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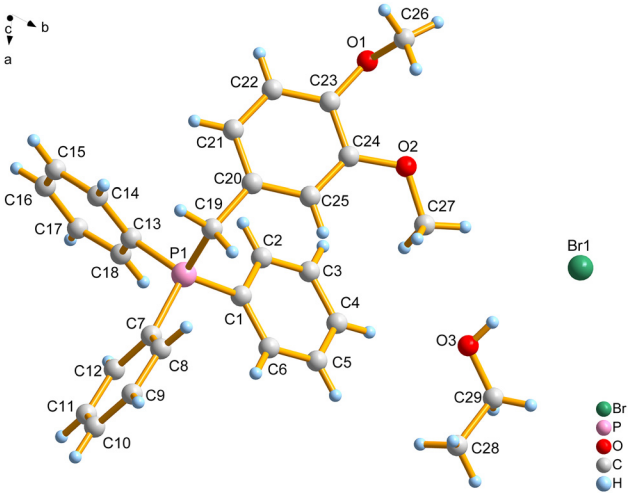
Crystal structure of (3,4-dimethoxybenzyl) triphenylphosphonium bromide ethanol solvate, $C_{29}H_{32}BrO_3P$



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Abstract

$C_{29}H_{32}BrO_3P$, triclinic, $P\bar{1}$ (no. 2), a = 9.9536(3) Å, b = 12.6359(6) Å, c = 12.8846(6) Å, α = 62.338(5)°, β = 75.402(3)°, γ = 69.765(4)°, V = 1338.54(12) Å^3, Z = 2, $R_{gt}(F)$ = 0.0459, $wR_{ref}(F^2)$ = 0.1274, T = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data. The list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

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Table 1: Data collection and handling.

Crystal:	Clear light white needle
Size:	0.03 × 0.02 × 0.01 mm
Wavelength:	Cu $K\alpha$ radiation (1.54184 Å)
μ:	2.87 mm^{-1}
Diffractometer, scan mode:	Rigaku Synergy, ω scans
θ_{max}, completeness:	66.6°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	14309, 4724, 0.064
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 4,207
$N(param)_{refined}$:	319
Programs:	Bruker,[1] SHELX,[2,3] Olex2 [4]

1 Source of materials

A solution of (3,4-dimethoxybenzyl)triphenylphosphonium bromide (0.5 mmol) in 5 mL of ethanol was prepared by ultrasonic treatment for 15 min to ensure complete dissolution. The resulting precursor was filtered and left at room temperature, yielding some crystals after five days.

2 Experimental details

Diffraction data were collected using a Rigaku diffractometer.[1] The crystal structure was solved with SHELXT and refined by using SHELXL within the Olex2.[2–4]

3 Comment

This compound contains a (3,4-dimethoxybenzyl)triphenylphosphonium (**DOMTP**) cation, bromide anion and one ethanol molecule. The **DOMTP** molecule has one positive charge, the bromide ion has one negative charge. The bond distances of DOMTP fall within the normal range reported in the literature.[5–10]

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Conflict of interest: The authors declare no conflicts of interest regarding this article.

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