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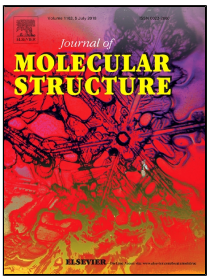

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EXPERIMENTAL AND THEORETICAL STUDY OF THE ACYLATION REACTION OF AMINOPYRAZOLES WITH ARYL AND METHOXYMETHYL SUBSTITUENTS

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Abstract

As a result of the chain of transformations from 1,3-butanedione with aryl and methoxy substituents through nitrosation and cyclization with hydrazine, the corresponding nitrosopyrazoles and aminopyrazoles were synthesized. According to this scheme, eight new previously unknown compounds were obtained. Their structures were established by the methods of IR, UV, ^{1}H NMR, ^{13}C NMR spectroscopy and mass spectrometry. DFT method of quantum-chemical calculations showed that obtained aminopyrazoles can exist as two tautomers; it was also confirmed by NMR ^{1}H spectroscopy data. In the case of acylation, an isomer is formed, where aryl substituent takes place in the fifth, rather than in the third position of the pyrazole ring, as shown by the DFT calculations.

Keywords: nitrosopyrazoles, aminopyrazoles, acylation, tautomerism.

1. Introduction

It is known that many pyrazole derivatives exhibit different types of biological activity [1-10]. However, thousands of substances are synthesized or obtained from natural raw materials, but only some of them are ultimately effective in the creation of medicines [11]. The reasons of that are still unclear, because the strong theory, connecting the structure of mentioned compounds with their pharmaceutical properties, does not exist. Therefore, it seems important to obtain new previously unknown compounds, including new pyrazole derivatives, which can exhibit biological activity. We need more amount of experimental information to establish correlation between structure of these compounds and their potential properties and use.

In the present work we obtained aminopyrazoles with aryl and methoxymethyl substituents and investigated the reaction of their acylation. This direction of synthesis was chosen due to the fact that presence of pharmacophore amino or acetamide groups in the molecule provides the

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