Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Isobutyltriphenylphosphonium bromide

Edmund W. Czerwinski

Department of Human Biological Chemistry and Genetics, Sealy Center for Structural Biology, University of Texas Medical Branch, Galveston, Texas 77555-0647, USA

Correspondence e-mail: edcz@xray.utmb.edu

Key indicators

Single-crystal X-ray study
T = 102 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.112
Data-to-parameter ratio = 16.4

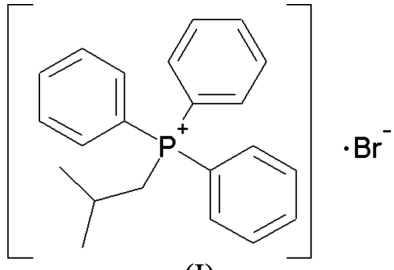
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 August 2004
Accepted 18 August 2004
Online 28 August 2004

At 102 K, the isobutyl group of the title compound, $C_{22}H_{24}P^+\cdot Br^-$, is in the extended conformation. However, the isopropyl moiety is in the eclipsed conformation with respect to the H atoms on the C atom attached to the P atom. The benzene rings are in the propeller configuration usually found in this family of triphenylphosphonium compounds.

Comment

The title compound, (I), is the seventh crystal structure in a series of alkyl-substituted triphenylphosphonium bromide compounds from this laboratory (Czerwinski, 1986, 2004; Ponnuswamy & Czerwinski, 1986; Czerwinski & Ponnuswamy, 1988*a*,*b*, 1989). The atom labelling is consistent with the previously reported structures.



(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

$C_{22}H_{24}P^+\cdot Br^-$
M_r = 399.29
Monoclinic, $P2_1/c$
a = 11.3309 (3) Å
b = 9.8033 (2) Å
c = 17.7075 (3) Å
β = 106.487 (1)°
V = 1886.08 (7) Å^3
Z = 4
D_x = 1.406 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 19 309 reflections
θ = 4.1–70.1°
μ = 3.75 mm^{-1}
T = 102 (2) K
Prism, colorless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker AXS diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.37, T_{max} = 0.685
18 578 measured reflections
3555 independent reflections
2997 reflections with $I > 2\sigma(I)$
R_{int} = 0.089
θ_{max} = 70.3°
h = −13 → 11
k = −11 → 11
l = −21 → 21

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.112$
$S = 1.13$
3555 reflections
217 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0659P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.035$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.68$ e Å^{-3}

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

C11—C12	1.541 (4)	C21—P	1.801 (3)
C11—P	1.791 (3)	C31—P	1.799 (2)
C12—C13	1.526 (3)	C41—P	1.798 (3)
C12—C14	1.539 (4)		
C12—C11—P	116.77 (18)	C46—C41—P	122.40 (19)
C13—C12—C14	110.0 (2)	C42—C41—P	117.4 (2)
C13—C12—C11	110.9 (2)	C11—P—C41	112.00 (12)
C14—C12—C11	110.2 (2)	C11—P—C31	111.26 (12)
C22—C21—P	117.8 (2)	C41—P—C31	109.71 (12)
C26—C21—P	122.20 (19)	C11—P—C21	110.30 (12)
C32—C31—P	121.77 (19)	C41—P—C21	107.68 (12)
C36—C31—P	118.6 (2)	C31—P—C21	105.65 (12)
P—C11—C12—C13	−102.2 (2)	C42—C41—P—C11	56.8 (2)
P—C11—C12—C14	135.71 (19)	C32—C31—P—C11	9.5 (3)
C12—C11—P—C41	52.7 (2)	C36—C31—P—C11	−168.3 (2)
C12—C11—P—C31	−70.5 (2)	C22—C21—P—C11	56.3 (2)
C12—C11—P—C21	172.64 (18)	C26—C21—P—C11	−128.0 (2)
C46—C41—P—C11	−126.9 (2)		

Following anisotropic refinement, all H atoms were placed in geometrically idealized positions. The C—H distances were constrained to ride on their parent atoms within the range of 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* (Farrugia, 1999).

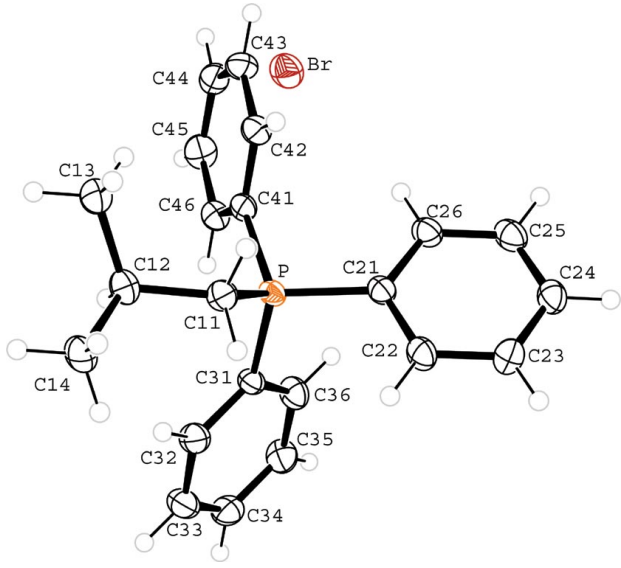


Figure 1
View of the title compound, showing the atom-labelling scheme (50% probability displacement ellipsoids). H atoms are represented by small spheres.

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (2001). *SAINT-Plus.* Data Version 1.6. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2002). *PROTEUM.* Version 1.38. Bruker AXS Inc., Madison, Wisconsin, USA.
Czerwinski, E. W. (1986). *Acta Cryst.* C**42**, 236–239.
Czerwinski, E. W. (2004). *Acta Cryst.* E**60**, o1442–o1443.
Czerwinski, E. W. & Ponnuswamy, M. N. (1988*a*). *Acta Cryst.* C**44**, 862–865.
Czerwinski, E. W. & Ponnuswamy, M. N. (1988*b*). *Acta Cryst.* C**44**, 1862–1864.
Czerwinski, E. W. & Ponnuswamy, M. N. (1989). *Acta Cryst.* C**45**, 1034–1039.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Ponnuswamy, M. N. & Czerwinski, E. W. (1986). *Acta Cryst.* C**42**, 1019–1022.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.