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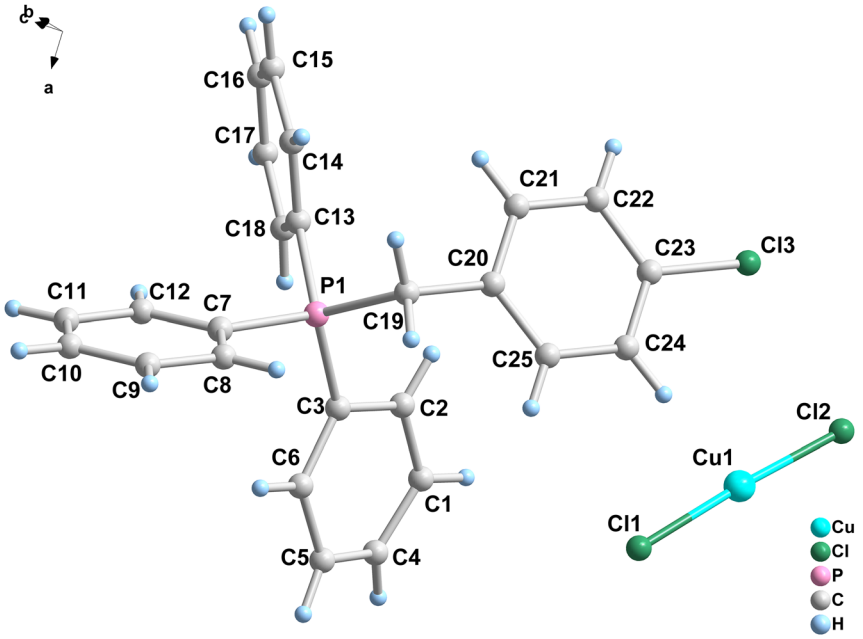
Crystal structure of [(4-chlorobenzyl) triphenylphosphonium] dichloridocopper(I), $\{[C_{25}H_{21}ClP]^{+}[CuCl_2]^{-}\}_n$



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Abstract

$C_{25}H_{21}Cl_3CuP$, monoclinic, *Cc* (no. 9), a = 8.69340(10) Å, b = 17.5173(3) Å, c = 16.2068(3) Å, β = 99.765(2)°, V = 2432.29(7) Å^3, Z = 4, $R_{gt}(F)$ = 0.0391, $wR_{ref}(F^2)$ = 0.1044, 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 colourless block
Size:	0.10 × 0.08 × 0.06 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	4.99 mm^{-1}
Diffractometer, scan mode:	Rigaku Synergy, ω scan
θ_{max}, completeness:	73.7°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	10986, 3790, 0.043
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3,614
$N(param)_{refined}$:	299
Programs:	Rigaku,[1] SHELX,[2,4] Olex2[3]

1 Source of materials

The 0.5 mmol of (4-chlorobenzyl)triphenylphosphonium chloride and CuCl (0.5 mmol) were added in 0.5 mL HCl and 5 mL CH_3CH_2OH. Then, the 100 μL H_3PO_2 was added to prevent Cu^+ from oxidation. The mixture was maintained at room temperature for 15 days, the well-shaped crystals were obtained.

2 Experimental details

The diffraction data were collected on a Rigaku.[1] The structure was determined using SHELXT program within the Olex2 and refined with SHELXL.[2–4] The structural picture was finished using Diamond.[5]

3 Comment

In this research, a zero-dimensional copper(I)-based metal halide was reported. As is shown in the figure, the asymmetric unit contains a (4-chlorobenzyl)triphenylphosphonium cation, $[CuCl_2]^-$ anion. And the distances of Cu1–Cl1, Cu1–Cl2 are 2.093 Å, 2.091 Å within the normal range of the literature which have been reported.[6,7]

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

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