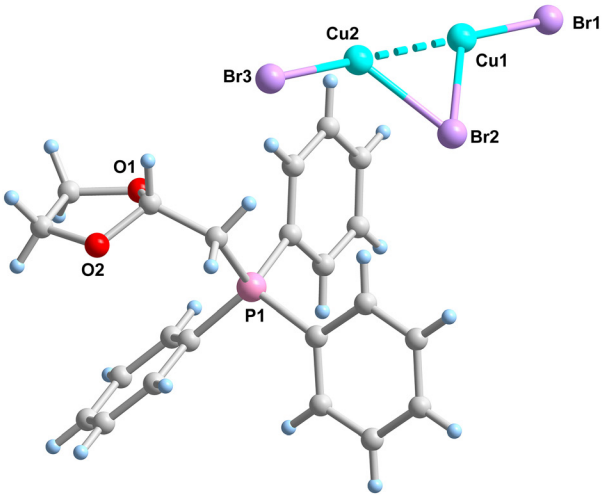
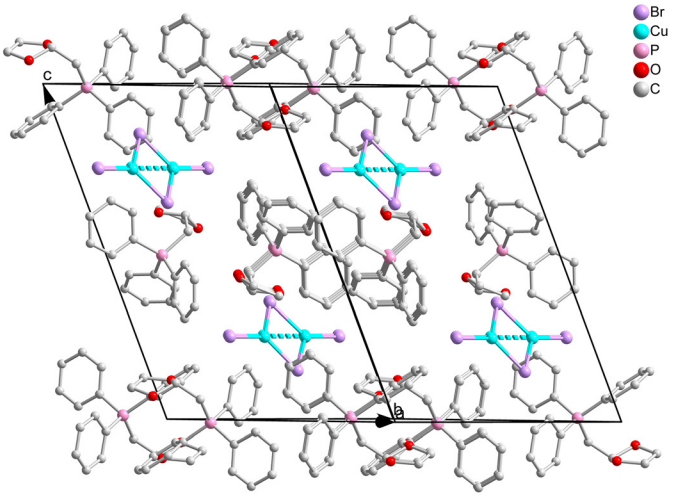
Xinyang Li, Xinyu Zhao, Meiying Wang and Xiuhua Li*

Crystal structure of bis [(1,3-dioxolan-2-ylmethyl) triphenylphosphonium] tetrabromidodicopper(I), $C_{22}H_{22}Br_2CuO_2P$





https://doi.org/10.1515/ncrs-2025-0347
Received August 7, 2025; accepted October 5, 2025;
published online October 23, 2025

Abstract

$C_{22}H_{22}Br_2CuO_2P$, monoclinic, $C2/c$ (no. 15), a = 17.5804(15) Å, b = 15.1053(7) Å, c = 19.4144(16) Å, β = 119.893(11)°, V = 4469.7(7) Å^3, Z = 8, $R_{gt}(F)$ = 0.0367, w$R_{ref}(F^2)$ = 0.0765, T = 305(1) K.

CCDC no.: 2478485

Table 1 contains the crystallographic data and 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:	Clear light colourless block
Size:	0.08 × 0.07 × 0.07 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	4.64 mm^{-1}
Diffractometer, scan mode:	XtaLAB Synergy, ω scans
θ_{max}, completeness:	25.0°, 100 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	19236, 3936, 0.052
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2869
$N(param)_{refined}$:	255
Programs:	Rigaku,[1] Olex2,[2] SHELX[3,4]

1 Source of materials

A mixture of (1,3-dioxolan-2-ylmethyl)triphenylphosphonium bromide (0.5 mmol) and CuBr (0.5 mmol) were dissolved in 5 mL of dichloromethane/ethanol solution (v/v, 3:2) under continuous stirring. Subsequently, 100 µL of hypophosphorous acid and 50 µL of hydrobromic acid were added dropwise to the solution. The resulting precursor solution was filtered and kept at room temperature. After four days, a number of single crystals were obtained.

2 Experimental details

The X-ray diffraction data were collected using a Rigaku diffractometer.[1] Using Olex2 software, the structure was solved with SHELXT program and refined with SHELXL package.[2–4] The hydrogen atom positions were fixed geometrically at the calculated distances.

***Corresponding author: Xiuhua Li**, School of Biological and Pharmaceutical Engineering, Jilin Agricultural Science and Technology College, 132101 Jilin, China, E-mail: lixiuhua@jlnku.edu.cn. https://orcid.org/0009-0008-3862-0711
Xinyang Li, Xinyu Zhao and Meiying Wang, School of Biological and Pharmaceutical Engineering, Jilin Agricultural Science and Technology College, 132101 Jilin, China

Open Access. © 2025 the author(s), published by De Gruyter. This work is licensed under the Creative Commons Attribution 4.0 International License.

3 Comment

Low-dimensional metal halide materials have attracted significant attention as emerging candidates for X-ray scintillators, owing to their high photoluminescence quantum yields (PLQYs) and large Stokes shifts.[5,6] Among them, copper(I)-based metal halides have been widely investigated due to their low toxicity. In this work, one copper(I)-based metal halide has been synthesized. The title compound crystallizes in monoclinic space group *C*2/*c*. As shown in picture, its structure consists of (1,3-dioxolan-2-ylmethyl)triphenylphosphonium cation, one half of a $[Cu_2Br_4]^{2-}$ anion. The bond lengths of Cu1–Br1, Cu1–Br2, Cu2–Br2, Cu2–Br3 are 2.270, 2.457, 2.388, 2.314 Å respectively. Furthermore, the $[Cu_2Br_4]^{2-}$ cluster processes Cu···Cu metal-metal interaction, of which its distance is 2.717 Å. Two copper(I) centers (Cu1, Cu2) were connected by two μ–Br bridges. In addition, its packing structure is zero-dimensional (*cf.* right part of the picture).[7–10]

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.
Research funding: This work was funded by scientific research project of Jilin Agricultural Science and Technology College, No. [2012303].

References

1. Rigaku Corporation. CrysAlis^{PRO}; Rigaku Corporation: Yarnton, Oxfordshire, England, 2015.
2. Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. Olex2: A Complete Structure Solution, Refinement and Analysis Program. *J. Appl. Crystallogr.* **2009**, *42*, 339–341.
3. Sheldrick, G. M. Shelxt – Integrated Space-Group and Crystal-Structure Determination. *Acta Crystallogr.* **2015**, *A71*, 3–8.
4. Sheldrick, G. M. Crystal Structure Refinement with Shelxl. *Acta Crystallogr.* **2015**, *C71*, 3–8.
5. Wang, Q.-Q.; Li, H.-B.; Tong, H.; Zhu, J.-L.; Fan, J.-L.; Pan, S.-F.; Zhou, Z.-N.; Liu, W.; Ouyang, G.-F. Copper Mixed-Halide Hybrids with Intrinsic Broadband White-Light Emission for Wled Application with Ultrahigh Color Rendering Index. *Small* **2025**, *21*, 2500660.
6. Lin, N.; Li, Y.-X.; Liu, Y.; Sun, K.-Q.; Zhang, H.-Y.; Lei, X.-W.; Chen, Z.-W. Broadband Blue Light Emissions of One-Dimensional Hybrid CuI) Halides with Ultrahigh Anti-Water Stability. *Dalton Trans.* **2024**, *53*, 16577–16584.
7. Niu, C.-Y.; Jiang, H. Crystal Structure of (1,3-Dioxolan-2-ylmethyl) triphenylphosphonium bromide, $C_{22}H_{22}BrO_2P$. *Z. Kristallogr. – N. Cryst. Struct.* **2025**, *240*, 687–688.
8. Willett, R. D.; Twamley, B. Novel Double Layer Salts of Copper(I) Bromide with *N*-Substituted Ethylenediammonium Cations. *Inorg. Chem.* **2004**, *43*, 954–957.
9. Niu, C.-Y.; Jiang, H. Crystal Structure of {[(4-Fluorophenyl)methyl] triphenylphosphonium}dibromocopper(I), $[C_{25}H_{21}FP]^+[CuBr_2]^-$. *Z. Kristallogr. – N. Cryst. Struct.* **2025**, *240*, 167–169.
10. Meng, H.; Zhu, W.; Zhou, Z.; Zhou, R.; Yan, D.; Zhao, Q.; Liu, S. High-Efficiency Luminescent Organic–Inorganic Hybrid Manganese(II) Halides Applied to X-ray Imaging. *J. Mater. Chem. C* **2022**, *10*, 12286.