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(Triphenylarsine)iodinemonobromine: a charge-transfer adduct in which arsenic selectively bonds to iodine

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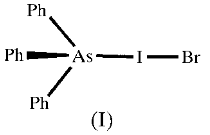
The title molecule, (iodobromo)triphenylarsenic(III), $[As(BrI)(C_6H_5)_3]$, has a dart shape, with the phenyl rings arranged in a propeller conformation [I—As—C—C 61.3 (4), 43.8 (4) and 54.1 (4)°]. There is no indication that the halogen atoms have mixed site occupancies. Packing forces displace the I atom away from one phenyl ring [I—As—C 117.3 (2)°] towards the other two [I—As—C 109.8 (2) and 108.3 (2)°] and produce an even more pronounced leaning of the terminal bromine [As—I—Br 174.78 (2)°].

Comment

This work is a continuation of our investigation into adducts formed between group VA donors and the heavier halogens. Both Ph_3PI_2 [Godfrey *et al.*, 1991; I—P—C—C 38 (1), 45 (1) and 57 (1)°] and Ph_3PBr_2 [Bricklebank *et al.*, 1992; Br—P—C—C 43.0 (9), 49.1 (9) and 57.7 (8)°] have similar shapes to the title molecule, (I). However, at 2.5904 (8) Å, the As—I bond in (I) is shorter than any of the analogous bonds in the various polymorphs of Ph_3AsI_2 (Abbas *et al.*, 1994; Beagley *et al.*, 1988), which range from 2.613 (2) to 2.653 (2) Å. Interestingly, if a Lewis acid competes for the terminal iodine in Ph_3AsI_2, the As—I bond is shortened below the Ph_3AsIBr value, *e.g.* 2.485 (1) Å when GaI_3 is used as the Lewis acid (Baker *et al.*, 1994). This suggests that the As—I bond is short in (I) because the Br—I bonding is weaker than the corresponding I—I interaction. In contrast to the disordered $Ph_3PI_{1.29}Br_{0.71}$ structure (Bricklebank *et al.*, 1993), where P is attached to Br in 14 (2)% of the molecules, the structure of (I) contains no As—Br bonds.



(I)

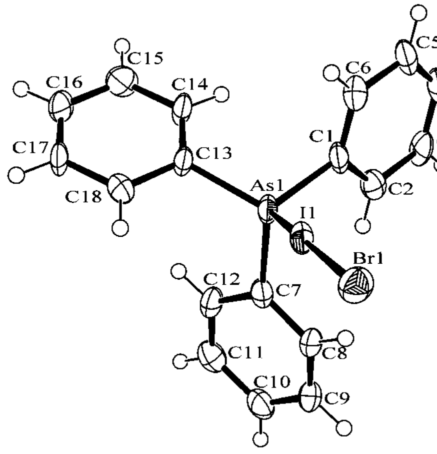


Figure 1
View of the structure of (I) showing the atom-numbering scheme and 50% probability displacement ellipsoids. H atoms are shown as spheres of arbitrary radii.

Experimental

Triphenylarsine (1.98 g, 7.25 mmol) was added to diethyl ether (*ca* 75 ml) under dry argon and a saturated ether solution of IBr (1.5 g, 7.25 mmol) was then added (Godfrey, 1993). A yellow solid precipitated immediately and was recrystallized from diethyl ether to give orange crystals suitable for X-ray analysis.

Crystal data

$[As(BrI)(C_6H_5)_3]$
$M_r = 513.03$
Monoclinic, $P2_1/c$
$a = 9.1198\ (13)$ Å
$b = 9.960\ (2)$ Å
$c = 19.483\ (3)$ Å
$\beta = 92.176\ (12)°$
$V = 1768.4\ (6)$ Å^3
$Z = 4$
$D_x = 1.927$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 13.33$–$16.41°$
$\mu = 5.919$ mm^{-1}
$T = 203\ (2)$ K
Needle, orange
0.25 × 0.15 × 0.11 mm

Data collection

Nonius MACH3 diffractometer
$2\theta/\omega$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.386$, $T_{max} = 0.521$
3270 measured reflections
3065 independent reflections
2360 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 24.98°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 11$
$l = -23 \rightarrow 23$
3 standard reflections every 150 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.089$
$S = 1.023$
3065 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0503P)^2 + 2.5099P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.65$ e Å^{-3}
$\Delta\rho_{min} = -0.99$ e Å^{-3}
Extinction correction: *SHELX*97 (Sheldrick, 1997)
Extinction coefficient: 0.00015 (19)

Table 1
Selected geometric parameters (Å, °).

I1—As1	2.5904 (8)	As1—C7	1.911 (6)
I1—Br1	2.8546 (8)	As1—C13	1.920 (5)
As1—C1	1.906 (5)		
As1—I1—Br1	174.78 (2)	C1—As1—I1	109.76 (17)
C1—As1—C7	107.2 (2)	C7—As1—I1	108.30 (17)
C1—As1—C13	107.1 (2)	C13—As1—I1	117.26 (18)
C7—As1—C13	106.8 (2)		

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *Software*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELX*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELX*97; molecular graphics: *ORTEP*-3 (Farrugia, 1997) and *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELX*97.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: CF1314). Services for accessing these data are described at the back of the journal.

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