

Communication

6-Amino-3-(prop-2-en-1-yl)-9H-purin-3-ium Tetracopper(I) Hexabromide: Synthesis and X-ray Structure Determination

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Abstract: 6-Amino-3-(prop-2-en-1-yl)-9H-purin-3-ium tetracopper(I) hexabromide [(C₅H₅N₅(C₃H₅)₂Cu₄Br₆) (1) is synthesized in this paper. The title compound is characterized by Raman spectroscopy and single crystal X-ray diffraction: monoclinic, Sp.gr. *P*2₁/*c*, *Z* = 2, unit cell dimensions: *a* = 8.6870(3), *b* = 9.7447(2), *c* = 16.4418(4) Å, β = 100.681(3)°, *V* = 1367.72(7) Å³ at 150 K. The peculiarities of the metal coordination and distribution of weak interactions are analyzed. The significant role of hydrogen bonds in the construction of 1 crystal structure is shown.

Keywords: adenine; allyl derivative; crystal structure; intermolecular interaction



Citation: Pavlyuk, O.V.; Slyvka, Y.I.; Goreschnik, E.A.; Mys'kiv, M.G. 6-Amino-3-(prop-2-en-1-yl)-9H-purin-3-ium Tetracopper(I) Hexabromide: Synthesis and X-ray Structure Determination. *Molbank* **2022**, *2022*, M1401. <https://doi.org/10.3390/M1401>

Academic Editor: Rodrigo Abonia

Received: 31 May 2022

Accepted: 24 June 2022

Published: 5 July 2022

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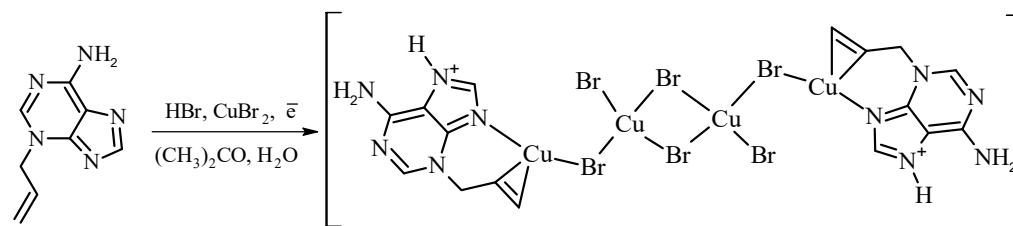
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1. Introduction

Both metallic copper and copper compounds are widely used in many branches of modern science and technology [1]. In turn, copper-containing complexes with unsaturated olefin ligands are attractive as catalysts in fine organic synthesis [2,3] in terms of their unique biochemical role [4] and interesting physical properties [5], as well as productive tools in the crystal engineering of coordination compounds [6,7], etc. In recent years, close attention has been paid to the crystal structure and properties of Cu(I) π-complexes with allyl-substituted heterocyclic ligands due to the possibility of the synchronous coordination of one metal atom with several organic linkers and the subsequent emergence of unique topological units [8–10].

However, adenine as a purine base is directly involved in the construction of nucleotides of nucleic acids (DNA and RNA). The mentioned heterocyclic nucleus incorporated in various derivatives, primarily attracts the attention of researchers due to its indirect participation in the transmission of hereditary information [11], its possible control of microorganisms, and the therapeutic effect of these microorganisms in medical practice [12,13]. Moreover, due to the presence of several coordination centers, the adenine nucleus is very interesting in the context of implementing diverse possibilities for coordination with metal ions. It is possible for all donor N atoms of *N*-substituted adenine to act as Lewis bases and to form bonds with metal ions. However, in the coordination compounds of copper(II), cobalt(III) and other *d*-metal ions with *N*3-substituted adenine ligands, the coordination of the metal atom is involved only in the *N*7 atom of the heterocyclic nucleus [14,15]. A modification of the adenine ring by the allyl group would also significantly extend its coordination behavior regarding Cu(I), forming a strongly directed Cu(I)–(C=C) interaction.

Based on the above, in the present work, we focus on the structural characterization of the product of copper(I) bromide coordination with the adenine derivative 6-amino-3-(prop-2-en-1-yl)-9H-purin-3-ium (3-allyladenine) bromide({*AllAd*}Br) (Scheme 1).



Scheme 1. Synthesis of compound 1.

2. Results and Discussion

The Cu1 atom in the crystal structure of $[(C_5H_5N_5(C_3H_5))_2Cu_4Br_6]$ (**1**) is located in a planar–trigonal coordination environment built from a nitrogen atom of a five-membered heterocyclic core of adenine ligands (distance Cu–N 1.978(4) Å), C=C bond of the allyl group of the same cation (Cu–C distances are 2.039(4)–2.059(5) Å, Cu–*m*–1.932(1) Å (*m*–midpoint of C=C bond of allyl group), Table 1), and bromine atoms (Cu–Br–2.321(1) Å). Another crystallographically independent Cu2 metal atom forms a slightly deformed tetrahedral environment ($\tau_4' = 0.93$, [16]) from the bromine atoms (Cu–Br–2.462(1)–2.499(1) Å).

Table 1. Selected geometric parameters (Å, °) of $[(C_5H_5N_5(C_3H_5))_2Cu_4Br_6]$.

Bond	<i>d</i> , Å	Angle	ω , °
Cu(1)–N(1)	1.978(4)	N(1)–Cu(1)–Br(1)	113.3(1)
Cu(1)–C(7)	2.039(4)	N(1)–Cu(1)–C(7)	93.7(2)
Cu(1)–C(8)	2.059(5)	N(1)–Cu(1)–C(8)	131.5(2)
Cu(1)–Br(1)	2.321(1)	C(7)–Cu(1)–C(8)	38.9(2)
Cu(1)– <i>m</i>	1.932(1)	Br(1)–Cu(2)–Br(3) ⁱ	111.03(3)
Cu(2)–Br(1)	2.484(1)	Br(2)–Cu(2)–Br(1)	102.54(3)
Cu(2)–Br(2)	2.462(1)	Br(2)–Cu(2)–Br(3) ⁱ	106.31(3)
Cu(2)–Br(3)	2.478(1)	Br(2)–Cu(2)–Br(3)	109.25(3)
Cu(2)–Br(3) ⁱ	2.499(1)	Br(3)–Cu(2)–Br(1)	111.27(3)
		Br(3)–Cu(2)–Br(3) ⁱ	115.50(2)

ⁱ Symmetry code: (i) $-x + 2, -y + 1, -z + 1$.

The linkage role of the two halogen atoms Br(3) causes the formation of dimers $\{Cu_2Br_6\}$. This is quite common among inorganic fragments in copper halide coordination compounds. These units occurs as isolated anions of the same composition [17] or as part of polyanions (for example, linear $\{CuBr_2\}_n^{n-}$ [18], or more complex 2D, or even 3D skeletons [19]). The arrangement of metal coordination tetrahedra in these kind of building blocks, in our opinion, depends mainly on steric hindrances. In the case of isolated anions $[Cu_2Br_6]^{2-}$, the copper polyhedra are as far apart as possible and the torsion angle Br–Cu–Br–Cu is 0.0° (the same value is observed in the structure of the discussed compound). Instead, the inclusion of $\{Cu_2Br_6\}$ as the topological block in the three-dimensional framework slightly shifts the tetrahedra relative to each other (the value of the torsion angle increases, for example, to about 15° in the complicated fragment $\{Cu_9Cl_{16}\}$ [20]).

Another halogen atom—Br(1)—acts as a bridge between the polyhedra of the crystallographically independent Cu(1) and Cu(2) atoms. As a result, the topological unit of the composition $\{[C_5H_5N_5(C_3H_5)Cu_2Br_3]_2\}$ (Figure 1) plays a key role in constructing the crystal structure of the discussed compound.

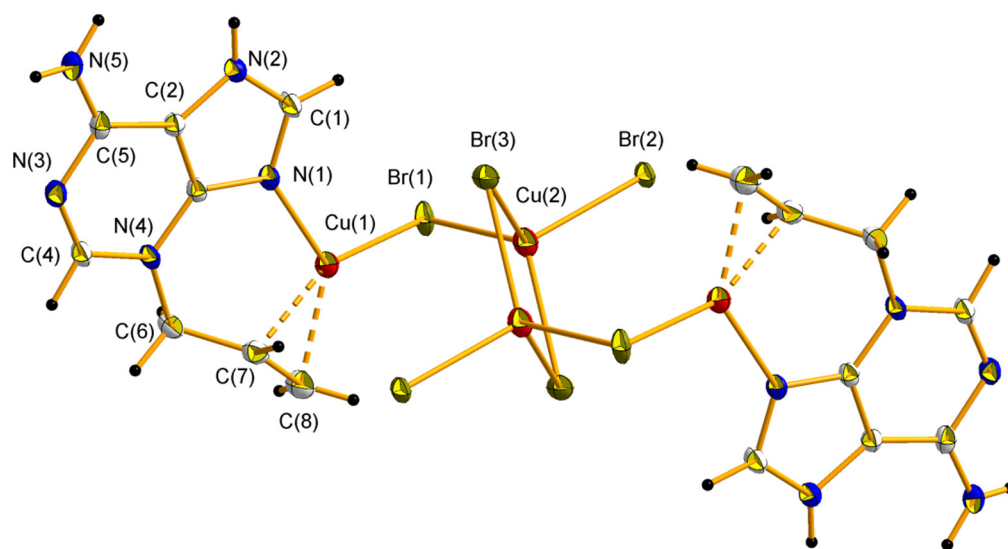


Figure 1. Dimeric topological unit $\{[AllAdCu_2Br_3]_2\}$ in crystal structure of $[(C_5H_5N_5(C_3H_5))_2Cu_4Br_6]$. Thermal ellipsoids are drawn at the 50% probability level.

Isolated topological units with formal stoichiometry $L_2Cu_4Hal_6$ are also common among coordination compounds of copper and, for example, were observed in the structure of the $[(3,2-pypzpy)_2(Cu_4I_6)]_n$ compound [21] based on 1-methyl-3-(1-(pyridin-2-yl)-1*H*-pyrazol-3-yl)pyridin-1-ium. However, according to the Cambridge Structural Database [22], compound **1** is the first known example of a structure with the $\{Cu_4Hal_6\}$ motif, which is π -attached (through the $Cu^I-(C=C)$ interaction) to the olefin group of the π , σ -ligand. A somewhat similar copper(I) halide fragment has previously been observed only in π -ligands, such as *N*-allylpiperazinium [23] and *N*-propargylamonium [24].

Based on the presence in the crystal structure of the compound $[AllAd_2Cu_4Br_6]$ isolated topological units with $\{(C_5H_5N_5(C_3H_5)Cu_2Br_3)_2\}$ composition are important to explore the supramolecular interactions that bind these blocks in a three-dimensional framework. The analysis of the geometry of hydrogen contacts (Table 2) displays the presence of quite noticeable interactions where the acceptors are nitrogen (of the adenine nucleus of the ligand) and carbon atoms (from the allyl group of the ligand), and donor–bromine anions. The corresponding bonds are formed both within the $\{(C_5H_5N_5(C_3H_5)Cu_2Br_3)_2\}$ dimer and between individual topological blocks by connecting them into a three-dimensional grid. The Hirshfeld surface analysis confirms the conclusion that they play an important role in the construction of the structure, since the total contribution to the surface area for $X-H\cdots Br$ contacts is 39.2% (Figure 2).

Table 2. Selected hydrogen bonds' geometric parameters (\AA , $^\circ$) of $[(C_5H_5N_5(C_3H_5))_2Cu_4Br_6]$.

Bond	$d(D-H)$, \AA	$d(H\cdots A)$, \AA	$d(D\cdots A)$, \AA	$\omega(D-H\cdots A)$, $^\circ$
$N(2)-H(2)\cdots Br(2)$ ⁱⁱ ¹	0.89(7)	2.34(7)	3.215(4)	168(6)
$N(5)-H(5A)\cdots Br(2)$ ⁱⁱ	0.88(6)	2.60(6)	3.460(5)	166(5)
$N(5)-H(5B)\cdots Br(3)$ ⁱⁱⁱ	0.73(7)	2.79(7)	3.521(5)	174(6)
$C(4)-H(4)\cdots Br(1)$ ^{iv}	0.99(5)	2.76(6)	3.624(5)	146(4)

¹ Symmetry codes: ⁽ⁱⁱ⁾ $1-x, 1-y, 1-z$; ⁽ⁱⁱⁱ⁾ $1-x, -y, 1-z$; ^(iv) $x, -1+y, z$.

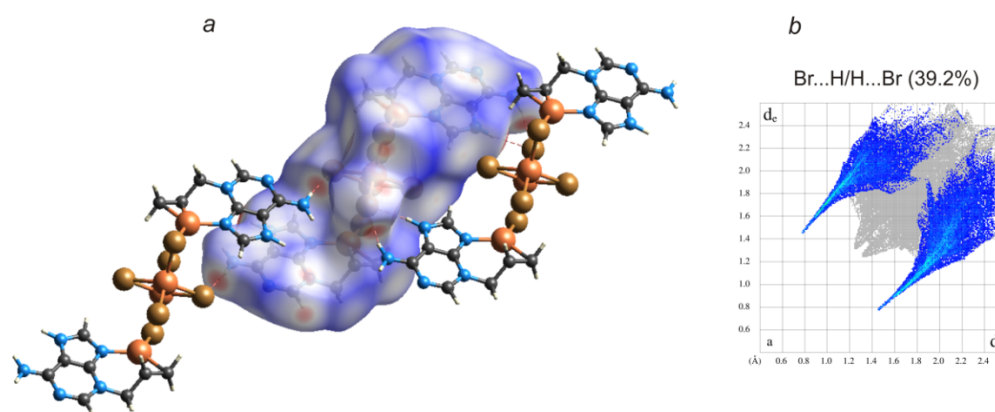


Figure 2. (a) Hirshfeld surface for the title molecule mapped with d_{norm} over the range of -0.506 to 1.324 a.u. (b) Fingerprint plot resolved into $\text{O}\cdots\text{H}/\text{H}\cdots\text{O}$ contacts. Neighboring molecules associated with hydrogen bonds are also shown.

3. Materials and Methods

First, 3-(2-propen-1-yl)-3*H*-purin-6-amine (3-allyladenine) was synthesized according to the reported procedure [25].

Crystals of the title compound (**1**) were obtained under the alternating-current electrochemical technique [26] starting from an acetone solution of copper(II) bromide and 3-(2-propen-1-yl)-3*H*-purin-6-amine, which was acidified by two drops of 48% hydrobromic acid. The mixture was carefully stirred and then was placed into a small test tube with subsequent alternating-current reduction (frequency 50 Hz, voltage 1.0 V) and after 10 days only few yellowish crystals of the title compound appeared on the copper wire electrodes (Scheme 1).

Diffraction data for the **1** single crystal were collected on an Agilent Gemini A four-circle diffractometer with an Atlas CCD detector. The collected data were processed with the CrysAlis PRO program (version 1.171.40.57a) [27]. The structure was solved by ShelXT and refined by the least squares method on F^2 by ShelXL software with the following graphical user interface of OLEX² [28–30]. Atomic displacements for non-hydrogen atoms were refined using an anisotropic model. N-bound hydrogen atoms were derived from difference Fourier synthesis and refined isotropically. Other hydrogen atoms were placed on geometrically calculated positions and refined as riding atoms with relative isotropic displacement parameters. The figures were prepared using DIAMOND 3.1 software (Bonn, Germany).

The Platon program was used to analyze the geometric features of the distribution of weak interactions [31]. The Hirshfeld surface for the structure $[\text{C}_5\text{H}_5\text{N}_5(\text{C}_3\text{H}_5)\text{Cu}_2\text{Br}_3]$ was constructed using the Crystal Explorer software package [32]. Crystal data for $[(\text{C}_5\text{H}_5\text{N}_5(\text{C}_3\text{H}_5))_2\text{Cu}_4\text{Br}_6]$: $M = 1086.04$ g/mol, monoclinic crystal system, space group $P2_1/c$, $Z = 2$, unit cell dimensions: $a = 8.6870(3)$, $b = 9.7447(2)$, $c = 16.4418(4)$ Å, $\beta = 100.681(3)^\circ$, $V = 1367.72(5)$ Å³ at 150 K; $\rho_{\text{calc}} = 2.637$ g/cm³, $R[F^2 > 2\sigma(F^2)] = 0.036$ for 3016 reflections and $wR(F_2) = 0.096$ for all 3417 reflections. These data have been deposited at the Cambridge Crystallographic Data Centre as CCDC 2176152, including the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via <https://www.ccdc.cam.ac.uk/structures/>.

Raman spectrum from **1** (see supplementary materials) was recorded with a Horiba Jobin–Yvon LabRAM HR spectrometer with the use of the 632.81 nm excitation line of a He–Ne laser (17 mW). Before data recording, the instrument scale was calibrated using a silicon polycrystalline plate (a characteristic band at 521 cm^{−1}).

Supplementary Materials: The following supporting information can be downloaded online. Figure S1. Raman spectrum of $[\text{C}_5\text{H}_5\text{N}_5(\text{C}_3\text{H}_5)_2\text{Cu}_4\text{Br}_6]$.

Author Contributions: O.V.P., investigation, software, writing—original draft; Y.I.S., conceptualization, methodology, investigation; E.A.G., software, investigation; M.G.M., software, investigation. All authors have read and agreed to the published version of the manuscript.

Funding: The authors thank the Ministry of Education and Science of Ukraine for financial support of this project (Grant No. 0120U102028) and the Slovenian Research Agency (research core funding No. P1-0045; Inorganic Chemistry and Technology).

Data Availability Statement: The X-ray data are deposited at CCDC as stated above.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Bellussi, G.; Bohnet, M.; Bus, J.; Drauz, K.; Greim, H.; Jackel, K.-P.; Karst, U.; Kleemann, A.; Kreysa, G.; Laird, T.; et al. *Ullmann's Encyclopedia of Industrial Chemistry*; Wiley-VCH: Chichester, UK, 2011.
2. Wang, X.-S.; Zhao, H.; Li, Y.-H.; Xiong, R.-G.; You, X.-Z. Olefin-Copper(I) Complexes and their Properties. *Top. Catal.* **2005**, *35*, 43–61. [[CrossRef](#)]
3. Tang, C.; Zhang, R.; Zhu, B.; Fu, J.; Deng, Y.; Tian, L.; Guan, W.; Bi, X. Directed Copper-Catalyzed Intermolecular Heck-Type Reaction of Unactivated Olefins and Alkyl Halides. *J. Am. Chem. Soc.* **2018**, *140*, 16929–16935. [[CrossRef](#)] [[PubMed](#)]
4. Binder, B.M. Ethylene signaling in plants. *J. Biol. Chem.* **2020**, *295*, 7710–7725. [[CrossRef](#)] [[PubMed](#)]
5. Armaroli, N.; Accorsi, G.; Cardinali, F.; Listorti, A. Photochemistry and photophysics of coordination compounds: Copper. In *Photochemistry and Photophysics of Coordination Compounds I*; Springer: Berlin/Heidelberg, Germany, 2007; pp. 69–115.
6. Rickerby, J.; Steinke, J.H.G. Current Trends in Patterning with Copper. *Chem. Rev.* **2002**, *102*, 1525–1550. [[CrossRef](#)]
7. Zhang, J.; Xiong, R.-G.; Chen, X.-T.; Xue, Z.; Peng, A.S.-M.; You, X.-Z. Two-Dimensional Luminescent Rectangular Molecular Grids Containing Copper(I)–Olefin Bonds as Bridging Spacers. *Organometallics* **2002**, *21*, 235–238. [[CrossRef](#)]
8. Slyvka, Y.; Goresnik, E.; Pavlyuk, A.; Mys'Kiv, M. Copper(I) π -complexes with allyl derivatives of heterocyclic compounds: Structural survey of their crystal engineering. *Open Chem.* **2013**, *11*, 1875–1901. [[CrossRef](#)]
9. Fedorchuk, A.; Slyvka, Y.; Kinzhyballo, V.; Lis, T.; Mys'Kiv, M. An unusual diverse coordination of silver(I) with *N*-allylthiohydantoin ligand in the presence of benzene- and *p*-toluenesulfonate anions. *Inorg. Chim. Acta* **2019**, *484*, 79–86. [[CrossRef](#)]
10. Hordiichuk, O.; Slyvka, Y.I.; Kinzhyballo, V.V.; Goresnik, E.A.; Bednarchuk, T.; Bednarchuk, O.; Jędryka, J.; Kityk, I.; Mys'Kiv, M. Construction of heterometallic and mixed-valence copper(I/II) chloride π -complexes with 1,2,4-triazole allyl-derivative. *Inorg. Chim. Acta* **2019**, *495*, 119012. [[CrossRef](#)]
11. Ryu, S.-M.; Koo, T.; Kim, K.; Lim, K.; Baek, G.; Kim, S.-T.; Kim, H.S.; Kim, D.-E.; Lee, H.; Chung, E.; et al. Adenine base editing in mouse embryos and an adult mouse model of Duchenne muscular dystrophy. *Nat. Biotechnol.* **2018**, *36*, 536–539. [[CrossRef](#)]
12. Heithoff, D.M.; Sinsheimer, R.L.; Low, D.A.; Mahan, M.J. An Essential Role for DNA Adenine Methylation in Bacterial Virulence. *Science* **1999**, *284*, 967–970. [[CrossRef](#)]
13. Gaudelli, N.M.; Lam, D.K.; Rees, H.A.; Solá-Esteves, N.M.; Barrera, L.A.; Born, D.A.; Edwards, A.; Gehrke, J.M.; Lee, S.-J.; Liquori, A.J.; et al. Directed evolution of adenine base editors with increased activity and therapeutic application. *Nat. Biotechnol.* **2020**, *38*, 892–900. [[CrossRef](#)] [[PubMed](#)]
14. Sorrell, T.; Epps, L.A.; Kistenmacher, T.J.; Marzilli, L.G. Transition metal compounds of *N*(3)-alkylated 6-aminopurines. Synthesis and unusually high stability of bis(acetylacetonato)(nitro)*N*(3)-alkylated 6-aminopurine)cobalt(III) complexes. Crystal and molecular structure of the triacanthine complex. *J. Am. Chem. Soc.* **1978**, *100*, 5756–5763. [[CrossRef](#)]
15. Pérez-Yáñez, S.; Castillo, O.; Cepeda, J.; García-Terán, J.P.; Luque, A.; Román, P. Supramolecular architectures of metal–oxalato complexes containing purine nucleobases. *Inorg. Chim. Acta* **2011**, *365*, 211–219. [[CrossRef](#)]
16. Yang, L.; Powell, D.R.; Houser, R.P. Structural variation in copper(i) complexes with pyridylmethylamide ligands: Structural analysis with a new four-coordinate geometry index, τ_4 . *Dalton Trans.* **2007**, 955–964. [[CrossRef](#)]
17. Willett, R.D. Crystal structure of bis(*N*-methylethylenediammonium) hexabromodicuprate(I). *Inorg. Chim. Acta* **2004**, *357*, 1579–1582. [[CrossRef](#)]
18. Pavlyuk, A.; Davydov, V.N.; Mys'Kiv, M. Copper(I) Complexes with *N*-Allylquinolinium Bromide [C₉H₇N(C₃H₅)]CuBr₂ and [C₉H₇N(C₃H₅)]Cu₂Br₃: Synthesis and Crystal Structure. *Russ. J. Coord. Chem.* **2003**, *29*, 199–202. [[CrossRef](#)]
19. Peng, R.; Li, M.; Li, D. Copper(I) halides: A versatile family in coordination chemistry and crystal engineering. *Coord. Chem. Rev.* **2010**, *254*, 1–18. [[CrossRef](#)]
20. Martin, J.D.; Dattelbaum, A.M.; Thornton, T.A.; Sullivan, R.M.; Yang, J.; Peachey, M.T. Metal Halide Analogues of Chalcogenides: A Building Block Approach to the Rational Synthesis of Solid-State Materials. *Chem. Mater.* **1998**, *10*, 2699–2713. [[CrossRef](#)]
21. Xue, J.-Y.; Li, J.-C.; Li, H.-X.; Li, H.-Y.; Lang, J.-P. Chan–Lam cross-coupling reactions promoted by anionic copper(I)/iodide species with cationic methyl-(pyridinyl)-pyrazolylpyridin-1-ium. *Tetrahedron* **2016**, *72*, 7014–7020. [[CrossRef](#)]
22. Groom, C.R.; Bruno, I.J.; Lightfoot, M.P.; Ward, S.C. The Cambridge Structural Database. *Acta Crystallogr. Sect. B Struct. Sci. Crystallogr. Eng. Mater.* **2016**, *72*, 171–179. [[CrossRef](#)]

23. Shkurenko, A.A.; Davydov, V.N.; Mys'Kiv, M. Synthesis and Crystal Structure of Copper(I) Chloride π -Complexes with *N*-Allyl- and *N,N'*-Diallylpiperazinium Dichlorides: $[\text{C}_3\text{H}_5\text{NH}(\text{CH}_2)_4\text{NH}_2]\text{Cu}_2\text{Cl}_4$ and $[\text{C}_3\text{H}_5\text{NH}(\text{CH}_2)_4\text{NHC}_3\text{H}_5]_{0.5}\text{CuCl}_2$. *Russ. J. Coord. Chem.* **2003**, *29*, 445–450. [[CrossRef](#)]
24. Noshtchenko, G.; Kinzhybalo, V.; Lis, T.; Mykhalitchko, B. π -Complexes of Copper(I) with Terminal Alkynes. Synthesis and Crystal Structure of $[(\text{HC}\equiv\text{CCH}_2\text{NH}_3)(\text{Cu}_2\text{Br}_3)]$ π -Complex. *Z. Anorg. Allg. Chem.* **2007**, *633*, 306–309. [[CrossRef](#)]
25. Eder, E.; Lutz, D.; Jörns, M. Allylic compounds bind directly to DNA: Investigation of the binding mechanisms in vitro. *Chem. Interact.* **1987**, *61*, 97–108. [[CrossRef](#)]
26. Slyvka, Y.; Pokhodylo, N.T.; Goreshnik, E.; Pavlyuk, O.; Mys'Kiv, M. Syntheses and crystal structures of two copper(I)-halide π,σ -coordination compounds based on 2-[(prop-2-en-1-yl)sulfanyl]pyridine. *Acta Crystallogr.* **2021**, *77*, 1180–1184. [[CrossRef](#)] [[PubMed](#)]
27. Rigaku CrysAlisPro Software System; Version 1.171.40.57a; Rigaku Oxford Diffraction (Tokyo, Japan): 2019. Available online: <http://www.rigaku.com> (accessed on 1 September 2019).
28. Sheldrick, G.M. SHELXT—Integrated space-group and crystal-structure determination. *Acta Crystallogr.* **2015**, *A71*, 3–8. [[CrossRef](#)]
29. Sheldrick, G.M. Crystal structure refinement with SHELXL. *Acta Crystallogr.* **2015**, *71*, 3–8. [[CrossRef](#)]
30. 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. [[CrossRef](#)]
31. Spek, A.L. PLATON, an integrated tool for the analysis of the results of a single crystal structure determination. *Acta Crystallogr.* **1990**, *46*, 34. [[CrossRef](#)]
32. Spackman, P.R.; Turner, M.J.; McKinnon, J.J.; Wolff, S.K.; Grimwood, D.J.; Jayatilaka, D.; Spackman, M.A. CrystalExplorer: A program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals. *J. Appl. Crystallogr.* **2021**, *54*, 1006–1011. [[CrossRef](#)]