\text{H}2 \cdots \text{O}1^{\text{iii}}$ bond links the dimers into an infinite sheet (Fig. 3) propagating in (100). The $\text{As} \cdots \text{As}^{\text{ii}}$ and


Figure 1

The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radius. The hydrogen bond is indicated by a double-dashed line. [Symmetry code: (i) $-x, -y, -z$.]

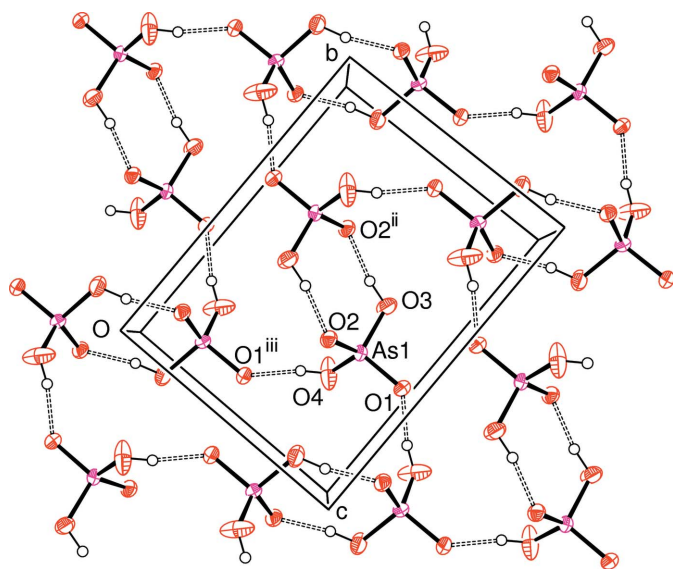


Figure 2
Detail of a part of a (100) hydrogen-bonded sheet of H_2AsO_4^- groups in (I), with hydrogen bonds indicated by double-dashed lines. Symmetry codes as in Table 2

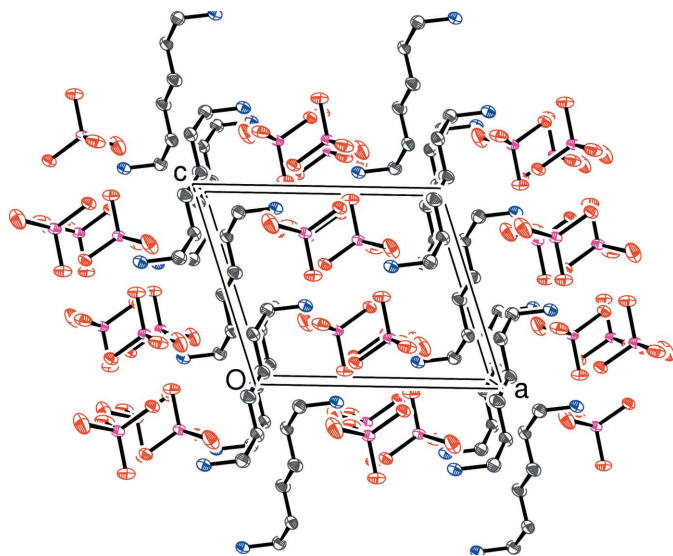


Figure 3
The packing in (I), viewed down [010], showing the (100) dihydrogen-arsenate layers mediated by the organic cations. H atoms have been omitted for clarity.

$\text{As}\cdots\text{As}^{\text{iii}}$ separations are 4.3922 (3) and 4.8900 (3) Å, respectively. A supramolecular $R_6^6(24)$ loop (Bernstein *et al.*, 1995) arises for each circuit of six tetrahedra within the sheet.

The anionic sheets are bridged by the organic cations, each of which participates in three nearly linear $\text{N}-\text{H}\cdots\text{O}$ interactions from its $-\text{NH}_3^+$ group (Table 2), resulting in a layered crystal structure (Fig. 3).

Guanidinium dihydrogenarsenate, $\text{CH}_6\text{N}_3\cdot\text{H}_2\text{AsO}_4$ (Wilkinson & Harrison, 2005), contains a hydrogen-bonded tetrahedral sheet topology similar to that in the title compound, despite the different cation–anion ratio in $\text{CH}_6\text{N}_3\cdot\text{H}_2\text{AsO}_4$.

Experimental

An aqueous 1,6-diaminohexane solution (0.5 M, 10 ml) was added to an aqueous H_3AsO_4 solution (0.5 M, 10 ml), resulting in a clear solution. A mass of chunks and blocks of (I) grew as the water evaporated over the course of a few days.

Crystal data

$\text{C}_6\text{H}_{18}\text{N}_2^{2+}\cdot 2\text{AsH}_2\text{O}_4^-$	$V = 737.27$ (6) Å ³
$M_r = 400.10$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 9.5237$ (5) Å	$\mu = 4.56$ mm ⁻¹
$b = 10.1029$ (5) Å	$T = 293$ (2) K
$c = 8.0747$ (4) Å	$0.33 \times 0.31 \times 0.13$ mm
$\beta = 108.385$ (1)°	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	7129 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 1999)	2649 independent reflections
$T_{\text{min}} = 0.314$, $T_{\text{max}} = 0.589$	2187 reflections with $I > 2\sigma(I)$
(expected range = 0.295–0.553)	$R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$	83 parameters
$wR(F^2) = 0.057$	H-atom parameters constrained
$S = 0.99$	$\Delta\rho_{\text{max}} = 0.52$ e Å ⁻³
2649 reflections	$\Delta\rho_{\text{min}} = -0.53$ e Å ⁻³

Table 1

Selected bond lengths (Å).

As1—O1	1.6501 (11)	As1—O4	1.6998 (13)
As1—O2	1.6656 (11)	As1—O3	1.7169 (11)

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O3}-\text{H1}\cdots\text{O2}^{\text{ii}}$	0.92	1.70	2.6103 (15)	169
$\text{O4}-\text{H2}\cdots\text{O1}^{\text{iii}}$	0.86	1.71	2.5613 (16)	170
$\text{N1}-\text{H3}\cdots\text{O2}$	0.89	2.01	2.8938 (17)	172
$\text{N1}-\text{H4}\cdots\text{O2}^{\text{iii}}$	0.89	2.12	2.9681 (19)	159
$\text{N1}-\text{H5}\cdots\text{O1}^{\text{iv}}$	0.89	1.89	2.7714 (16)	169

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

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. The other H atoms were positioned geometrically, with $\text{C}-\text{H} = 0.97$ Å and $\text{N}-\text{H} = 0.89$ Å, and refined as riding atoms. $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$ for all H atoms.

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; 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.

HSW thanks the Carnegie Trust for the Universities of Scotland for an undergraduate vacation studentship.

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