CONVERSIONS OF N-ACETONYL-3-METHYLISOQUINOLINIUM BROMIDE

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1-Methyl-N-acetonyl- or -N-phenacylisoquinolinium salts are converted by the action of soda or potash to the respective pyrrolo[2,1-a]isoquinolines [1, 2]. We have shown that by the action of potash on N-acetonyl-3-methylisoquinolinium bromide (I) there is formed not 2-methylpyrrolo[1,2-b]isoquinoline, but only the betaine, which is easily converted back to the starting salt by acid. When (I) is boiled with aqueous potash there is isolated from the reaction mixture, besides 3-methylisoquinoline, a 15% yield of 2-methyl-5,10-dihydropyrrolo[1,2-b]isoquinoline (II); this compound is formed by removal of a proton from the 3-methyl group and subsequent closure of the pyrrole ring and reduction of the pyridine ring. Pyrrolo[1,2-b]isoquinoline (II) is protonated in trifluoroacetic acid, and is acylated by trifluoroacetic anhydride in benzene at the α-position of the pyrrole ring.
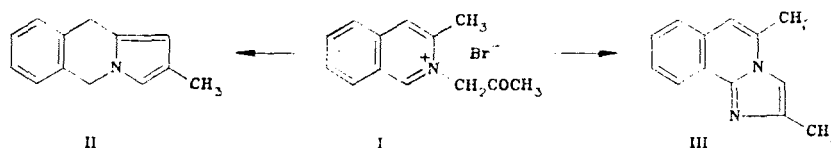
When potash is replaced by alcoholic ammonia solution (sealed ampul, 150°C, 20 h), besides 22% of (II) there is isolated from the reaction mixture 30% of 2,5-dimethylimidazo-[2,1-a]isoquinoline (III); this compound is formed by successive addition of ammonia at position 1 of the isoquinoline nucleus, attack by the amino group on the carbonyl carbon, and oxidation of the intermediate thus formed.

2-Methyl-5,10-dihydropyrrolo[1,2-b]isoquinoline (II, $C_{13}H_{13}N$). Mp 108°C (from hexane). PMR spectrum (in $CDCl_3$): 2.14 (3H, s, 2-CH_3), 4.00 (2H, s, 10-CH_2), 5.01 (2H, s, 5-CH_2), 5.87 (1H, s, 1-H), 6.50 (1H, s, 3-H), 7.20-7.29 (4H, m, aromatic protons).

2,5-Dimethylimidazo[2,1-a]isoquinoline (III, $C_{13}H_{12}N_2$). Mp 112°C (from hexane). PMR spectrum (in $CDCl_3$): 2.55 (3H, s, 2-CH_3), 2.60 (3H, s, 5-CH_3), 6.86 (1H, s, 6-H), 7.29 (1H, s, 3-H), 7.50-7.60 (2H, m, 8-H, 9-H), 7.64 (1H, d, J_{78} = 10 Hz, 7-H), 8.63 (1H, d, J_{109} = 10 Hz, 10-H).

The elemental composition agrees with the calculated values.

LITERATURE CITED

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