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**Key indicators**

 Single-crystal X-ray study  
 $T = 293\text{ K}$   
 Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 Disorder in main residue  
 $R$  factor = 0.029  
 $wR$  factor = 0.074  
 Data-to-parameter ratio = 29.0

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

## 2-Methylpiperazinium bis(dihydrogenarsenate)

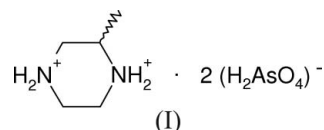
The title compound,  $\text{C}_5\text{H}_{14}\text{N}_2^{2+} \cdot 2\text{H}_2\text{AsO}_4^-$ , contains a network of centrosymmetric doubly protonated 2-methylpiperazinium cations, showing disorder of the methyl group, accompanied by dihydrogenarsenate anions. The component species interact by way of 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  $\text{H}_2\text{AsO}_4^-$  anions containing  $R_6^6(24)$  supramolecular loops.

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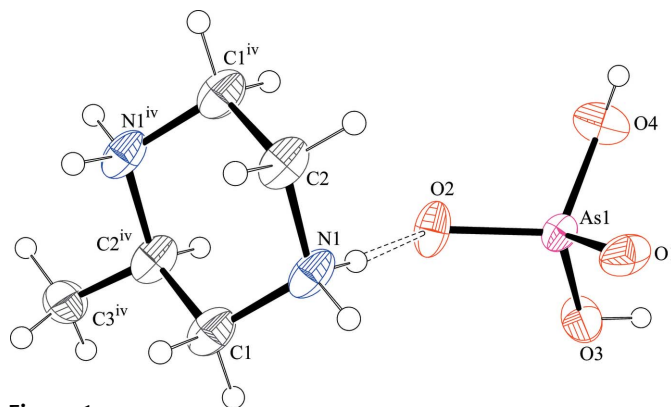
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**Comment**

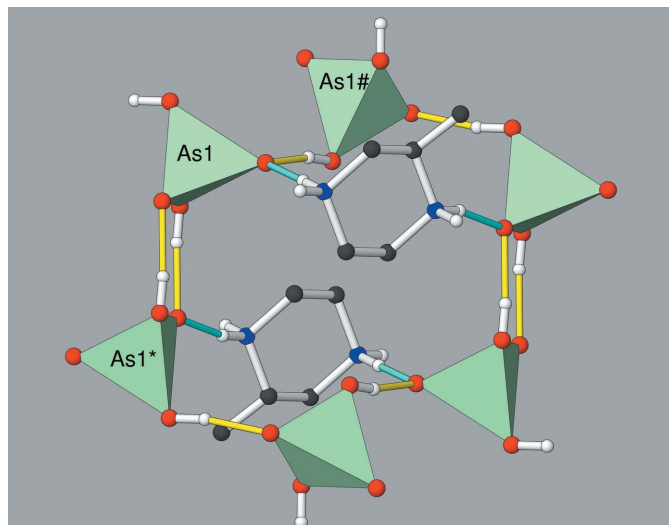
The title compound, (I) (Fig. 1), was prepared as part of our ongoing studies of hydrogen-bonding interactions in the molecular salts of oxo-anions (Wilkinson & Harrison, 2007).



The tetrahedral  $\text{H}_2\text{AsO}_4^-$  anion in (I) [mean  $\text{As}-\text{O} = 1.677(2)\text{ \AA}$ ], shows the usual distinction (Table 1) between protonated and unprotonated  $\text{As}-\text{O}$  bond lengths (Wilkinson & Harrison, 2007). The complete 2-methylpiperazinium dication is generated by inversion. This must result in disorder, as each dication is chiral at C2. Thus, the two enantiomers are superimposed in the long-range structure of the crystal, with all the atoms of the ring overlapped. A typical chair conformation for the six-membered ring arises, and atom C3 of the methyl group is equatorial to the ring in both disorder components.


**Figure 1**

The molecular structure of (I) (50% displacement ellipsoids and H atoms are drawn as spheres of arbitrary radius). The hydrogen bond is indicated by a double-dashed line. Only one disorder component of the cation is shown. [Symmetry code: (iv)  $-x, -y, 1 - z$ .]



**Figure 2**

Detail of a six-membered ring of  $\text{H}_2\text{AsO}_4^-$  groups in (I), in polyhedral representation, with attached organic cations. Only one disorder component of each cation is shown and the C-bound H atoms are omitted for clarity. The  $\text{H}\cdots\text{O}$  parts of the  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds are coloured yellow and the  $\text{H}\cdots\text{O}$  parts of the  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds are light blue. The  $\text{As1}^*$  and  $\text{As1}^\#$  tetrahedra are generated by the symmetry operations  $(1-x, 1-y, 1-z)$  and  $(1-x, \frac{1}{2}+y, \frac{3}{2}-z)$ , respectively.

As well as Coulombic forces, the component species in (I) interact by way of a network of anion-to-anion  $\text{O}-\text{H}\cdots\text{O}$  and cation-to-anion  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2). The hydrogen-bonding scheme and overall structure in (I) are very similar to those in piperazinium bis(dihydrogenarsenate), (II) (Wilkinson & Harrison, 2007). In both (I) and (II), the  $\text{H}_2\text{AsO}_4^-$  units are linked into infinite (100) layers by the  $\text{O}-\text{H}\cdots\text{O}$  bonds. A distinctive feature of the sheets are supra-molecular  $R_6^0(24)$  rings (Bernstein *et al.*, 1995) built up from six tetrahedra, the rings being stabilized by  $\text{N}-\text{H}\cdots\text{O}$  bonds from the organic cations (Fig. 2). For the two inter-tetrahedral  $\text{O}-\text{H}\cdots\text{O}$  interactions, the  $\text{As}\cdots\text{As}^i$  and  $\text{As}\cdots\text{As}^{ii}$  (see Table 2 for symmetry codes) separations for (I) are 4.3061 (3) and 4.7599 (3) Å, respectively, which are distinctly different from the values of 4.0148 (3) and 5.0190 (3) Å for the topologically equivalent network in (II).

## Experimental

To an aqueous racemic 2-methylpiperazine solution (10 ml, 0.5 M) was added an aqueous  $\text{H}_3\text{AsO}_4$  solution (10 ml, 0.5 M), resulting in a clear solution. Chunks and blocks of (I) grew as the water evaporated over the course of a few days; these were harvested by vacuum filtration and rinsed with acetone.

### Crystal data

$\text{C}_5\text{H}_{14}\text{N}_2^{2+}\cdot 2\text{AsH}_2\text{O}_4^-$	$V = 669.31 (5) \text{ \AA}^3$
$M_r = 384.06$	$Z = 2$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 6.7537 (3) \text{ \AA}$	$\mu = 5.02 \text{ mm}^{-1}$
$b = 8.1753 (4) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 12.7105 (5) \text{ \AA}$	$0.37 \times 0.12 \times 0.03 \text{ mm}$
$\beta = 107.501 (2)^\circ$	

### Data collection

Bruker SMART 1000 CCD diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 1999)  
 $T_{\min} = 0.258$ ,  $T_{\max} = 0.864$

6913 measured reflections  
2409 independent reflections  
1929 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.026$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.074$   
 $S = 1.06$   
2409 reflections

83 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.65 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.67 \text{ e \AA}^{-3}$

**Table 1**

Selected bond lengths (Å).

As1—O1	1.6477 (16)	As1—O3	1.6974 (16)
As1—O2	1.6531 (16)	As1—O4	1.7082 (17)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O4—H2 $\cdots$ O1 <sup>i</sup>	0.84	1.76	2.599 (3)	174
O3—H1 $\cdots$ O2 <sup>ii</sup>	0.86	1.70	2.548 (2)	169
N1—H4 $\cdots$ O2	0.90	1.79	2.689 (2)	175
N1—H3 $\cdots$ O1 <sup>iii</sup>	0.90	1.80	2.685 (2)	168

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

The C3 methyl group is disordered over two positions in the molecule. Crystal symmetry dictates equal occupancy for both components. The O-bound H atoms were found in a difference map and refined as riding in their as-found relative positions, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$  (see Table 2 for distances). The C- and N-bonded H atoms were placed in idealized positions ( $\text{C}-\text{H} = 0.96\text{--}0.97 \text{ \AA}$  and  $\text{N}-\text{H} = 0.90 \text{ \AA}$ ) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ . The methyl group was allowed to rotate, but not to tip, to best fit the electron density.

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) and ATOMS (Shape Software, 2004); software used to prepare material for publication: SHELXL97.

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