

Synthesis of (3-Aroyl-2-aryl-4-hydroxy-5-oxo-2,5-dihydro-1*H*-pyrrol-1-yl)acetonitriles and Their Reaction with Hydrazine Hydrate

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Received December 3, 2018; revised February 10, 2019; accepted February 21, 2019

Abstract—Three-component reaction of methyl 4-aryl-2,4-dioxobutanoates with aromatic aldehyde and 2-aminoacetonitrile sulfate in glacial acetic acid in the presence of anhydrous sodium acetate afforded previously unknown (3-aryol-2-aryl-4-hydroxy-5-oxo-2,5-dihydro-1*H*-pyrrol-1-yl)acetonitriles. The reaction involved intermediate formation of Schiff base, followed by Michael-type addition of the dioxo ester to the C=N bond and cyclization of the addition product, methyl 3-aryol-4-aryl-4-(cyanomethylamino)-2-oxobutanoate. The cyclization product reacted with hydrazine hydrate at the aroyl carbonyl group to give the corresponding hydrazone which was converted in 1,4-dioxane to the cyclic form, [3,4-diaryl-6a-hydroxy-6-oxo-3a,4,6,6a-tetrahydropyrrolo[3,4-*c*]pyrazol-5(1*H*)-yl]acetonitrile, without elimination of the second water molecule. When the reaction of (3-aryol-2-aryl-4-hydroxy-5-oxo-2,5-dihydro-1*H*-pyrrol-1-yl)acetonitriles with hydrazine hydrate was carried out in boiling acetic acid, [3,4-diaryl-6-oxo-2,6-dihydropyrrolo[3,4-*c*]pyrazol-5(4*H*)-yl]acetonitriles were obtained as a result of dehydration of initially formed [3,4-diaryl-6a-hydroxy-6-oxo-3a,4,6,6a-tetrahydropyrrolo[3,4-*c*]pyrazol-5(1*H*)-yl]acetonitriles as shown by special experiment. The structures of [6a-hydroxy-6-oxo-3,4-diphenyl-3a,4,6,6a-tetrahydropyrrolo[3,4-*c*]pyrazol-5(1*H*)-yl]acetonitrile and [4-(4-methoxyphenyl)-6-oxo-3-phenyl-2,6-dihydropyrrolo[3,4-*c*]pyrazol-5(4*H*)-yl]acetonitrile were determined by X-ray analysis.

Keywords: three-component reaction, (3-aryol-2-aryl-4-hydroxy-5-oxo-2,5-dihydro-1*H*-pyrrol-1-yl)acetonitriles, 2-aminoacetonitrile sulfate, hydrazine hydrate, [3,4-diaryl-6a-hydroxy-6-oxo-3a,4,6,6a-tetrahydropyrrolo[3,4-*c*]pyrazol-5(1*H*)-yl]acetonitriles, [3,4-diaryl-6-oxo-2,6-dihydropyrrolo[3,4-*c*]pyrazol-5(4*H*)-yl]acetonitriles.

DOI: 10.1134/S1070428019070054