DIMERIZATION OF 1-VINYL-4,5,6,7-TETRAHYDROINDOLE UNDER THE INFLUENCE OF HCl

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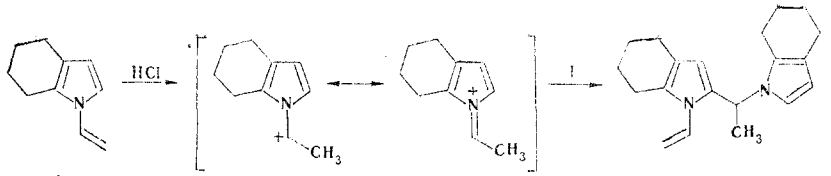
It is known that 1-vinylindole and other N-vinyl derivatives of the pyrrole series undergo polymerization at the double bond (for example, see [1]) or form polymeric charge-transfer complexes in the presence of halogens and hydrogen halides [1]. However, when we treated 1-vinyl-4,5,6,7-tetrahydroindole (I) with HCl we obtained, in addition to a polymer, dimer III — the product of electrophilic attack by immonium cation II on the pyrrole ring of the I molecule.



One drop of concentrated HCl was added to 1 g (0.007 mole) of indole I. After 50 h, the bright-red polymerizate was extracted with hot hexane, and the extract was cooled to precipitate 0.2 g (20%) of pinkish crystals of 1-vinyl-2-[1-(1,4,5,6,7-tetrahydroindolyl)ethyl]-4,5,6,7-tetrahydroindole (III) with mp 114°C; the results of elementary analysis of this product were in agreement with the formula. Mass spectrum (m/z): 294 (M^+) and 174 (splitting out of a 4,5,6,7-tetrahydroindolyl radical). PMR spectrum (d_6-acetone): 6.43 (1H, q, C–H), 6.23 (1H, d, 7-H), 6.01 (1H, s, 4-H), 5.67 (1H, d, 8-H), 5.17 (1H, q, 5-H), 4.73 (1H, d, A-H), 4.70 (1H, d, B-H), 2.46 (8H, m, 9-H, 12-H, 13-H, 16-H), 1.71 (8H, m, 10-H, 11-H, 14-H, 15-H), and 1.54 ppm (3H, d, 6-H); spin-spin coupling constants (SSCC) (Hz): $^3J_{7+8}$ = 3.5, $^3J_{AC}$ = 16.0, $^3J_{BC}$ = 9.0, $^2J_{AB}$ = 0, and $^3J_{5+6}$ = 7.0. IR spectrum: 580, 870, 970, 1380, 1490, 1530, 1640 cm^{-1} (frequencies of the N-vinyl group and the pyrrole ring [2]). UV spectrum in ethanol, λ_{max} ($\varepsilon \cdot 10^{-3}$): 208 (26.5) and 247 nm (14.6), in agreement with the literature data [3] for N-vinylpyrroles.

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