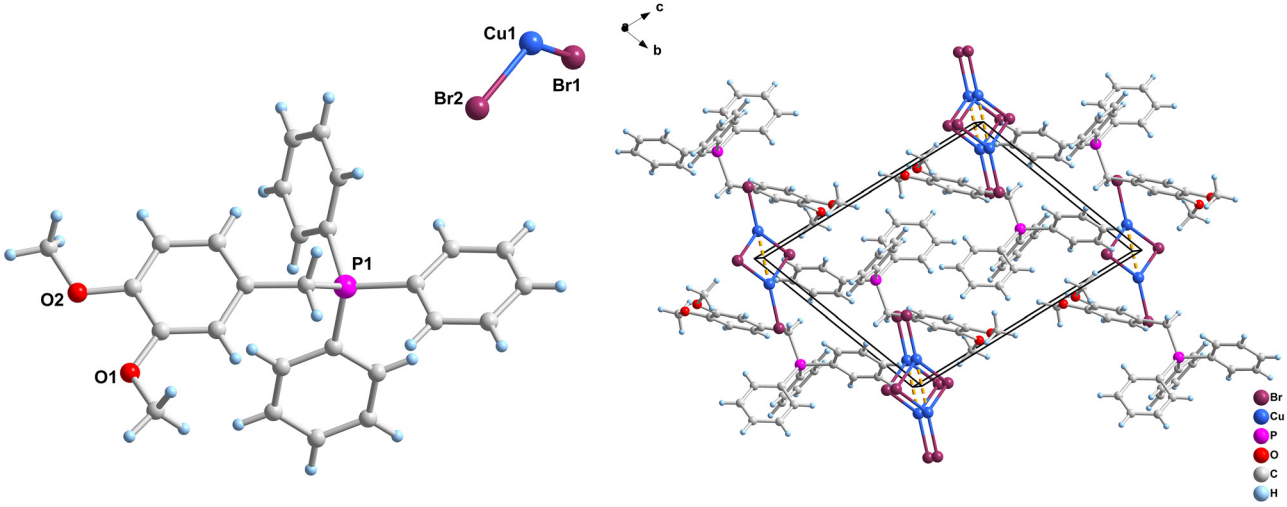
Jiayan Wang, Qianyou Su, Yuan Gao, Liguo Li and Xiuhua Li*

Crystal structure of bis[(3,4-dimethoxybenzyl) triphenylphosphonium]di-μ2-bromido-dibromidodicopper(I)



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Abstract

$C_{54}H_{52}Br_4Cu_2O_4P_2$, triclinic, $P\bar{1}$ (no. 2), a = 9.9855(4) Å, b = 10.5557(4) Å, c = 13.3955(5) Å, α = 69.662(3)°, β = 78.316(3)°, γ = 79.167(3)°, V = 1285.81 Å^3, Z = 1, R_{gt} (F) = 0.0446, wR_{ref} (F^2) = 0.1110, T = 305.00(10) K.

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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.

Table 1: Data collection and handling.

Crystal:	Block, clear light colourless
Size:	0.12 × 0.1 × 0.1 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	4.04 mm^{-1}
Diffractometer, scan mode:	XtaLAB Synergy R, ω-scans
θ_{max}, completeness:	25°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	13810, 4543, 0.032
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3,632
$N(param)_{refined}$:	300
Programs:	CrysAlis^{PRO},[1] SHELX,[2,3] OLEX2[4]

1 Source of materials

The (3,4-dimethoxybenzyl)triphenylphosphonium bromide (0.5 mmol) and CuBr (0.5 mmol) were placed into a clean glass vial. Subsequently, 2 mL of ethanol, 100 μL of hydrobromic acid, and 200 μL of hypophosphorous acid were added, and the mixture was stirred for 15 min. The CH_2Cl_2 (2 mL) was then introduced to form a clear solution. The resulting solution was filtered and left at room temperature to allow for slow evaporation. After five days, colorless transparent single crystals were obtained.

2 Experimental details

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

***Corresponding author: Xiuhua Li**, School of Biological and Pharmaceutical Engineering, Jilin Agricultural Science and Technology College, 132101 Jilin, Jilin, China, E-mail: lixiuhua@jlnku.edu.cn. https://orcid.org/0009-0008-3862-0711
Jiayan Wang, Qianyou Su, Yuan Gao and Liguo Li, School of Biological and Pharmaceutical Engineering, Jilin Agricultural Science and Technology College, 132101 Jilin, Jilin, China

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The H atoms were placed in geometrically idealized positions.

3 Comment

Among zero-dimensional metal halides, copper(I)-based halides have emerged as promising competitors for optoelectronic functional materials, owing to their abundant coordination configurations, high photoluminescence quantum yields (P_{LQYS}), and exceptional structural designability, etc.[5,6] In this work, one zero-dimensional copper(I)-based halide was synthesized. As shown in left part of the picture, its asymmetric unit contains one (3,4-dimethoxybenzyl)triphenylphosphonium (**DOMBTP**) cation and one half of a $Cu_2Br_4^{2-}$ anion. The bonds lengths of Cu1–Br1, Cu1–Br2 are 2.305, 2.412 Å, falling within the normal range reported in the literature.[7,8] As shown in right part of the picture, its packing structure is zero-dimensional, containing $[Cu_2Br_4]^{2-}$ clusters and **DOMBTP** organic ligands.

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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