Thermodynamics of the formation of complexes between aniline derivatives and proton acceptors in solution.

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Streszczenie

The $M^{(0)}$, $M^{(1)}$ and spectral moments of the ν(NH) bands of aniline derivatives as well as their complexes with various proton acceptors in solution were determined in the temperature range 285–330K. Studied compounds were: aniline; 4-metoxytetrafluoraniline; 2,3,5,6-tetrafluoraniline and 4-aminotetrafluorpyridine. The coefficients of linear Y=aT+b regression of the spectral moments $M^{(0)}$, $M^{(1)}$ and with temperature were determined for the free amino groups as well as for 1:1 complexes with various proton acceptors in CCl_4 solutions. An analysis of the influence of temperature on the spectral characteristics of monomers and their 1:1 complexes with various proton acceptors was performed. The heat formation (ΔH_1) of the 1:1 complexes with proton acceptors was determined using the dependence of the equilibrium constants on temperature.On the basis of the “rule of intensity”: the ΔH_2 for the complexes of 1:2 stoichiometry was calculated, allowing the estimation of the relation $\Delta H_1/\Delta H_2$.It was shown that ΔH_1 is larger than ΔH_2 recalculated for a single bond.Comparison of the dynamics characteristics of the N-H bonds in amino groups in complexes of different stoichiometry proves that the hydrogen bonds in 1:1 complexes is stronger than in the complexes of 1:2 stoichoimetry.

Słowa kluczowe

aniline derivatives, hydrogen bonding, spectral characteristics of NH stretching bands, temperature effects, enthalpy of complex formation

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