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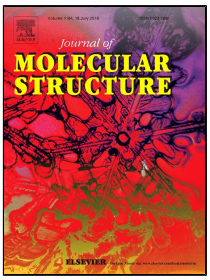

Crystal packing, high-temperature phase transition, second-order nonlinear optical and biological activities in an hybrid material: [(S)-$C_7H_{16}N_2$][$CuBr_4$]

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Crystal packing, high-temperature phase transition, second-order nonlinear optical and biological activities in an hybrid material: [(S)-$C_7H_{16}N_2$][$CuBr_4$]

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Abstract

The directed synthesis of non-centrosymmetric copper (II) bromo-complex has been achieved through the use of homochiral organic molecule. Reaction containing (S)-(–)-3-aminoquinuclidine, $CuBr_2$, HBr and H_2O were subjected to mild hydrothermal conditions, resulting in the growth of single crystals of [(S)-$C_7H_{16}N_2$][$CuBr_4$]. The compound crystallizes in the non polar space group $P2_12_12_1$(No. 19), which exhibits the enantiomorphic crystal class 222 (D_2). In the crystal structure, the tetrabromocuprate(II) anion is connected to three organic cations through N–H···Br hydrogen bonds to form cation-anion-cation molecular units, which are held together by means of offset face-to-face interactions to give one-dimensional chains. DSC measurements indicated that the compound [(S)-$C_7H_{16}N_2$][$CuBr_4$] underwent a reversible phase transition at 80°C. [(S)-$C_7H_{16}N_2$][$CuBr_4$] is more than 1.2 times as efficient as KDP in second harmonic generation; making it a potentially attractive material for non-linear optical applications. The synthesized product was also screened for in vitro antioxidant and antimicrobial activities, while showing favorable antioxidant activities against DPPH as well as the discoloration of β-carotene.

Keywords: chiral crystal; metal complex; second harmonic generation; phase transition; biological activities.