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RING-CHAIN TAUTOMERISM IN THE 2-PHENYLHEXAHYDROPYRIMIDINE – 1-BENZYLIDENEAMINO-3-AMINOPROPANE SYSTEMS

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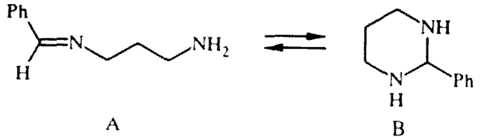
In principle hexahydropyrimidines are capable of ring-chain tautomerism with participation of a linear form — 1-alkylidene(arylidene)amino-3-aminopropane. This property has been observed in a few N-substituted derivatives [1]. However all known 1,3-unsubstituted hexahydropyrimidines (including hexahydropyrimidine [1-3], and its 2-alkyl- [2-5] and 2,2-dialkylsubstituted homologs [1, 2]) exist only in the cyclic form. We have found that the product (I) obtained from the reaction of benzaldehyde with propylene diamine in a 1:1 ratio in solution showed evidence of the ring-chain tautomerism A ⇄ B:



I

2-Phenylhexahydropyrimidine (I). Equimolar amounts of benzaldehyde and propylene diamine were mixed in one twentieth of the amount of benzene, the mixture was dried over potassium hydroxide and the solvent was removed in vacuum. The residue was extracted three times with one twentieth of the amount of hexane, dried over potash, and the solvent was evaporated in vacuum to give a quantitative yield of oil. ^{1}H NMR Spectrum ($CDCl_3$, δ, ppm): form A (10%): 7.99 (1 H, s, H–C=N), 3.39 (2H, t, 1-H) (signal of $\underline{CH_2}NH_2$ was hidden below the more intense signals of the methylene protons of form B). Form B (90%): 4.20 (1H, s, 2-H), 2.89 (2H, m, 4,6-H_e), 2.54 (2H, m, 4,6-H_a). The signals for H_{arom} at 7.02-7.53 (5 H, m, H_{arom}), CCH_2C at 1.40 (m, 2H), and NH at 1.29 ppm (s, 2H) are broad for both forms. ^{13}C NMR Spectrum ($CDCl_3$, δ, ppm): form A: 159.4 (C=N), 58.2 (C_1), 38.7 (C_3), 33.6 (C_2). Form B: 73.2 (C_2), 45.0 ($C_{4,6}$), 26.0 (C_5). There are 8 signals in the range 125.2-141.7 ppm for C_{arom} of both forms.

Elemental analysis for compound I are within limits of 0.3% of the calculated values. ^{1}H and ^{13}C NMR spectra were recorded with a Tesla BS-487 instrument (100 and 20.41 Hz respectively).

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