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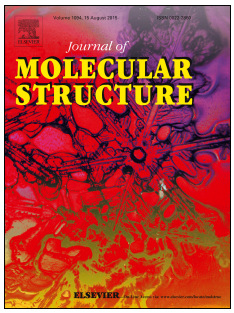

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New esters with thioxoimidazoquinazoline ring – synthesis, spectral characterization and quantum mechanical modelling

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Abstract: In present work, new esters with a thioxoimidazoquinazoline ring were obtained in a reaction of 1-phenyl-2H,6H-3-thioxoimidazo[1,5-c]quinazolin-5-one with ethyl bromoacetate. The obtained esters - 2-(ethoxycarbonylmethyl)-1-phenyl-6H-3-thioxoimidazo[1,5-c]quinazoline-5-one and 2,6-bis(ethoxycarbonylmethyl)-1-phenyl-3-thioxoimidazo[1,5-c]quinazoline-5-one, were isolated at high yield and characterized by instrumental methods: elemental analysis, IR, ^{1}H- and ^{13}C-NMR, UV and MS-ESI spectroscopies. 2-(ethoxycarbonylmethyl)-1-phenyl-6H-3-thioxoimidazo[1,5-c]quinazolin-5-one is formed as the only product of the equimolar reaction. Quantum-mechanical modelling carried out with the use of the DFT method explained the substitution course. Moreover, the quantum calculations and the spectroscopic analysis exclude the presence of a product with ester group linked via sulfur atom. It was calculated that 99.96 % of the monoester is formed at position No. 2. The reason for the reaction's chemoselectivity is the distribution of electron density in the 1-phenyl-2H,6H-3-thioxoimidazo[1,5-c]quinazolin-5-one molecule. Only the second mole of ethyl bromoacetate reacts with nitrogen atom No. 6, and diester is formed. Quantum-mechanical calculations allowed to determine the composition of 2-(ethoxycarbonylmethyl)-1-phenyl-6H-3-thioxoimidazo[1,5-c]quinazoline-5-one and 2,6-bis(ethoxycarbonylmethyl)-1-phenyl-3-thioxoimidazo[1,5-c]quinazoline-5-one conformers. Furthermore, the conformer compositions of mono and diesters of 1-phenyl-2H,6H-3-thioxoimidazo[1,5-c]quinazolin-5-one were compared with those ones of 1-phenyl-2H,6H-imidazo[1,5-c]quinazoline-3,5-dione.

Keywords: thioxoimidazoquinazoline ring, ester, synthesis, structure characterization, quantum-mechanical calculations

Introduction

Heterocyclic compounds containing a sulfur atom are interesting substances, since many of them can have biologically activity [1-3]. Derivatives of imidazolines with sulfur atoms also arouse great interest. A number of 2-thioxoimidazolines and their derivatives exhibit significant biological activities [4, 5], e.g. inflammatory activity [6], inhibitory activity of gentamycin nephrotoxicity [7] and dopamine β-hydroxylase, and anti-aggregating activity against collagen [8].