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Pentyltriphenylphosphonium bromide

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At 102 K, the two torsion angles of the pentyl group nearest to P in the title compound, $C_{23}H_{26}P^{+}\cdot Br^{-}$, correspond to the extended conformation. However, the remaining torsions are *gauche*−. The phenyl rings are in the propeller configuration usually found in this family of triphenylphosphonium compounds.

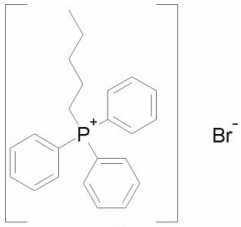
Key indicators

Single-crystal X-ray study
T = 102 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.089
Data-to-parameter ratio = 16.3

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

Comment

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



(I)

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

$C_{23}H_{26}P^{+}\cdot Br^{-}$
M_r = 413.32
Monoclinic, $P2_1/c$
a = 11.6338 (4) Å
b = 10.3522 (3) Å
c = 17.2434 (5) Å
β = 104.393 (2)°
V = 2011.54 (11) Å^3
Z = 4
D_x = 1.365 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 20273 reflections
θ = 3.9–68.2°
μ = 3.53 mm^{-1}
T = 102 (2) K
Prism, colorless
0.28 × 0.18 × 0.15 mm

Data collection

Bruker PROTEUM CCD plate diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.36, T_{max} = 0.59
19502 measured reflections
3684 independent reflections
2694 reflections with $I > 2\sigma(I)$
R_{int} = 0.098
θ_{max} = 68.4°
$h = -14 \rightarrow 13$
$k = -8 \rightarrow 12$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.089
S = 0.94
3684 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected geometric parameters (Å, °) for (I).

C11—C12	1.537 (4)	C14—C15	1.508 (4)
C11—P	1.804 (3)	C21—P	1.805 (3)
C12—C13	1.533 (4)	C31—P	1.802 (3)
C13—C14	1.532 (4)	C41—P	1.799 (3)
C12—C11—P	112.9 (2)	C46—C41—P	122.0 (2)
C13—C12—C11	112.1 (2)	C42—C41—P	118.6 (2)
C14—C13—C12	114.8 (2)	C41—P—C31	110.68 (13)
C15—C14—C13	112.7 (3)	C41—P—C11	107.97 (13)
C26—C21—P	122.0 (2)	C31—P—C11	110.93 (14)
C22—C21—P	117.6 (2)	C41—P—C21	109.18 (14)
C32—C31—P	121.3 (2)	C31—P—C21	106.95 (13)
C36—C31—P	119.0 (2)	C11—P—C21	111.14 (14)
P—C11—C12—C13	173.0 (2)	C36—C31—P—C11	−179.3 (2)
C11—C12—C13—C14	−69.6 (3)	C12—C11—P—C41	46.6 (2)
C12—C13—C14—C15	−63.8 (3)	C12—C11—P—C31	−74.9 (2)
C46—C41—P—C11	−119.5 (3)	C12—C11—P—C21	166.3 (2)
C42—C41—P—C11	58.3 (3)	C26—C21—P—C11	−120.8 (3)
C32—C31—P—C11	−2.4 (3)	C22—C21—P—C11	62.5 (3)

Systematic absences were rejected during refinement. All H atoms were placed in geometrically idealized positions, and were constrained to ride on their parent atoms, with C—H 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: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

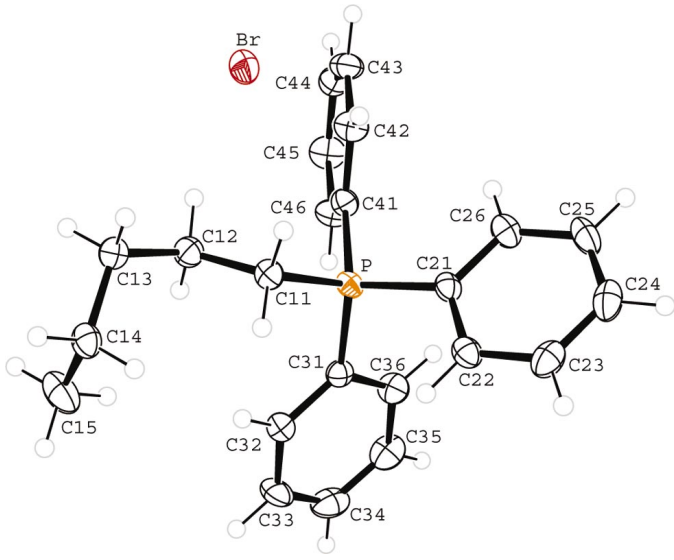


Figure 1
View of the title compound, showing the atom-labeling scheme (50% probability displacement ellipsoids).

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