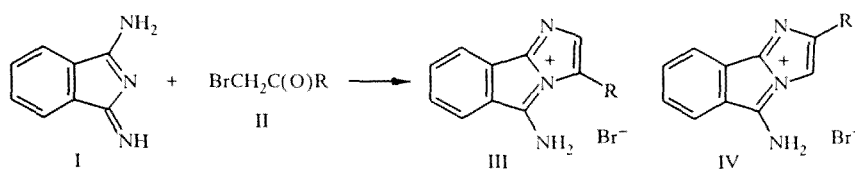


REACTION OF AMINO-IMINO-1H-ISOINDOLE WITH α -BROMOKETONES

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The reaction of 1-amino substituted azoles with α -halogenated carbonyl compounds is frequently used to produce $[d,e]$ annulated imidazole rings [1-4]. However similar condensations in the 3-amino-1-imino-1H-isoindole series have not yet been reported.

Using as examples the reactions of 3-amino-1-imino-1H-isoindole (I) with phenacyl bromide and its *p*-chloro-(bromo)derivatives (II) we have shown for the first time that this route can be used for the preparation of derivatives of 5-aminoimidazo[2,1-*a*]isoindoles (III, IV):



II-IV a R=Ph, b R=C₆H₄Br-*p*, c R=C₆H₄Cl-*p*

As a rule hydrogen bromides of two isomers are formed. If the reagents are boiled in isopropanol the 3-arylimidazoisoindoles (III) predominate (3:1), whereas if the reaction is carried out in ethanol at room temperature the 2-aryl isomers (IV) are the major products (10:1).

The isomers are separated by successive treatment of the mixtures with acetone and toluene; the salts IV are practically insoluble in acetone.

5-Amino-3-phenylimidazo[2,1-*a*]isoindolium Bromide (IIIa, C₁₆H₁₂BrN₃). Yield 25%. M.p. > 250°C (acetone-toluene). ¹H NMR spectrum (DMSO-D₆): 7.35-8.25 (10 H, m, arom. H), 8.77 (s), 8.97 (s), 9.36 ppm (2 H, s, NH).

5-Amino-2-phenylimidazo[2,1-*a*]isoindolium Bromide (IVa, C₁₆H₁₂BrN₃). Yield 8%. M.p. > 250°C. ¹H NMR spectrum (DMSO-D₆): 7.47-7.80 (10 H, m, arom. H), 7.93 (1 H, s, 3-H), 9.48 (s), 9.23 ppm (2 H, s, NH).

5-Amino-3-(4-bromophenyl)imidazo[2,1-*a*]isoindolium Bromide (IIIb, C₁₆H₁₁Br₂N₃). Yield 25%. M.p. > 250°C (acetone-toluene). ¹H NMR spectrum (DMSO-D₆): 7.50-8.30 (9 H, m, arom. H), 8.77 (s), 8.99 (s), 9.08 (s), 9.36 ppm (2 H, s, NH).

5-Amino-2-(4-bromophenyl)imidazo[2,1-*a*]isoindolium Bromide (IVb, C₁₆H₁₁Br₂N₃). Yield 7%. M.p. > 250°C. ¹H NMR spectrum (DMSO-D₆): 7.65-8.32 (9 H, m, arom. H), 8.01 (1 H, s, 3-H), 9.26 (1 H, s), 9.50 ppm (1 H, s, NH).

5-Amino-3-(4-chlorophenyl)imidazo[2,1-*a*]isoindolium Bromide (IIIc, C₁₆H₁₁BrClN₃). Yield 24%. M.p. > 250°C (acetone-toluene). ¹H NMR spectrum (DMSO-D₆): 7.50-8.35 (9 H, m, arom. H), 8.77 (s), 8.99 (s), 9.04 (s), 9.76 ppm (2 H, s, NH).

5-Amino-2-(4-chlorophenyl)imidazo[2,1-*a*]isoindolium Bromide (IVc, C₁₆H₁₁BrClN₃). Yield 7%. M.p. > 250°C. ¹H NMR spectrum (DMSO-D₆): 7.50-8.30 (9 H, m, arom. H), 8.00 (1 H, s, 3-H), 9.27 (1 H, s), 9.51 ppm (1 H, s, NH).

Results of elemental analyses corresponded to calculated values.

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