FIRST EXAMPLE OF THE RECYCLIZATION OF AN IMIDAZO[4,5-c]PYRIDINE DERIVATIVE TO A SUBSTITUTED BENZIMIDAZOLE

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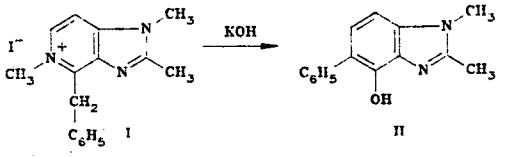
Quaternary pyridinium salts are known to react with bases via ring opening, followed by ring closure, to give amino- and hydroxybenzene derivatives [1, 2]. We have demonstrated that an analogous reaction takes place easily when 4-benzyl-1,2,5-trimethyl-1H-imidazo[4,5-c]-pyridinium iodide (I) is heated in aqueous alcohol solutions of base. As a result of this conversion of the pyridinium ring with the methylene group of the side chain, 4-hydroxy-5-phenyl-1,2-dimethylbenzimidazole (II) is formed in nearly quantitative yield. Compounds such as II are not easily accessible via the traditional methods of benzimidazole synthesis.

The structure of compound II was established based on its PMR, IR, and mass spectra, as well as the agreement of its elemental analysis with the calculated values.



I II

Iodide I. This was prepared by addition of methyl iodide to 4-benzyl-1,2-dimethylimidazo-[4,5-c]pyridine [3] in acetone (25°C, 24 h). Yield 45%, mp 244-245°C (from ethanol). PMR spectrum (CF_3COOH): 3.18 (3H, s, 2-CH_3), 4.22 (3H, s, 1-CH_3), 4,40 (3H, s, 5-CH_3), 5.00 (2H, s, 4-CH_2), 7.12-7.43 (5H, m, C_6H_5), 8.33 (1H, d, J = 6.5 Hz, 7-H), 8.87 ppm (1H, d, J = 6.5 Hz, 6-H).

Benzimidazole II. A mixture of 0.6 g (1.6 mmole) of iodide I and a solution of 1.7 g (30 mmole) potassium hydroxide in 10 ml alcohol and 0.5 ml water was refluxed for 2 h under a weak stream of argon. The alcohol was evaporated in vacuo and the oily residue was treated with 1-2 ml of water. The resulting precipitate was filtered, washed with water (3 ml) and dried. Yield 0.36 g (95%), mp 247-248°C (reprecipitated from a solution in 10% H_2SO_4 by the addition of ammonia). PMR spectrum (CF_3COOH): 2.92 (3H, s, 2-CH_3), 4.02 (3H, s, 1-CH_3), 7.53 (5H, s, C_6H_5), 7.30 (1H, d, j = 8.5 Hz, 6-H), 7.59 ppm (1H, d, J = 8.5 Hz, 7-H). IR spectrum (chloroform): 3470 cm^{-1} (OH). M^+ 238.

LITERATURE CITED

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