Spectroscopic and structural consequences of intramolecular hydrogen bond formation in *ortho*-dimethylaminomethylphenol.

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Streszczenie

Ab initio and density functional calculations are applied to analyse the structure of the Mannich base *ortho*-dimethylaminomethylphenol with emphasis on a detailed description of the properties of the intramolecular hydrogen bond. The calculated structures of the components, phenol and dimethylbenzylamine, are compared to the geometries of the hydrogen-bonded and open forms of the Mannich base. Additionally, the gas-phase infrared spectra of the Mannich base and of dimethylbenzylamine are presented. The experimental spectra are confronted with theoretical infrared spectra and interpreted with the aid of a detailed normal coordinate analysis. Trends in the modifications of computed harmonic force constants upon closure of the intramolecular hydrogen bond are monitored and discussed.

Słowa kluczowe

Ab initio calculations, DFT methods, Mannich bases, Dimethylbenzylamine, Ortho-dimethylaminomethylphenol, Intramolecular hydrogen bonding, Gas-phase IR spectra

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