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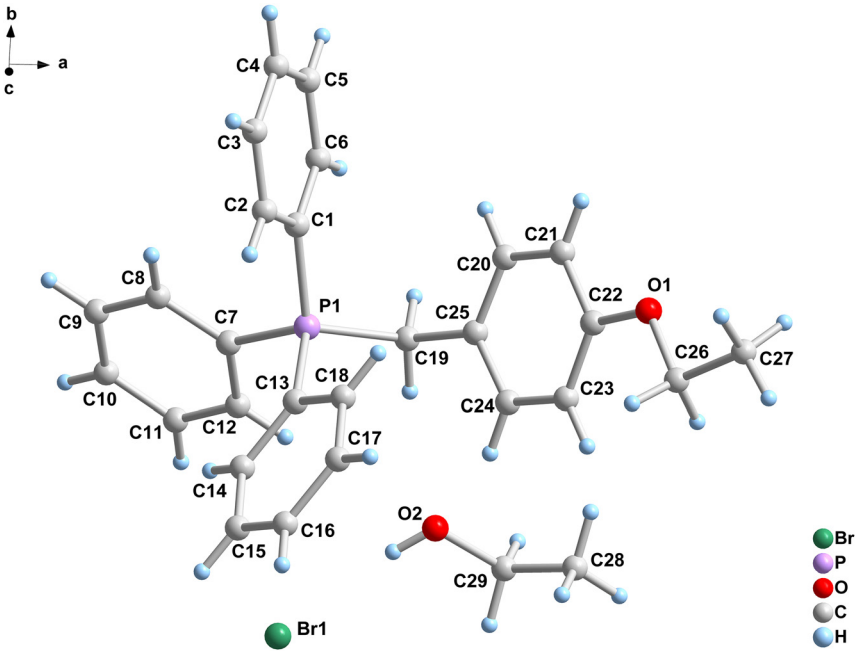
Crystal structure of (4-ethoxybenzyl) triphenylphosphonium bromide ethanol solvate, $C_{29}H_{32}BrO_2P$



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Abstract

$C_{29}H_{32}BrO_2P$, monoclinic, $P2_1/c$ (no. 14), a = 8.52420(10) Å, b = 13.5027(5) Å, c = 23.3580(4) Å, β = 95.359(1)°, V = 2676.75(11) Å^3, Z = 4, $R_{gt}(F)$ = 0.0386, w$R_{ref}(F^2)$ = 0.1039, T = 298(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 1: Data collection and handling.

Crystal:	Clear light white block
Size:	0.15 × 0.12 × 0.05 mm
Wavelength:	Cu $K\alpha$ radiation (1.54184 Å)
μ:	2.83 mm^{-1}
Diffractometer, scan mode:	XtaLAB Synergy, φ and ω scans
θ_{max}, completeness:	74.0°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	27232, 5370, 0.049
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 4,755
$N(param)_{refined}$:	302
Programs:	Rigaku,[1] Olex2,[2] SHELX[3]

1 Source of materials

The (4-ethoxybenzyl)triphenylphosphonium bromide (1 mmol) was dissolved in 10 mL of ethanol with ultrasonic treatment for 10 min to ensure complete dissolution. The solution was left at room temperature, and crystals formed over two weeks.

2 Experimental details

The data were collected using Rigaku,[1] the structure was determined by SHELXT program within Olex2 and refined

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.38673 (3)	0.33943 (2)	0.30595 (2)	0.06821 (12)
P1	0.41039 (5)	0.75498 (4)	0.36406 (2)	0.04065 (13)
O1	1.06112 (19)	0.85741 (12)	0.51771 (7)	0.0568 (4)
C1	0.3805 (2)	0.88594 (16)	0.37184 (9)	0.0452 (4)
C2	0.3158 (3)	0.92478 (18)	0.41920 (11)	0.0578 (5)
H2	0.290625	0.883476	0.448868	0.069*
C3	0.2888 (3)	1.0258 (2)	0.42195 (13)	0.0704 (7)
H3	0.245622	1.052272	0.453708	0.084*
C4	0.3252 (3)	1.08705 (19)	0.37816 (13)	0.0656 (6)
H4	0.307068	1.154786	0.380469	0.079*
C5	0.3883 (3)	1.04869 (18)	0.33114 (12)	0.0602 (6)
H5	0.412448	1.090558	0.301592	0.072*
C6	0.4162 (3)	0.94829 (17)	0.32724 (10)	0.0536 (5)
H6	0.458474	0.922435	0.295129	0.064*
C7	0.2628 (2)	0.70777 (17)	0.31111 (9)	0.0476 (4)
C8	0.1225 (3)	0.7583 (2)	0.29925 (12)	0.0653 (6)
H8	0.105419	0.818045	0.317521	0.078*
C9	0.0073 (3)	0.7190 (3)	0.25973 (15)	0.0825 (9)
H9	−0.087021	0.752774	0.251009	0.099*
C10	0.0328 (4)	0.6304 (3)	0.23366 (13)	0.0855 (10)
H10	−0.044631	0.604605	0.207113	0.103*
C11	0.1706 (4)	0.5790 (3)	0.24601 (13)	0.0800 (8)
H11	0.185429	0.518455	0.228360	0.096*
C12	0.2873 (3)	0.6175 (2)	0.28475 (10)	0.0611 (6)
H12	0.381360	0.583261	0.293102	0.073*
C13	0.3936 (2)	0.69225 (16)	0.43112 (9)	0.0451 (4)
C14	0.2981 (3)	0.60871 (18)	0.43245 (11)	0.0560 (5)
H14	0.237673	0.588142	0.399379	0.067*
C15	0.2936 (3)	0.5565 (2)	0.48321 (12)	0.0683 (7)
H15	0.229209	0.501087	0.484238	0.082*
C16	0.3834 (3)	0.5859 (2)	0.53208 (11)	0.0691 (7)
H16	0.380276	0.550036	0.565931	0.083*
C17	0.4780 (3)	0.6682 (2)	0.53115 (10)	0.0646 (7)
H17	0.538845	0.687664	0.564381	0.077*
C18	0.4834 (3)	0.72240 (19)	0.48107 (10)	0.0552 (5)
H18	0.546435	0.778562	0.480710	0.066*
C19	0.6046 (2)	0.73222 (16)	0.34067 (9)	0.0448 (4)
H19A	0.615370	0.662262	0.332462	0.054*
H19B	0.615301	0.768641	0.305448	0.054*
C20	0.7830 (3)	0.86107 (16)	0.39172 (10)	0.0504 (5)
H20	0.741219	0.908108	0.365486	0.060*
C21	0.8917 (3)	0.88977 (16)	0.43566 (10)	0.0530 (5)
H21	0.922483	0.955773	0.438934	0.064*
C22	0.9562 (2)	0.82069 (16)	0.47530 (10)	0.0467 (4)
C23	0.9125 (3)	0.72215 (16)	0.46899 (11)	0.0533 (5)
H23	0.956886	0.674764	0.494478	0.064*
C24	0.8021 (3)	0.69465 (16)	0.42442 (11)	0.0520 (5)
H24	0.773217	0.628414	0.420483	0.062*
C25	0.7339 (2)	0.76310 (15)	0.38566 (9)	0.0430 (4)
C26	1.1206 (3)	0.7922 (2)	0.56268 (11)	0.0628 (6)
H26A	1.164677	0.733310	0.546633	0.075*
H26B	1.036467	0.772266	0.585457	0.075*
C27	1.2456 (4)	0.8470 (2)	0.59942 (14)	0.0789 (8)
H27A	1.321262	0.873633	0.575613	0.118*
H27B	1.297360	0.802414	0.627086	0.118*
H27C	1.198184	0.900034	0.619080	0.118*
O2	0.6779 (2)	0.49137 (14)	0.33182 (9)	0.0734 (5)
H2A	0.599244	0.457031	0.324527	0.110*
C28	0.9493 (4)	0.4590 (3)	0.35911 (18)	0.1018 (11)
H28A	1.037721	0.420563	0.349344	0.153*
H28B	0.925960	0.442720	0.397413	0.153*
H28C	0.974118	0.528193	0.357139	0.153*
C29	0.8142 (4)	0.4372 (3)	0.31919 (17)	0.0937 (10)
H29A	0.838676	0.453283	0.280534	0.112*
H29B	0.791696	0.366901	0.320440	0.112*

by SHELXL.[2–4] The structural picture was finished using Diamond.[5]

3 Comment

In this study, the compound consists of the (4-ethoxybenzyl) triphenylphosphonium (**4EOTP**) organic cation, one bromide anion, and one ethanol molecule. The **4EOTP** molecule carries a positive charge, with the bromide ion acting as the counter anion. The bond distances of the four benzene rings of the **4EOTP** cation fall within the typical range reported in the literature.[6–8]

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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References

1. Rigaku Corporation, CrysAlis^{PRO}; Rigaku Corporation: Yarnton, Oxfordshire, England, 2015.
2. Sheldrick, G. M. SHELXT – Integrated Space-Group and Crystal-structure Determination. *Acta Crystallogr.* **2015**, *A71*, 3–8.
3. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Crystallogr.* **2009**, *42*, 339–341.

4. Sheldrick, G. M. Crystal Structure Refinement with SHELXL. *Acta Crystallogr.* **2015**, *C71*, 3–8.
5. Brandenburg, K. DIAMOND. *Visual Crystal Structure Information System. Ver. 3.2*; Crystal Impact: Bonn, Germany, 2012.
6. Jiang, J. K.; Jiang, H. Crystal Structure of (4-bromobenzyl) triphenylphosphonium Bromide Ethanol Solvate, $C_{52}H_{48}Br_4OP_2$. *Z. Kristallogr. N. Cryst. Struct.* **2024**, *239*, 495–496.
7. Lin, N.; Wang, R. C.; Zhang, S. Y.; Lin, Z. H.; Chen, X. Y.; Li, Z. N.; Lei, X. W.; Wang, Y. Y.; Yue, C. Y. 0D Hybrid Cuprous Halide as an Efficient Light Emitter and X-Ray Scintillator. *Laser Photonics Rev.* **2023**, *17*, 2300427.
8. Smit, J. B. M.; Marais, C.; Malan, F. P.; Bezuidenhout, B. C. B. Crystal Structure of (2,4-dimethoxybenzyl) triphenylphosphonium trifluoroacetate —trifluoroacetic acid (1/1), $C_{31}H_{27}F_6O_6P$. *Z. Kristallogr. New Cryst. Struct.* **2019**, *234*, 621–623.