Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Trimethylarsonium iodide

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(s–C) = 0.007 Å
R factor = 0.029
wR factor = 0.078
Data-to-parameter ratio = 22.4

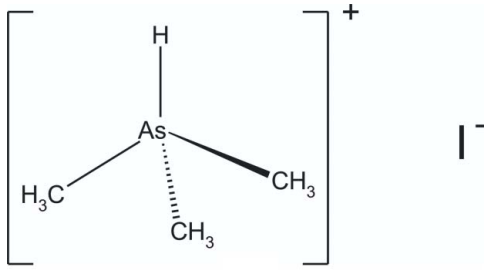
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 15 November 2005
Accepted 17 November 2005
Online 23 November 2005

The title compound, $C_3H_{10}As^+\cdot I^-$, contains discrete $[(CH_3)_3AsH]^+$ cations with a distorted tetrahedral geometry for the central As atom, which lies on a mirror plane. Weak van der Waals contacts are observed between the I atom and the H atoms in the range 3.15 (1)–3.25 (1) Å.

Comment

$[(CH_3)_4As]^+$ cations have been reported with a variety of different counteranions. Tetramethylarsonium halides, for example, have been characterized by X-ray structural analysis for the heavier halides bromide (Collins *et al.*, 1963) and iodide (Assenmacher & Jansen, 1995), whereas the chloride compound has not yet been characterized by single-crystal structure analysis, although Debye–Scherrer investigations have revealed that it is isostructural with $(CH_3)_4AsBr$ (Ang & Dunell, 1976). In contrast, the trimethylarsonium cation has been characterized only twice. In both $[(CH_3)_3AsH][As_2F_{11}]$ and $[(CH_3)_3AsH][SbF_6]$ (Minkwitz *et al.*, 1999), relatively large counteranions are needed to stabilize the $[(CH_3)_3AsH]^+$ cations in the solid state.



(I)

The title compound, $(CH_3)_3AsHI$, (I), is the first example of a discrete trimethylarsonium cation crystallizing with a halide counteranion. The As atom, which lies on a mirror plane, exhibits a distorted tetrahedral environment, with As—C distances of 1.923 (5) and 1.927 (8) Å, which are similar to those observed in $[(CH_3)_3AsH][As_2F_{11}]$ [1.894 (5)–1.908 (5) Å].

The I^- counteranion exhibits long-range van der Waals interactions with its surrounding H atoms [I···H 3.15 (1)–3.25 (1) Å]; these stabilize the arrangement of (I) in the crystal packing (Fig. 2).

Experimental

GeI_4 (580.19, 1.0 mmol), As_2Se_3 (193.4 mg, 0.5 mmol), Se (79.0 mg, 1.0 mmol) and K_2CO_3 (138.2 mg, 1.0 mmol) were heated to 433 K in CH_3OH (0.8 ml) in a sealed glass tube. After 2 d, the contents were

cooled to room temperature to afford colourless crystals of (I) in 52% yield.

Crystal data

$C_3H_{10}As^+\cdot I^-$
M_r = 247.93
Orthorhombic, *Pnma*
a = 14.174 (3) Å
b = 8.0458 (16) Å
c = 6.2037 (12) Å
V = 707.5 (2) Å^3
Z = 4
D_x = 2.328 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 21 reflections
θ = 6.2–15.0°
μ = 9.04 mm^{-1}
T = 292 (2) K
Block, colourless
0.41 × 0.33 × 0.21 mm

Data collection

Siemens *P*4 four-circle diffractometer
ω scans
Absorption correction: ψ scan (*XPREP* in *SHELXTL*; Sheldrick, 1995)
T_{min} = 0.040, T_{max} = 0.152
671 measured reflections
671 independent reflections
576 reflections with $I > 2\sigma(I)$
θ_{max} = 25.0°
$h = 0 \rightarrow 16$
$k = -9 \rightarrow 0$
$l = 0 \rightarrow 7$
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.078
S = 1.16
671 reflections
30 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.82 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0286 (17)

Table 1
Selected geometric parameters (Å, °).

As—C1	1.923 (6)	As—C2	1.927 (8)
C1^i—As—C1	98.9 (3)	C1—As—C2	97.8 (2)

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

H atoms were located in a difference electron-density map but were refined with fixed individual displacement parameters [U_{iso}(H) = 1.5U_{eq}(C)] using a riding model, with C—H = 0.96 Å. The idealized As—H bond length is 1.40 Å.

Data collection: *R3m/V* (Siemens, 1989); cell refinement: *R3m/V*; data reduction: *XDISK* (Siemens, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL97*.

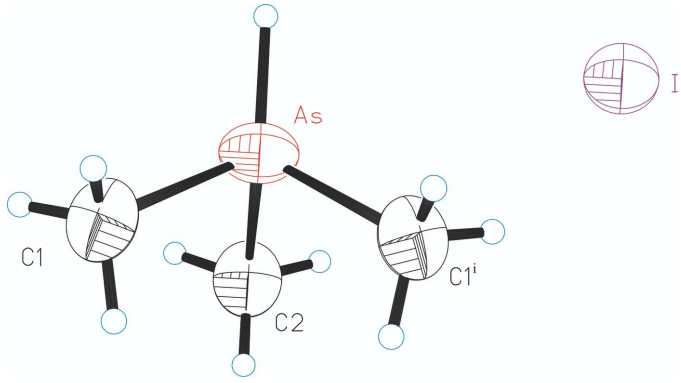


Figure 1
The structure of (I). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $x, \frac{1}{2}-y, z$.]

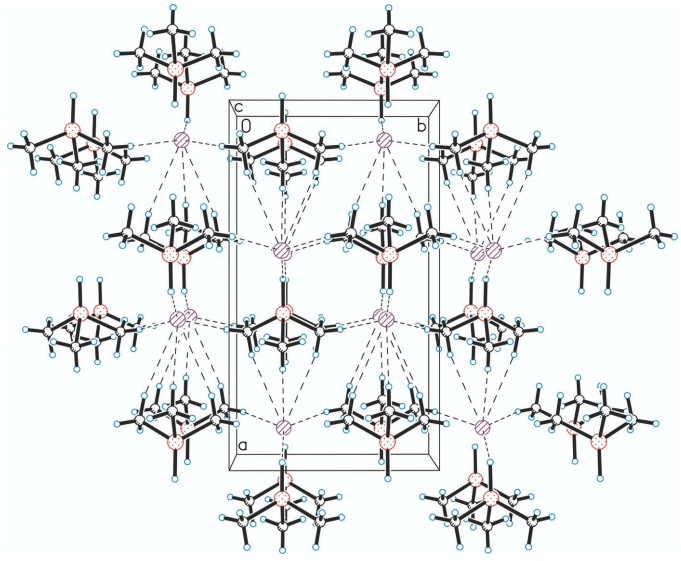


Figure 2
Projection of the structure of (I) perpendicular to the *ab* plane, showing the weak van der Waals interactions (dashed lines) of the I atoms. Atom colour codes: I purple, As red, C black and H blue.

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