

FTIR study of the hydrogen bond symmetry in protonated homodimers of pyridine and collidine in solution.

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Streszczenie

FTIR spectra of the protonated homodimers of pyridine and of 2,4,6-trimethylpyridine in solution in dichloromethane have been studied in the temperature interval from 290 to 160 K. It was found that the frequencies of the symmetrical and antisymmetrical CN vibrations are affected by hydrogen bonding strong enough to discriminate between the spectral pattern of hydrogen bonded and protonated pyridines. The experimental results obtained confirm asymmetric structure of both the systems even in low-polar solvent. Optimized structure, energy, vibrational spectrum and potential energy profile for proton transfer coordinate have been studied by DFT/B3LYP method. The calculation predicts that for the studied homodimers the proton transfer coordinate is involved not only in the stretching vibration $\nu(\text{NH})$, but also in the rings vibrations $\nu(\text{CN})$. As a result, inside a certain interval of the $\text{N}\cdots\text{H}$ distances the frequency of $\nu(\text{CN})$ band should be strongly affected by H/D substitution.

Słowa kluczowe

hydrogen bonding, FTIR spectra, Homodimers, Pyridine–pyridinium complex, Collidine–collidinium complex

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