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Triphenyl(propyl)phosphonium bromide

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.090
Data-to-parameter ratio = 16.0

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

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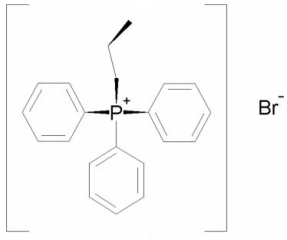
At 102 K, the propyl group of the title compound, $C_{21}H_{22}BrP$, is in the extended conformation. The phenyl rings are in the propeller configuration usually found in this family of triphenylphosphonium compounds.

Comment

This is the sixth crystal structure of a series of alkyl-substituted triphenylphosphonium bromide compounds from this laboratory (Czerwinski, 1986; Ponnuswamy & Czerwinski, 1986; Czerwinski & Ponnuswamy, 1988*a*,*b*, 1989). The atom labeling used here is consistent with earlier structures.



(I)

The propyl group is in the extended conformation. The phenyl rings are in the expected propeller configuration.

Experimental

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

Crystal data

$C_{21}H_{22}P^{+}\cdot Br^{-}$
M_r = 385.27
Monoclinic, $P2_1/c$
a = 10.7932 (2) Å
b = 9.8543 (2) Å
c = 17.8692 (3) Å
β = 103.967 (1)°
V = 1844.37 (6) Å^3
Z = 4
D_x = 1.387 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 18618 reflections
θ = 5.1–68.2°
μ = 3.81 mm^{-1}
T = 100 (2) K
Prism, colorless
0.35 × 0.35 × 0.30 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: none
17895 measured reflections
3349 independent reflections
2945 reflections with $I > 2\sigma(I)$
R_{int} = 0.098
θ_{max} = 68.3°
$h = -12 \rightarrow 10$
$k = -11 \rightarrow 8$
$l = -19 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.07
3349 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.0077P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

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

C11—P	1.793 (2)	C31—P	1.797 (2)
C21—P	1.7980 (19)	C41—P	1.8020 (19)
C12—C11—P	113.98 (13)	C11—P—C31	110.52 (10)
C26—C21—P	122.49 (14)	C11—P—C21	110.50 (9)
C22—C21—P	117.07 (15)	C31—P—C21	106.86 (9)
C32—C31—P	121.65 (16)	C11—P—C41	109.36 (9)
C36—C31—P	118.29 (16)	C31—P—C41	110.82 (9)
C42—C41—P	116.91 (15)	C21—P—C41	108.74 (9)
C46—C41—P	122.58 (15)		
P—C11—C12—C13	−150.20 (17)	C36—C31—P—C11	174.01 (15)
C12—C11—P—C31	72.36 (16)	C26—C21—P—C11	123.93 (17)
C12—C11—P—C21	−169.57 (14)	C22—C21—P—C11	−58.36 (18)
C12—C11—P—C41	−49.90 (17)	C42—C41—P—C11	−53.23 (18)
C32—C31—P—C11	−2.73 (19)	C46—C41—P—C11	128.55 (17)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.95–1.00 Å, and with U_{iso}(H) = 1.2U_{eq}(C). Systematic absences were omitted during the final refinement.

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).

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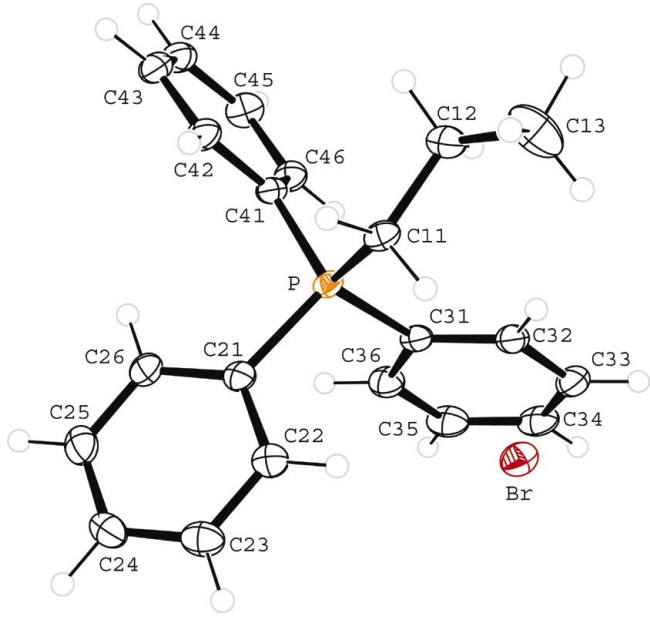

Figure 1
View of the title compound showing the atom-labelling scheme and 50% probability displacement ellipsoids.

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