MECHANISM OF THE CONDENSATION REACTION BETWEEN 1-ARYL- AND HETEROARYL-1,4-DIHYDRO-3(2*H*)-ISOQUINOLINONES AND ALDEHYDES

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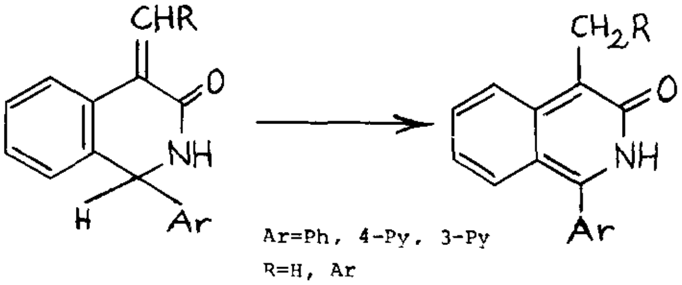
According to our investigations /1/ the reaction of 1-aryl-1,4-dihydro-3(2*H*)-isoquinolinones with aromatic aldehydes or with *in situ* formaldehyde yields new 1,4-disubstituted 3(2*H*)-isoquinolinones, through 4-arylidene /alkylidene/ intermediates.



Ar=Ph, 4-Py, 3-Py
R=H, Ar

In case Ar=phenyl, the reaction can be carried out in the presence of a strong base /e.g. NaH/, when Ar=pyridyl, in polyphosphoric acid medium /PPA/, too. Compounds labelled with deuterium were synthetized and using the method of rearrangement of isotope isomers we have established, that in the presence of a strong base the product was formed by the intermolecular migration of the C-1 hydrogen. As this migration of the hydrogen as a proton or radical can be excluded, our results made a hydride transfer mechanism probable.

In case of the 1-pyridyl-derivatives /Ar=4-Py or 3-Py/ the reaction was performed in perdeuterated PPA,in which medium the migration of the hydride ion is impossible.The NMR spectra of the products showed that in the perdeuterated PPA deuterium incorporation into the C-4 methylene group took place,one of the hydrogens was completely substituted.In this case the transformation takes place by a proton splitting off and subsequently by a proton up-take from the medium.

The lecture outlines the proposed mechanism of the transformation under acidic and basic conditions, respectively.

/1/ L.Hazai,Gy.Deák,G.Tóth,J.Volford,J.Tamás: J.Heterocyclic Chem.19,49/1982/.