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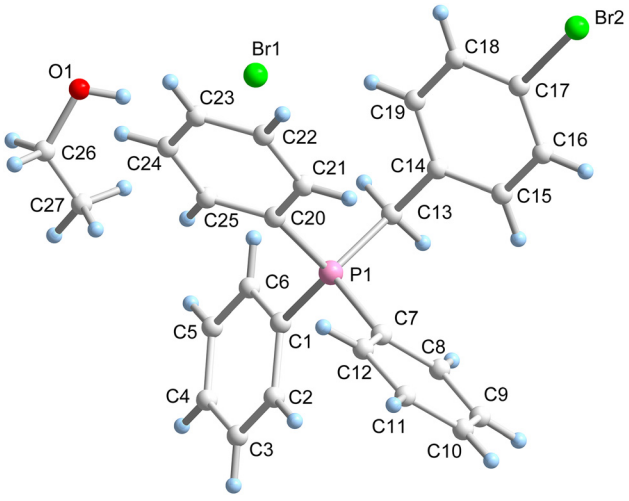
Crystal structure of (4-bromobenzyl) triphenylphosphonium bromide ethanol solvate, $C_{52}H_{48}Br_4OP_2$



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Abstract

$C_{52}H_{48}Br_4OP_2$, orthorhombic, *Pccn* (no. 56), a = 20.173(5) Å, b = 12.224(3) Å, c = 18.858(5) Å, V = 4650.2(19) Å^3, Z = 4, $R_{gt}(F)$ = 0.0395, $wR_{ref}(F^2)$ = 0.0906, T = 289(2) K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.10 × 0.08 × 0.05 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	3.57 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	25.0°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	25,098, 4105, 0.081
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2915
$N(param)_{refined}$:	282
Programs:	Bruker [1], SHELX [2, 4], Olex2 [3], Diamond [5]

1 Source of materials

The (4-bromobenzyl)triphenylphosphonium bromide (0.512 g, 1 mmol) was added in 15 mL CH_3CH_2OH/CH_2Cl_2 (v/v, 2/1). After ultrasonic treating for several minutes, the raw materials could dissolve fully to form clear solution, the precursor solution was filtered by using PTFE and was maintained at room temperature to obtain some crystals after several days.

2 Experimental details

The data were collected using Bruker [1], the structure of crystal was solved by SHELXT [2] program within Olex2 [3] and refined by SHELXL [4]. The graphics were finished using Diamond [5].

3 Comment

With the development of chemistry of materials, more and more organophosphates were studied for wide applications, such as continuous-wave Raman laser [6], scintillator [7], WLED [8] and so on. The asymmetric unit of title compound contains a (4-bromobenzyl)triphenylphosphonium (**4BTP**) molecule, one bromide ion and one ethanol molecule. The organic molecule **4BTP** has a positive charge, the free bromide ions act as counter anions. The bond distances of the four benzene-rings coming from **4BTP** are in normal range of literatures [9, 10]. There is a weak interaction between hydrogen atom of the hydroxy group and free bromide ion.

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.60875 (2)	0.02703 (4)	0.63414 (2)	0.04739 (14)
Br2	0.22297 (2)	0.05967 (5)	0.73003 (2)	0.07133 (19)
P1	0.47759 (5)	0.26520 (8)	0.50936 (5)	0.0332 (2)
C1	0.54599 (19)	0.2710 (3)	0.44869 (17)	0.0363 (9)
C2	0.5442 (2)	0.3407 (3)	0.39029 (19)	0.0447 (10)
H2	0.507946	0.386423	0.383462	0.054*
C3	0.5961 (2)	0.3421 (4)	0.3425 (2)	0.0562 (12)
H3	0.594715	0.388221	0.303242	0.067*
C4	0.6496 (2)	0.2751 (4)	0.3533 (2)	0.0645 (13)
H4	0.684564	0.276355	0.321209	0.077*
C5	0.6525 (2)	0.2064 (4)	0.4105 (2)	0.0625 (13)
H5	0.689384	0.161868	0.417219	0.075*
C6	0.6006 (2)	0.2033 (3)	0.4584 (2)	0.0494 (11)
H6	0.602253	0.155972	0.496956	0.059*
C7	0.40844 (18)	0.3357 (3)	0.47074 (18)	0.0371 (9)
C8	0.3762 (2)	0.2874 (3)	0.4139 (2)	0.0486 (11)
H8	0.390622	0.220295	0.396421	0.058*
C9	0.3226 (2)	0.3392 (4)	0.3833 (2)	0.0616 (13)
H9	0.301314	0.307299	0.344802	0.074*
C10	0.3005 (2)	0.4376 (4)	0.4093 (3)	0.0653 (14)
H10	0.263655	0.471082	0.389222	0.078*
C11	0.3327 (2)	0.4862 (4)	0.4647 (2)	0.0593 (13)
H11	0.317830	0.553111	0.481947	0.071*
C12	0.3874 (2)	0.4362 (3)	0.4955 (2)	0.0464 (10)
H12	0.409714	0.470169	0.532566	0.056*
C13	0.45652 (18)	0.1232 (3)	0.52261 (18)	0.0360 (9)
H13A	0.445479	0.090810	0.477150	0.043*
H13B	0.494991	0.084996	0.541053	0.043*
C14	0.39935 (19)	0.1067 (3)	0.57266 (18)	0.0353 (9)
C15	0.3346 (2)	0.1085 (3)	0.5492 (2)	0.0489 (11)
H15	0.326140	0.117551	0.501118	0.059*
C16	0.2821 (2)	0.0974 (4)	0.5954 (2)	0.0572 (12)
H16	0.238672	0.100936	0.578963	0.069*
C17	0.2951 (2)	0.0809 (4)	0.6663 (2)	0.0480 (10)
C18	0.3587 (2)	0.0774 (3)	0.6916 (2)	0.0471 (10)
H18	0.366701	0.066306	0.739652	0.056*
C19	0.4109 (2)	0.0905 (3)	0.64466 (19)	0.0442 (10)
H19	0.454261	0.088576	0.661468	0.053*
C20	0.49723 (18)	0.3215 (3)	0.59479 (18)	0.0347 (9)
C21	0.4465 (2)	0.3423 (3)	0.64311 (18)	0.0433 (10)
H21	0.402387	0.336335	0.629123	0.052*
C22	0.4620 (2)	0.3717 (3)	0.7119 (2)	0.0504 (11)
H22	0.428248	0.385871	0.744278	0.061*
C23	0.5268 (3)	0.3801 (4)	0.7325 (2)	0.0597 (13)
H23	0.536822	0.399315	0.778992	0.072*
C24	0.5769 (2)	0.3606 (4)	0.6855 (2)	0.0643 (13)
H24	0.620799	0.367146	0.700012	0.077*
C25	0.5626 (2)	0.3310 (3)	0.61603 (19)	0.0479 (10)
H25	0.596747	0.317774	0.584022	0.058*
O1[a]	0.7276 (5)	0.2056 (8)	0.6800 (5)	0.118 (3)
H1[a]	0.692658	0.181434	0.664279	0.177*
C26[a]	0.7601 (8)	0.2610 (17)	0.6280 (5)	0.059 (3)
H26A[a]	0.762937	0.337167	0.642184	0.071*
H26B[a]	0.805074	0.233083	0.625714	0.071*
C27[a]	0.7364 (6)	0.258 (2)	0.5671 (4)	0.063 (4)
H27A[a]	0.771085	0.269770	0.533031	0.094*
H27B[a]	0.703385	0.313853	0.562177	0.094*
H27C[a]	0.716617	0.187569	0.559045	0.094*

[a]Occupancy: 0.5.

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