Deuterium isotope effect on ^{13}C NMR spectra of ortho Mannich bases.

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Streszczenie

The deuterium isotope effect upon ^{13}C NMR spectra was studied for ortho Mannich bases of varying ΔpK_a value [$\Delta pK_a = pK_a(NH^+) - pK_a(OH)$]. The Δ values [$\Delta = \delta^{13}C(OH) - \delta^{13}C(OD)$] for different positions in the phenyl ring are consistent with calculations of charge distribution by means of MNDO — PM3 method and assuming that deuteration leads to a weakening of the hydrogen bonding. In the critical range of ΔpK_a, where the proton transfer appears, the inversion of the sign of the isotope effect for the carbon atom in position 1 takes place. Strong dependence of the Δ value on temperature was revealed for 2-(N,N-diethylaminomethyl)-3,4,5,6-tetrachlorophenol showing the proton transfer equilibrium.

Adres publiczny

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