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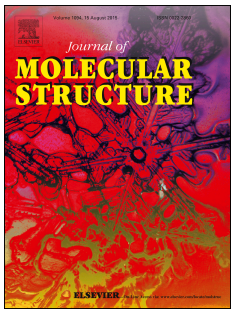

DFT calculations, crystal structure, Hirshfeld surface analyses and antibacterial studies of a new tetrachlorocuprate salt: $(C_6H_{16}N_2O)[CuCl_4]$

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DFT calculations, crystal structure, Hirshfeld surface analyses and antibacterial studies of a new tetrachlorocuprate salt: $(C_6H_{16}N_2O)[CuCl_4]$

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ABSTRACT

A novel tetrachlorocuprate salt $(C_6H_{16}N_2O)[CuCl_4]$ was synthesized and its crystal structure determined by single crystal X-ray diffraction analysis. This compound crystallizes in the monoclinic space group *Pn* with unit cell parameters *a*=7.71302(11), *b*=6.33580(8), *c*=13.10453(19)Å, β =104.9526(15)°, *V*=618.710(15)Å^3 and one cation and one anion in the asymmetric unit. Its crystal structure consists of $[CuCl_4]^{2-}$ anions surrounded by $[C_6H_{16}N_2O]^{2+}$ cations. N−H···Cl, N−H···O and O−H···Cl hydrogen bonding interactions link the entities into a three-dimensional framework. Theoretical calculations at the DFT/B3LYP/LanL2DZ level of theory provided good consistency between the calculated and experimental vibrational spectra and with the observed geometries of the ions. Compared with reference drugs, the compound exhibited moderate activity against gram-negative bacteria, while it showed modest activity against fungal and the gram-positive strains, except for S. aureus.

keywords: inorganic-organic hybrid material, tetrachlorocuprate, X-ray diffraction, Hirshfeld surface, DFT, antibacterial activity.