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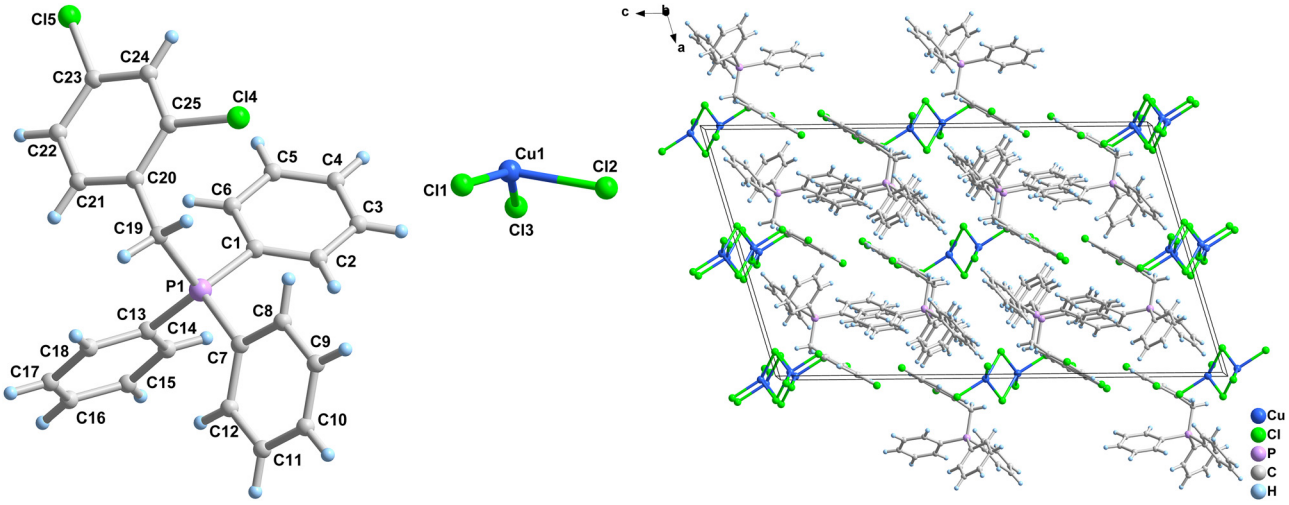
Crystal structure of [(2,4-dichlorobenzyl) triphenylphosphonium] trichloridocopper(II), $[C_{25}H_{20}Cl_2P]^+[CuCl_3]^-$



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Abstract

$C_{25}H_{20}Cl_5CuP$, monoclinic, $I2/a$ (no. 15), a = 16.8258(3) Å, b = 11.0938(2) Å, c = 28.8065(4) Å, β = 106.359(2)°, V = 5159.39(16) Å^3, Z = 8, $R_{gt}(F)$ = 0.0418, $wR_{ref}(F^2)$ = 0.1161, T = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data.

Table 1: Data collection and handling.

Crystal:	Clear orangish orange needle
Size:	0.12 × 0.08 × 0.07 mm
Wavelength:	Cu *Kα* radiation (1.54184 Å)
μ:	6.64 mm^{-1}
Diffractometer, scan mode:	Rigaku Synergy, ω scans
θ_{max}, completeness:	66.6°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	24294, 4557, 0.081
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4,070
$N(param)_{refined}$:	290
Programs:	Rigaku,[1] Olex2,[2] SHELX[3,4]

1 Source of materials

The (2,4-dichlorobenzyl)triphenylphosphonium chloride (1 mmol) and $CuCl_2$ (0.5 mmol) were added in 10 mL of CH_3OH and 0.3 mL HCl, forming a clear and homogeneous solution. After several days, the single crystals were obtained.

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2 Experimental details

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

3 Comment

This study reports a copper(II)-based metal halide, comprising a (2,4-dichlorobenzyl)triphenylphosphonium cation, and a [$CuCl_3$]$^-$ anion. The distances of Cu1–Cl1, Cu1–Cl2 and Cu1–Cl3 are 2.186 Å, 2.196 Å, 2.304 Å within the normal range.[5,6] Also all derived geometric parameters in the cation are in the expected ranges.[7,8] The packing structure is zero-dimensional (*cf.* right part of the picture).

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