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Butyltriphenylphosphonium bromide

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At 106 K, the three C atoms closest to P in the butyl group of the title compound, $C_{22}H_{24}BrP$, are in an extended conformation. However, unlike the longer alkylamine substituted triphenylphosphonium compounds, the terminal torsion angle in the butyl group is *gauche*. The phenyl rings are in the propeller configuration usually found in this family of triphenylphosphonium compounds.

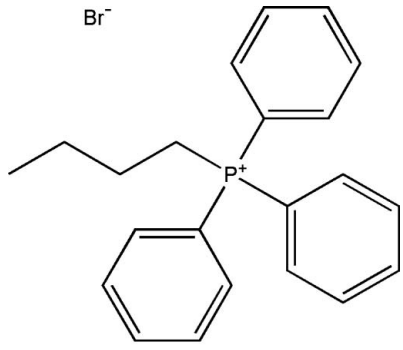
Key indicators

Single-crystal X-ray study
T = 106 K
Mean σ(C–C) = 0.04 Å
R factor = 0.034
wR factor = 0.095
Data-to-parameter ratio = 15.8

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

Comment

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



(I)

Experimental

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

Crystal data

$C_{22}H_{24}P^{+}\cdot Br^{-}$
M_r = 399.29
Monoclinic, $P2_1/c$
a = 11.1332 (2) Å
b = 10.0822 (3) Å
c = 17.4142 (4) Å
β = 104.058 (1)°
V = 1896.15 (8) Å^3
Z = 4
D_x = 1.399 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 19602 reflections
θ = 5.1–68.3°
μ = 3.73 mm^{-1}
T = 106 (2) K
Prism, colorless
0.43 × 0.25 × 0.15 mm

Data collection

Bruker CCD diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1985, 1987, 1995)
T_{min} = 0.235, T_{max} = 0.574
18937 measured reflections
3427 independent reflections
3037 reflections with $I > 2\sigma(I)$
R_{int} = 0.079
θ_{max} = 68.3°
$h = -13 \rightarrow 12$
$k = -9 \rightarrow 11$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 1.4293P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.034$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.095$	$\Delta\rho_{max} = 0.49$ e Å^{-3}
$S = 1.14$	$\Delta\rho_{min} = -0.70$ e Å^{-3}
3427 reflections	
217 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

C11—C12	1.540 (4)	C21—P	1.806 (3)
C11—P	1.800 (3)	C31—P	1.800 (3)
C12—C13	1.530 (4)	C41—P	1.801 (3)
C13—C14	1.521 (4)		
C12—C11—P	112.72 (17)	C42—C41—P	117.2 (2)
C13—C12—C11	111.6 (2)	C11—P—C31	110.40 (13)
C14—C13—C12	113.8 (2)	C11—P—C41	108.52 (12)
C26—C21—P	122.3 (2)	C31—P—C41	110.80 (12)
C22—C21—P	117.5 (2)	C11—P—C21	111.61 (12)
C36—C31—P	118.7 (2)	C31—P—C21	106.82 (12)
C32—C31—P	121.5 (2)	C41—P—C21	108.69 (12)
C46—C41—P	122.9 (2)		
P—C11—C12—C13	170.88 (19)	C32—C31—P—C11	0.4 (3)
C11—C12—C13—C14	−73.6 (3)	C46—C41—P—C11	−123.8 (2)
C12—C11—P—C31	−76.5 (2)	C42—C41—P—C11	55.7 (2)
C12—C11—P—C41	45.1 (2)	C26—C21—P—C11	−116.7 (2)
C12—C11—P—C21	164.85 (19)	C22—C21—P—C11	64.6 (2)
C36—C31—P—C11	−176.6 (2)		

All H atoms were placed in geometrically idealized positions. The C—H distances were constrained to ride on their parent atoms, with distances in the range 0.95–1.00 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$.

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: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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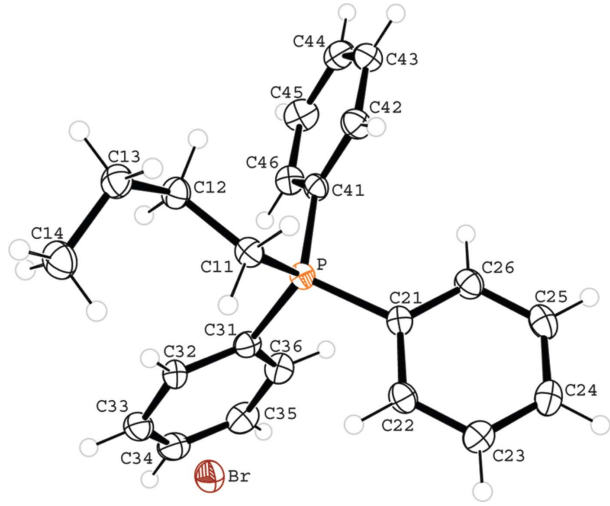

Figure 1
View of the title compound, showing the atom-labeling scheme and 50% probability displacement ellipsoids.

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