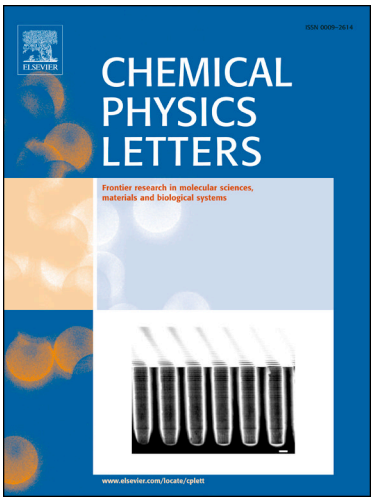

Frontiers article

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

Yu. Slyvka, A.A. Fedorchuk, E. Goreshnik, G. Lakshminarayana, I.V. Kityk, P. Czaja, M. Mys'kiv

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Synthesis, structural and NLO properties of the novel copper (I) *p*-toluenesulfonate 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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