Pyramidal nitrogen inversion hindered by a strong intramolecular hydrogen bond in 2-diethylaminomethylphenols.

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Streszczenie

In the 'H NMR spectra of 2-diethylaminomethyl-3,4,6-trichlorophenoi (1) below 260 K, an additional splitting of the CH, signal was found, which can be ascribed to the hindered nitrogen inversion. In the molecule of the 0- methylated derivative (2) this process is fast (on the NMR time-scale) down to 150 K. The frequencies and the activation parameters of the nitrogen inversion in (1) were measured by DNMR, which indicated that the inversion requires a preliminary stage of breaking an intramolecular hydrogen bond. The activation enthalpy, AH:",, of the inversion stage was evaluated as 28.5 f 6.7 kJ mol-'.

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