Dynamic, electooptical and energetic nonequivalency of NH bonds in 1:1 and 1:2 complexes of aminopyridines with proton acceptors.

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The influence of the $–NH_2$ group position in the pyridine ring on the proton donor ability of N–H groups in hydrogen bonding as well as on the spectral behaviour of stretching and bending vibrations of aminopyridines has been studied. The proton donor ability was shown to increase in the row: *meta*-, *ortho*-, and *para*-aminopyridines. It was established tha N–H bonds in *ortho*-aminopyridine were not equivalent, and the evaluation of their dynamic nonequivalence was made. The influence of temperature on the spectral characteristics of the absorption bands of the stretching vibrations of amine groups in the free and hydrogen bonded molecules in CCl_4 has been studied (in temperature range 290–330 K), the formation constants of the complexes have been determined, enthalpy of the 1:1 complexes formation ($-\Delta H_1$) between *ortho*- and *meta*-aminopyridines with dimethylformamide, dimethylsulphoxide and hexamethylphosphoramide has been calculated in temperature range 290–330 K. The 1:2 complexes of *ortho*-, *meta*- and *para*-aminopyridines with acetonitrile, tetrahydrofurane, dimethylsulphoxide, hexamethylphosphoramide were studied at the indoor temperature. Enthalpy of the 1:2 complex ($-\Delta H_2$) was estimated on the basis of 'intensity rule'; $-\Delta H_1=\alpha\Delta B^{1/2}$ assuming that α parameter does not depend on the composition of a complex.The vibrational and electrooptical tasks were solved for the free and H-bounded molecules of aminopyridines as well as its complexes of the 1:1 and 1:2 compositions. Dynamic, electrooptical and energetic nonequivalency of NH bonds of aminogroups in aminopyridines was studied quantitatively. The independent calculations of dynamic constants proved mentioned above nonequivalency of NH bonds.Correlations between spectral characteristics of the absorption bands, geometric, dynamic and electrooptical parameters of $–NH_2$ group in aminopyridines in the free and hydrogen bonded molecules have been established. Those correlations allow to determine the most important molecular characteristics obtained on the basis of spectral measurements in the range of the absorption bands of the stretching vibrations of aminogroup.

Słowa kluczowe

Aminopyridines, Hydrogen bonds, Dynamic, Electrooptical and energetic non equivalency of NH bonds, Correlations

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