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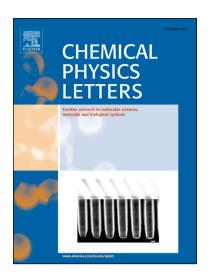
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ACCEPTED MANUSCRIPT

Synthesis, structural and NLO properties of the novel copper (I) ptoluenesulfonate π -complex with 1-allyloxybenzotriazole

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Abstract

Using the alternating-current electrochemical technique, a novel π -complex $[Cu_2(Alobtr)_2(H_2O)_2](CH_3C_6H_4SO_3)_2$ (1) was obtained starting from copper(II) p-toluenesulfonate and the 1-allyloxybenzotriazole (Alobtr) ethanol solution. The structure 1 should be considered as the first known example of $Cu^I(p\text{-CH}_3C_6H_4SO_3)$ π -coordination compound. Alobtr molecule acts as a chelate π , σ -ligand (being attached to the Cu(I) by means of allylic C=C bond and the two triazole N atoms) and forms centrosymmetric $[Cu_2(Alobtr)_2(H_2O)_2]^{2+}$ dimers. Cationic fragments and $p\text{TsO}^-$ anions are connected by means of (Ow)H....O hydrogen bonds into 1D chains. Laser stimulated third harmonic generation for fundamental wavelength 1540 nm is explored.

Keywords: copper(I); π -complex; 1,2,3-triazole derivatives; crystal structure; ac-electrochemical technique

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