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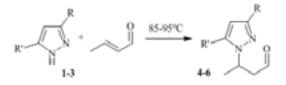
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Addition of pyrazoles to crotonaldehyde in the presence of water

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The synthesis of formylpropyl derivatives of pyrazoles (4-6) by the reaction of pyrazoles (1-3) with crotonaldehyde in the absence of catalyst and in neat has been studied in this work, the reactions proceed with up to 85-90% yields in 8-16 hours.



1,4 R = R'= H; 2,5 R = CH3, R' = H and R = H, R'= CH3; 3,6 R = R'= CH3

With the aim to decrease the duration of the reaction and avoiding the usage of organic solvents and taking into account the fact that the reaction between amines and conjugated systems can be easily carried out in aqueous medium [2,3,4] we performed the proposed synthesis in water. However, increase of yields or reduction of the reaction times have not been observed (4-5).

Unlike to the interaction of pyrazoles (1,2) with crotonaldehyde, in the case of 3,5-dimethylpirazole (3) a crystalline compound (7) was obtained with up to 60-65% yields. In order to determine the structure of the compound the monocrystal of (7) was investigated by X-ray analysis (XRD). According to XRD (fig. 1) (7) is a cyclic hemiacetal of the product of addition of second molecule of crotonaldehyde to the adduct of the first molecule to the 3,5-dimethylpyrazole.

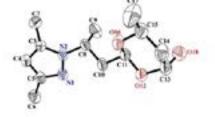
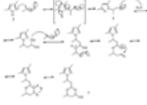


Figure 1: The structure of 2-(2-(3,5-dimethyl -1H-pyrazole -1-yl)propyl)-6-methyl -1,3-dioxan-4-ol (7) molecule without hydrogen atoms.

The somehow similar unusual behavior of 3,5-dimethylpyrazole (3) was observed also earlier the work [5]. The suggested mechanism of interaction is as follows:



Biography

H N Khachatryan is a PhD student. Her dissertation include "Aza-Michael reactions in azoles and further transformations of obtained adducts". She has seven published works in "Russian journal of general chemistry" and next work will be published soon. Aza-Michael reactions are known in literature but she don't use any catalysis and solvents. This is new technic to obtain products in high yields in low times. She continued her works to investigate properties of obtained adducts.

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