Influence of hydrogen bonding on the conformation of *ortho*-aminomethylphenol.

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Streszczenie

Intramolecular hydrogen bonding in *ortho*-aminomethylphenol is analysed with the aid of ab initio and density functional theory calculations. Selected properties of the components, phenol and benzylamine, are compared to those of the hydrogen-bonded form of the Mannich base as well as that of the non-hydrogen-bonded structure. Additionally, the gas phase infrared spectrum of benzylamine is analysed in terms of the possible conformations of the molecule.

Słowa kluczowe

Ab initio calculations, Mannich bases, Benzylamine, Ortho-aminomethylphenol, Intramolecular hydrogen bonding

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