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Article

Single Crystal Investigations, Hirshfeld Surface Analysis, DFT Studies, Molecular Docking, Physico-Chemical Characterization, and Biological Activity of a Novel Non-Centrosymmetric Compound with a Copper Transition Metal Precursor

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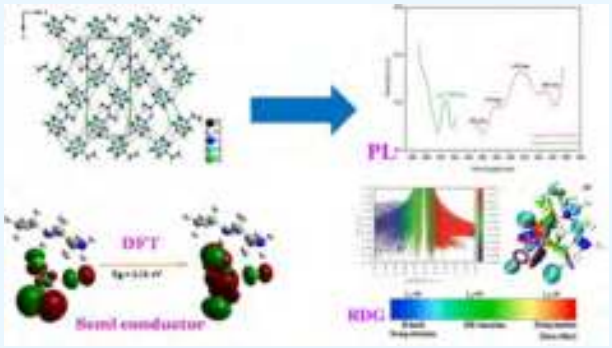
ABSTRACT: A novel organic−inorganic hybrid non-centrosymmetric superconductor material [2-ethylpiperazine tetrachlorocuprate(II)] has been synthesized and investigated by means of Fourier transform infrared spectroscopy, single-crystal X-ray crystallography, thermal analyses, and density functional theory (DFT) studies. The single-crystal X-ray analysis indicates that the studied compound crystallizes in the $P2_12_12_1$ orthorhombic space group. Hirshfeld surface analyses have been used to investigate non-covalent interactions. Organic cations $[C_6H_{16}N_2]^{2+}$ and inorganic moieties $[CuCl_4]^{2-}$ alternatively connect N−H···Cl and C−H···Cl hydrogen bonds. In addition, the energies of the frontier orbitals, highest occupied molecular orbital, lowest unoccupied molecular orbital, the reduced density gradient analyses and quantum theory of atoms in molecules analyses, and the natural bonding orbital are also studied. Furthermore, the optical absorption and photoluminescence properties were also explored. However, time-dependent/DFT computations were utilized to examine the photoluminescence and UV−vis absorption characteristics. Two different methods, 2, 2-diphenyl-1-picryhydrazyl radical and 2,2-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid radical scavenging, were used to evaluate the antioxidant activity of the studied material. Furthermore, the title material was docked to the SARS-CoV-2 variant (B.1.1.529) in silico to study the non-covalent interaction of the cuprate(II) complex with active amino acids in the spike protein.



INTRODUCTION

Over the years, crystal engineering approaches to integrate the inherent features of organic and inorganic materials into one material have drawn significant interest in the design of organic−inorganic materials. The hydrogen bonds N−H···Cl and C−H···Cl dominate the cohesive forces in these hybrid materials. Copper is an alluring transition metal with a d^9 electron system and exhibits a wide range of coordination compounds, particularly with coordination numbers four, five, and six.[1−4] Moreover, Cu(II) complexes can be used for a variety of biological and catalytic applications.[5,6]

Piperazines and their derivatives have intriguing pharmacological, cardiovascular, and autonomic properties. In addition, it has a wide range of applications due to its combination of organic and inorganic molecules, considering their pharmacological, optical, thermal, biological, and electrical properties, including photocatalysis and medicine.[7−14] Furthermore, the piperazine derivatives are a group of strongly basic amines capable of forming dications with normally all NH bonds capable of forming H bonds and have been used in pharmacological substances in a variety of therapeutic fields including antidepressants, antibiotics, antifungal, anticancer, and antipsychotic drugs.[15]

Herein, we describe the synthesis and structure investigations of a new hybrid inorganic−organic material $(C_6H_{16}N_2)[CuCl_4]$, abbreviated as 2EPCU, based on the piperazine cation and Cu^{2+} metal ion. Hirshfeld surface analysis has been proposed to understand the various intermolecular interactions. In addition, vibrational, UV−vis optical absorption, and photoluminescence (PL) studies were also performed. Furthermore, theoretical investigations employing quantum theory atom in molecule (QTAIM), reduced density gradient (RDG), natural bond orbital (NBO), and molecular electrostatic potential were carried out to assess the structural topology. In addition, the antioxidative properties of

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