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Isopentyltriphenylphosphonium bromide methanol solvate

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Key indicators

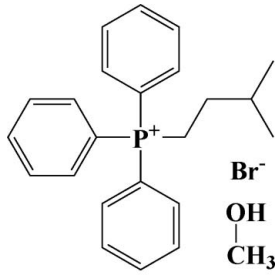
Single-crystal X-ray study
T = 102 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.105
Data-to-parameter ratio = 16.4

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

At 102 K, the isopentyl group of the title compound, $C_{23}H_{26}P^+\cdot Br^-$, is in the extended conformation. The phenyl rings are in the propeller configuration usually found in this family of triphenylphosphonium compounds. The methanol solvent molecule is hydrogen bonded to the bromide ion.

Comment

This is the tenth crystal structure of a series of alkyl-substituted triphenylphosphonium bromide compounds from this laboratory (Czerwinski, 1986, 2004*a*,*b*,*c*, 2005; Ponnuswamy & Czerwinski, 1986; Czerwinski & Ponnuswamy, 1988*a*,*b*, 1989). Atom labelling is consistent with earlier structures.



(I)

The shorter than normal C—O bond, as well as an anomalous peak near a methyl hydrogen of the methanol carbon, is most likely due to the Fourier ripple effects from the Br^- ion. All other bond lengths and bond angles are within normal limits. Hydrogen-bonding information is given in Table 1.

Experimental

The title compound was obtained from Lancaster Synthesis Ltd. Suitable crystals were grown by evaporation of a methanol solution at 294 K.

Crystal data

$C_{23}H_{26}P^+\cdot Br^-\cdot CH_4O$
M_r = 445.36
Monoclinic, $P2_1/c$
a = 8.7797 (1) Å
b = 18.3601 (5) Å
c = 14.6181 (3) Å
β = 108.775 (1)°
V = 2231.00 (8) Å^3
Z = 4
D_x = 1.326 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 3.26 mm^{-1}
T = 102 (2) K
Prism, colorless
0.4 × 0.35 × 0.35 mm

Data collection

Bruker SMART diffractometer
ω scans
Absorption correction: none
22024 measured reflections
4074 independent reflections
3546 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 68.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.105$
$S = 1.04$
4074 reflections
248 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 2.401P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.026$
$\Delta\rho_{max} = 0.9$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.364 (4)	C13—C15	1.521 (4)
C11—C12	1.541 (4)	C21—P	1.797 (3)
C11—P	1.805 (3)	C31—P	1.806 (3)
C12—C13	1.528 (4)	C41—P	1.792 (3)
C13—C14	1.519 (4)		
C12—C11—P	114.08 (18)	C46—C41—P	118.7 (2)
C13—C12—C11	112.8 (2)	C42—C41—P	121.1 (2)
C14—C13—C15	110.2 (2)	C41—P—C21	108.82 (13)
C14—C13—C12	110.3 (2)	C41—P—C11	111.17 (13)
C15—C13—C12	112.5 (2)	C21—P—C11	108.89 (12)
C26—C21—P	120.6 (2)	C41—P—C31	108.19 (12)
C22—C21—P	119.8 (2)	C21—P—C31	110.09 (13)
C32—C31—P	119.6 (2)	C11—P—C31	109.68 (13)
C36—C31—P	121.0 (2)		
P—C11—C12—C13	178.37 (19)	C22—C21—P—C11	50.3 (3)
C11—C12—C13—C14	164.9 (2)	C12—C11—P—C41	58.8 (2)
C11—C12—C13—C15	−71.6 (3)	C12—C11—P—C21	178.68 (19)
C46—C41—P—C11	−160.5 (2)	C12—C11—P—C31	−60.8 (2)
C42—C41—P—C11	24.0 (3)	C32—C31—P—C11	79.0 (2)
C26—C21—P—C11	−131.7 (2)	C36—C31—P—C11	−97.7 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···Br	0.82	2.51	3.329 (3)	173

H atoms were placed in geometrically idealized positions, and constrained to ride on their parent atoms, with C—H = 0.90–1.00 Å, O—H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O and methyl C).

Data collection: *PROTEUM* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

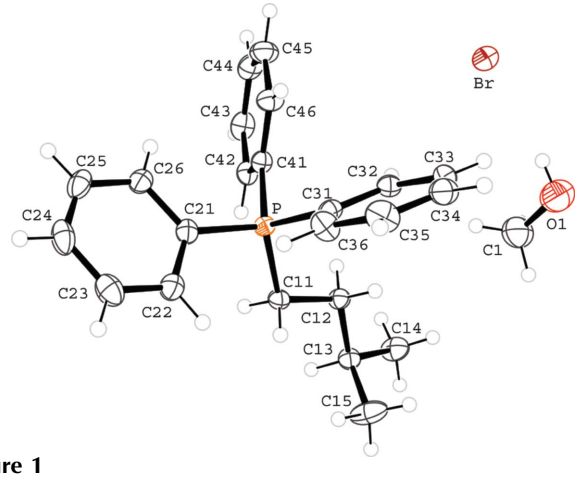


Figure 1
View of the title compound, showing the atom-labeling scheme (50% probability displacement ellipsoids)

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