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Yu.I. Slyvka, A.A. Fedorchuk, N.T. Pokhodylo, T. Lis, I.V. Kityk, M.G. Mys'kiv

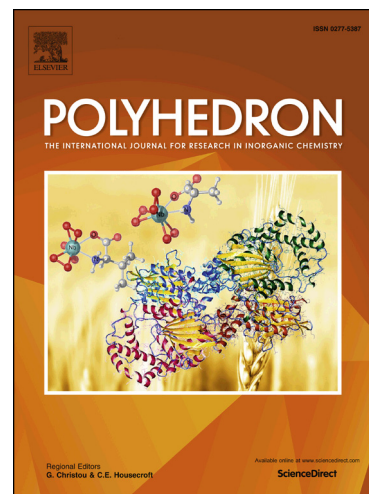
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A novel copper(I) sulfamate π -complex based on the 5-(allylthio)-1-(3,5-dimethylphenyl)-1*H*-tetrazole ligand: alternating-current electrochemical crystallization, DFT calculations, structural and NLO properties studies

Yu.I. Slyvka^{a,*}, A.A. Fedorchuk^a, N.T. Pokhodylo^a, T. Lis^b, I.V. Kityk^{c,d}, M.G. Mys'kiv^a

^a*Faculty of Chemistry, Ivan Franko National University of Lviv, KyrylaiMefodiya Str., 6, 79005, Lviv, Ukraine*

^b*Faculty of Chemistry, University of Wrocław, Joliot-Curie 14, 50-383 Wrocław, Poland*

^c*Institute of Optoelectronics and Measuring Systems, Faculty of Electrical Engineering, Czestochowa University of Technology, 17 ArmiiKrajowej Str., 42-200 Czestochowa, Poland*

^d*Department of Physics, Eastern European National University, 13 Voli Avenue, 43025 Lutsk, Ukraine*

*Corresponding author: E-mail address: yurii.slyvka@lnu.edu.ua (Yu.I.Slyvka)

ABSTRACT

Using the alternating-current electrochemical technique, the novel π -complex [Cu^I(*m-dmphast*)NH₂SO₃] (**1**), based on the 5-(allylthio)-1-(3,5-dimethylphenyl)-1*H*-tetrazole (*m-dmphast*) ligand, was obtained and it was studied using single crystal X-ray diffraction as well as IR and UV–Vis spectroscopy. The structure **1** should be considered as the first known example of a metal sulfamate coordination compound with a tetrazole ligand. The copper(I) ion in **1** possesses a trigonal pyramidal environment, arranged from the N4 atom of the tetrazole core, the C=C bond from the S-allyl group of the same *m-dmphast* ligand and O and N atoms of the NH₂SO₃[−] anion. The sulfamate anion is coordinated to the two neighboring Cu(I) ions in a bridged mode, occupying a basal plane (through the N atom) and an apical (through an O atom) position of the two neighboring metal trigonal pyramids. The bicolor coherent photoinduced treatment by a nanosecond Nd:YAG laser at a wavelength of 1064 nm caused the occurrence of charge density acentricity, which in turn favours an occurrence of second harmonic generation described by third rank polar tensors, that are usually forbidden for centrosymmetrical crystals.

Keywords: tetrazole; copper(I) π -complex; crystal structure; *ac*-electrochemical technique; NLO properties

1. Introduction

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