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Ammonium 4-nitrophenylarsonate

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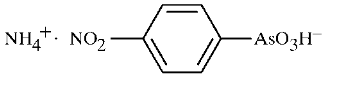
In the crystal structure of the title compound, $(NH_4)[AsO_2(OH)(C_6H_4NO_2)]$, the 4-nitrophenylarsonate anions and ammonium cations are linked through hydrogen bonds to form infinite chains along the *b* axis. The hydroxyl O atom of the 4-nitrophenylarsonate anion acts as both an acceptor and a donor of hydrogen bonds. All atoms are located in general positions.

Comment

The realm of phosphonate chemistry has developed rapidly and many new compounds have been prepared and characterized as a result of interest in their potential applications in the areas of sorption and ion exchange (Wang *et al.*, 1993), sensors (Cao *et al.*, 1992; Alberti & Polombari, 1989), nonlinear optics (Thompson, 1994; Ungashe *et al.*, 1992) and catalysis (Wan *et al.*, 1986). In contrast, arsonate chemistry has received only limited attention. To our knowledge, few studies have been undertaken of the synthesis and characterization of metal arsonates with the goal of preparing functional compounds analogous to the reported metal phosphonates (Huan *et al.*, 1990; Morizzi *et al.*, 2000). In this context, the synthesis and structure of the title compound, (I), are presented here.



(I)

The arsonate anion in (I) contains an As atom tetrahedrally connected to one C atom of the benzene ring and three O atoms (Nuttall & Hunter, 1996; Percino *et al.*, 2001). The As—O bond lengths range from 1.655 (3) to 1.732 (2) Å and the O—As—O angles vary from 108.8 (1) to 116.6 (1)°. The As—O5 (hydroxyl) bond is longer than the other two As—O bonds. The As—C distance of 1.930 (3) Å is close to that reported (1.95 Å) in the 4-aminobenzenearsonic acid complex (Shimada, 1961). The phenyl ring and nitro group are not coplanar, showing a dihedral angle of 6.4° between their mean planes.

The molecules of (I) are held together by an infinite chain of hydrogen bonds along the *b* axis (Fig. 2). The hydrogen bonds in this study have been considered with liberal distance cut-off criteria of $2.5 < D\cdots A < 3.0$ Å and angle cut-off criteria of $120 < D—H\cdots A < 180°$. Hydrogen-bond distances and angles are listed in Table 2.

From Fig. 2 it can be seen that there are five H atoms available for hydrogen bonding in the asymmetric unit, namely one from the arsonate hydroxyl group and the remaining four from the ammonium cation. There are three hydrogen bonds between the ammonium cation and O atoms from three different symmetry-related 4-nitrophenylarsonate anions. In dicyclohexylammonium arsonomethylphosphonate, the N atoms of the cation and the O atoms of the anion are also involved in hydrogen bonding (Falvello *et al.*, 1977). There is another hydrogen bond between the arsonate hydroxyl group and an arsonate O atom from another anion.

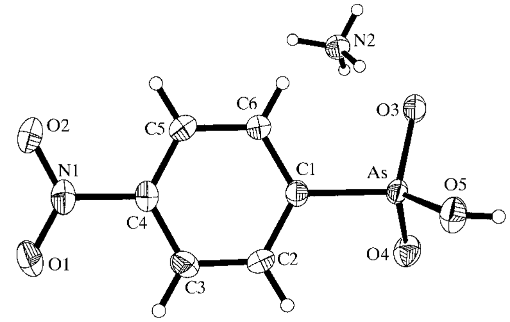


Figure 1
A view of the cation and anion of (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

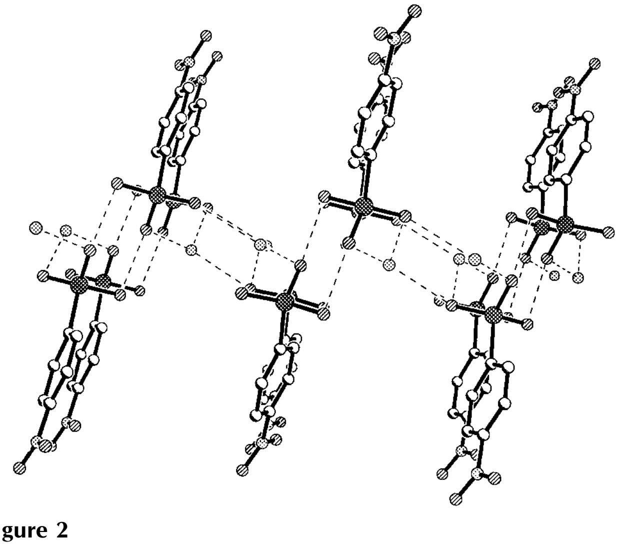


Figure 2
The infinite chains of (I) linked by hydrogen bonds (dashed lines) along the *b* axis.

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A comparison of the structure of (I) with that of benzenearsonic acid (Shimada, 1959) is interesting. The two structures are similar in having endless chains formed by the hydrogen bonds. However, in 4-aminobenzenearsonic acid, there are additional hydrogen bonds which connect these chains to form a beautiful network (Shimada, 1961).

In summary, the 4-nitrophenylarsonate anions and ammonium cations of (I) are linked through hydrogen bonds to form infinite chains along the *b* axis. The hydroxyl O atom of the 4-nitrophenylarsonate anion acts as both an acceptor and a donor of hydrogen bonds; as anticipated, the N atom of the ammonium cation acts only as a donor.

Experimental

An aqueous solution of ammonia was added to an aqueous solution of 4-nitrophenylarsonic acid until a pH of 6.5 was reached. Pale-yellow needle-shaped crystals of (I) were obtained after evaporating the solution at room temperature for a period of several weeks. Analysis calculated for $C_6H_9AsN_2O_5$: C 27.27, H 3.41%; found: C 27.41, H 3.26%. IR data (KBr, ν, cm^{-1}): 2814 (O—H), 1524 and 1349 (NO_2), 1089 (As—C), 1087 (As═O).

Crystal data

$(NH_4)[AsO_2(OH)(C_6H_4NO_2)]$
$M_r = 264.07$
Monoclinic, $P2_1/n$
$a = 11.670$ (3) Å
$b = 6.5073$ (16) Å
$c = 12.693$ (3) Å
$\beta = 107.975$ (18)°
$V = 916.9$ (4) Å^3
$Z = 4$
$D_x = 1.913$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
$\theta = 4.7$–8.9°
$\mu = 3.71$ mm^{-1}
$T = 293$ (2) K
Prism, pale yellow
0.52 × 0.36 × 0.23 mm

Data collection

Siemens *P*4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.223$, $T_{\max} = 0.426$
2283 measured reflections
1602 independent reflections
1285 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 25°$
$h = -1 \rightarrow 13$
$k = -1 \rightarrow 7$
$l = -15 \rightarrow 14$
3 standard reflections every 97 reflections intensity decay: none

Table 1
Selected geometric parameters (Å, °).

As—O4	1.655 (3)	C1—C6	1.392 (5)
As—O3	1.673 (3)	C1—C2	1.395 (5)
As—O5	1.732 (2)	C2—C3	1.372 (5)
As—C1	1.930 (3)	C3—C4	1.382 (5)
O1—N1	1.216 (4)	C4—C5	1.377 (5)
O2—N1	1.229 (4)	C5—C6	1.375 (5)
N1—C4	1.472 (5)		
O4—As—O3	116.59 (13)	C6—C1—As	119.6 (3)
O4—As—O5	109.22 (14)	C2—C1—As	120.2 (3)
O3—As—O5	108.79 (13)	C3—C2—C1	120.7 (4)
O4—As—C1	110.75 (14)	C2—C3—C4	117.8 (3)
O3—As—C1	107.48 (15)	C5—C4—C3	122.8 (3)
O5—As—C1	103.16 (13)	C5—C4—N1	118.4 (3)
O1—N1—O2	123.6 (3)	C3—C4—N1	118.8 (3)
O1—N1—C4	118.6 (3)	C6—C5—C4	119.2 (3)
O2—N1—C4	117.8 (3)	C5—C6—C1	119.4 (3)
C6—C1—C2	120.2 (3)		

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.077$
$S = 0.98$
1602 reflections
144 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0412P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.49$ e Å^{-3}
$\Delta\rho_{\min} = -0.57$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.0271 (17)

Table 2
Short O—H···O and N—H···O contacts (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H11···O3	0.92 (4)	1.89 (4)	2.813 (4)	176 (3)
N2—H12···O4$^{\rm i}$	0.86 (3)	1.97 (3)	2.819 (3)	169 (5)
N2—H13···O4$^{\rm ii}$	0.94 (5)	1.92 (5)	2.844 (4)	168 (4)
O5—H5···O3$^{\rm iii}$	0.82	1.87	2.638 (4)	156

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

All H atoms on C atoms were generated geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. The H atoms of the ammonium cation were located in a difference Fourier map and refined freely. The H atom of the hydroxyl group was generated theoretically and refined as a riding atom, with O—H = 0.82 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1196). Services for accessing these data are described at the back of the journal.

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