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Bis(tetraphenylarsonium) hexabromorhenate(IV)

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Key indicators

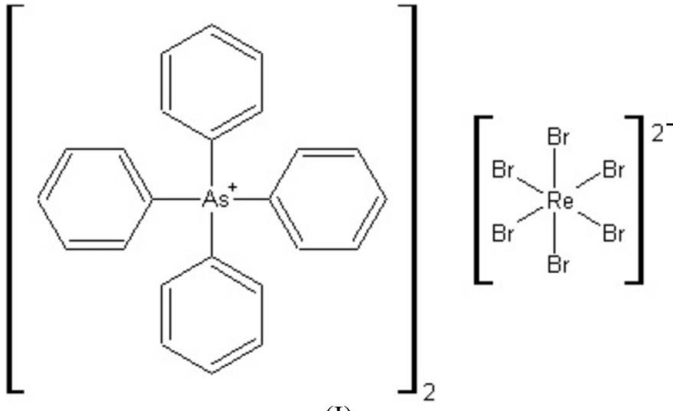
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.010 Å
R factor = 0.034
wR factor = 0.069
Data-to-parameter ratio = 15.6

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

The title compound, $(C_{24}H_{20}As)_2[ReBr_6]$, consists of tetraphenylarsonium cations and $[ReBr_6]^{2-}$ dianions, the latter lying on inversion centres. A possible C—H···Br interaction stabilizes the crystal packing.

Comment

The title complex, (I) (Fig. 1), is the first reported arsonium salt of the hexabromorhenate(IV) dianion. The Re atom occupies an inversion centre and is octahedrally coodinated by bromide anions. The Re—Br bond lengths in (I) (Table 1) are similar to those found in other hexabromorhenate(IV) dianions (Grundy & Brown, 1970). The cation and anion are linked by a weak C—H···Br bond (Table 2).



(I)

In the crystal packing of (I), each $[ReBr_6]^{2-}$ anion is surrounded by large organic cations, so there are no short metal–metal contacts: the shortest intermetallic distances in (I) are Re···Re^{ii} = 10.4085 (9), Re···Re^{iii} = 10.4157 (9) and Re···Re^{iv} = 10.8892 (9) Å [symmetry codes: (ii) $x-1, y, z$; (iii) $x, y-1, z$; (iv) $x-1, y-1, z$].

Experimental

$(NH_4)_2ReBr_6$ was obtained in a reaction of $(NH_4)ReO_4$ with H_3PO_2 in 7 *M* HBr (Watt & Thompson, 1963). A mixture of $(NH_4)_2ReBr_6$ (0.46 g), tetraphenylarsonium bromide monohydrate (0.40 g) and a solution of 1 ml of HBr in 50 ml of water was stirred for 5 h at 333 K. The color of the reaction mixture changed from dark violet–red to yellow–brown. After reaction, the mixture was cooled and the first crystalline product was obtained. X-ray quality crystals of (I) were obtained by recrystallization of the crude product from water at room temperature.

Crystal data

$(C_{24}H_{20}As)_2[ReBr_6]$
M_r = 1432.25
Triclinic, $P\overline{1}$
a = 10.4085 (9) Å
b = 10.4157 (9) Å
c = 12.1694 (9) Å
α = 92.565 (7)°
β = 99.915 (7)°
γ = 116.880 (9)°
V = 1147.85 (16) Å^3
Z = 1
D_x = 2.072 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 9.33 mm^{-1}
T = 100 (2) K
Prism, orange
0.13 × 0.10 × 0.07 mm

Data collection

Kuma KM-4-CCD diffractometer
ω scans
Absorption correction: numerical (*CrysAlis RED*; Oxford Diffraction, 2004)
T_{min} = 0.318, T_{max} = 0.598
9761 measured reflections
4040 independent reflections
2979 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.069
S = 0.93
4040 reflections
259 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0254P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.98 e Å^{-3}
$\Delta\rho_{min}$ = −1.16 e Å^{-3}

Table 1
Selected bond lengths (Å).

Re1—Br1	2.5023 (7)	Re1—Br2	2.5264 (7)
Re1—Br3	2.5197 (7)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C20—H20···Br1	0.93	2.86	3.671 (6)	147

The H atoms were positioned geometrically (C—H = 0.95 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier). The highest difference peak is 0.98 Å from atom Re1 and the deepest difference hole is 1.16 Å from Re1.

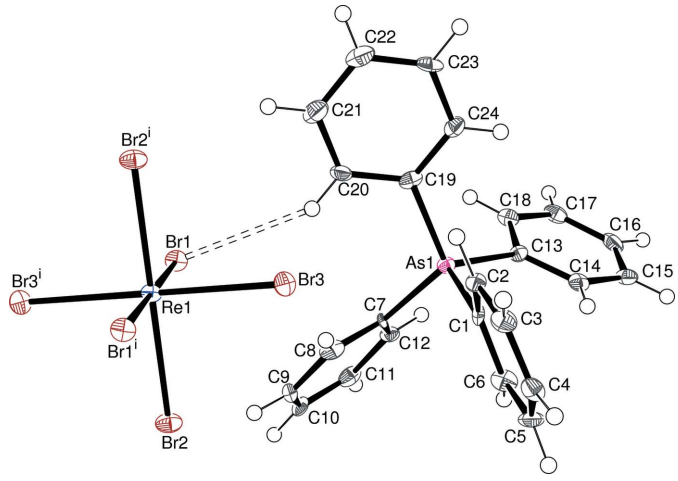


Figure 1
The structure of the ions of (I) showing 50% displacement ellipsoids for the non-H atoms. The C—H···Br interaction is indicated by a double-dashed line. [Symmetry code: (i) 1 − x, −y, 1 − z.]

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2004); data reduction: *CrysAlis RED*; 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*.

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