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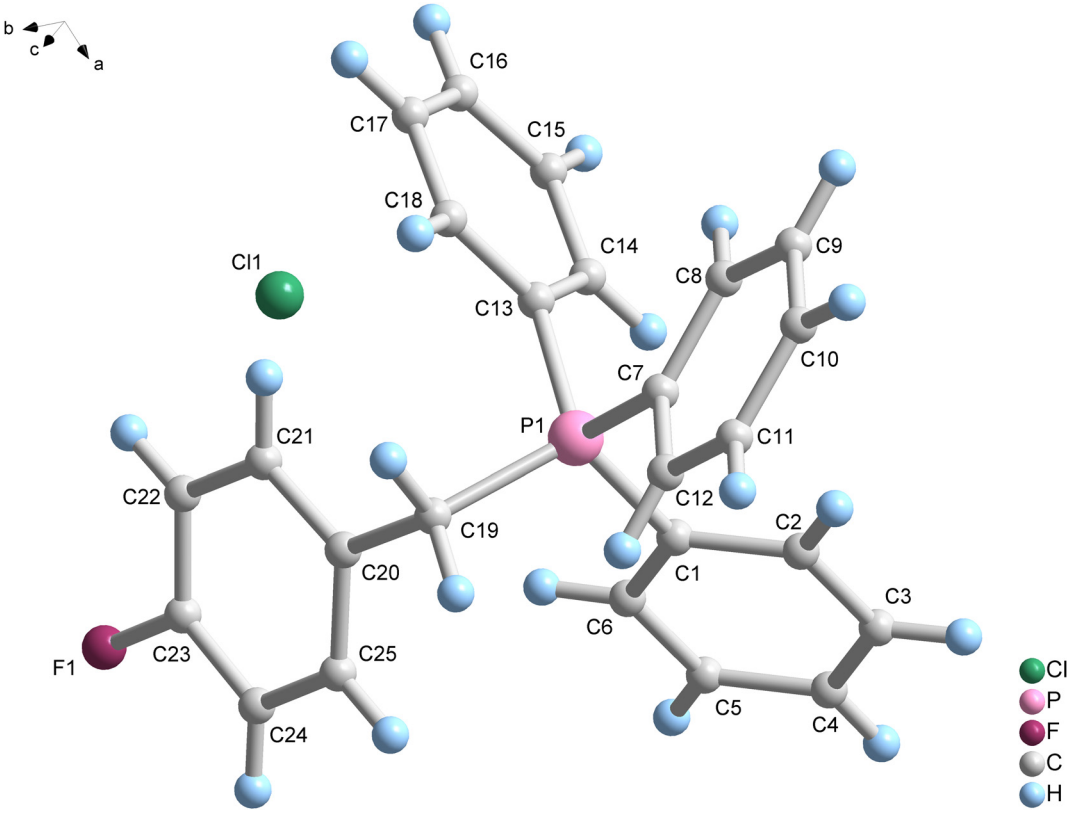
Crystal structure of (4-fluorobenzyl) triphenylphosphonium chloride, $C_{25}H_{21}ClFP$



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Abstract

$C_{25}H_{21}ClFP$, monoclinic, $P2_1/n$ (no. 14), a = 9.5700(2) Å, b = 13.9963(2) Å, c = 15.8793(4) Å, β = 101.024(2)°, V = 2087.70(8) Å^3, Z = 4, $R_{gt}(F)$ = 0.0401, $wR_{ref}(F^2)$ = 0.1112, T = 150 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.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size	0.10 × 0.08 × 0.05 mm
Wavelength:	Cu Kα radiation (1.54184 Å)
μ:	2.47 mm^{-1}
Diffractometer, scan mode:	XtaLAB Synergy, ω
θ_{max}, completeness:	74.0°, > 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	21953, 4162, 0.059
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3,625
$N(param)_{refined}$:	254
Programs:	CrysAlis^{PRO},[1] SHELX,[2, 4] Olex2,[3] Diamond[5]

1 Source of materials

The (4-fluorobenzyl)triphenylphosphonium chloride (1 mmol) powder was dissolved in 20 mL CH_3CH_2OH/CH_2Cl_2 (v/v, 3/1) and

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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}
Cl1	0.21195 (5)	0.55056 (3)	0.40263 (3)	0.05661 (16)
P1	0.38891 (4)	0.28069 (3)	0.51413 (2)	0.03576 (14)
F1	0.2445 (2)	0.45622 (11)	0.87330 (10)	0.0932 (5)
C1	0.49317 (18)	0.19181 (12)	0.57991 (11)	0.0439 (4)
C2	0.5756 (2)	0.12802 (15)	0.54332 (14)	0.0579 (5)
H2	0.577025	0.131371	0.483743	0.069*
C3	0.6557 (3)	0.05942 (18)	0.5942 (2)	0.0780 (7)
H3	0.711756	0.015629	0.569151	0.094*
C4	0.6546 (3)	0.05442 (17)	0.68017 (19)	0.0783 (8)
H4	0.711401	0.008138	0.714735	0.094*
C5	0.5712 (3)	0.11637 (17)	0.71682 (15)	0.0749 (7)
H5	0.569693	0.112114	0.776349	0.090*
C6	0.4896 (3)	0.18473 (15)	0.66679 (13)	0.0614 (5)
H6	0.431216	0.226791	0.691870	0.074*
C7	0.43612 (18)	0.28030 (11)	0.41021 (10)	0.0383 (3)
C8	0.3565 (2)	0.22778 (15)	0.34412 (13)	0.0556 (5)
H8	0.274511	0.194046	0.353119	0.067*
C9	0.3966 (3)	0.22448 (17)	0.26486 (13)	0.0658 (6)
H9	0.342363	0.188339	0.219436	0.079*
C10	0.5147 (3)	0.27347 (16)	0.25220 (13)	0.0627 (5)
H10	0.542459	0.270542	0.197934	0.075*
C11	0.5938 (2)	0.32701 (16)	0.31719 (13)	0.0603 (5)
H11	0.674371	0.361669	0.307154	0.072*
C12	0.5560 (2)	0.33035 (13)	0.39704 (12)	0.0487 (4)
H12	0.611123	0.366289	0.442287	0.058*
C13	0.20389 (17)	0.25121 (12)	0.50260 (10)	0.0408 (4)
C14	0.1588 (2)	0.16700 (14)	0.53512 (12)	0.0505 (4)
H14	0.226078	0.121356	0.562254	0.061*
C15	0.0141 (3)	0.15054 (17)	0.52741 (15)	0.0670 (6)
H15	−0.018153	0.092762	0.548640	0.080*
C16	−0.0827 (2)	0.21701 (19)	0.48938 (18)	0.0725 (6)
H16	−0.181568	0.205826	0.486031	0.087*
C17	−0.0385 (2)	0.29947 (17)	0.45612 (16)	0.0656 (6)
H17	−0.106663	0.344623	0.429064	0.079*
C18	0.1051 (2)	0.31715 (14)	0.46181 (13)	0.0512 (4)
H18	0.135965	0.373871	0.438053	0.061*
C19	0.41812 (18)	0.39995 (11)	0.55822 (10)	0.0399 (3)
H19A	0.521107	0.414409	0.566525	0.048*
H19B	0.367759	0.445944	0.515596	0.048*
C20	0.37000 (18)	0.41610 (11)	0.64221 (11)	0.0405 (4)
C21	0.2280 (2)	0.43245 (13)	0.64512 (13)	0.0507 (4)
H21	0.159459	0.434567	0.593260	0.061*
C22	0.1847 (2)	0.44580 (15)	0.72317 (15)	0.0613 (5)
H22	0.087395	0.456128	0.725404	0.074*
C23	0.2859 (3)	0.44363 (14)	0.79620 (14)	0.0629 (6)
C24	0.4271 (3)	0.43041 (16)	0.79644 (13)	0.0659 (6)
H24	0.494821	0.430732	0.848679	0.079*
C25	0.4696 (2)	0.41645 (14)	0.71837 (12)	0.0526 (4)
H25	0.567527	0.407081	0.717098	0.063*

10 µL 0.01 mol/L HCl. After several minutes, the colorless solution was obtained, and kept at room temperature to get some block crystals after two weeks.

2 Experimental details

The data were collected using Rigaku,[1] the structure was determined by SHELXT program within Olex2 and refined by SHELXL.[2–4] The graphics was made using Diamond.[5]

3 Comment

In this investigation, the title compound contains one (4-fluorobenzyl)triphenylphosphonium (**4FTP**) cation with one positive charge and one chloride ion as a counter anion. The bond distances of the four benzene-rings coming from **4FTP** are in normal range.[6–9]

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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