

On the properties of microsolvated molecules in the ground (S_0) and excited (S_1) states: The anisole-ammonia 1:1 complex

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Streszczenie

State-of-the-art spectroscopic and theoretical methods have been exploited in a joint effort to elucidate the subtle features of the structure and the energetics of the anisole-ammonia 1:1 complex, a prototype of microsolvation processes. Resonance enhanced multiphoton ionization and laser-induced fluorescence spectra are discussed and compared to high-level first-principles theoretical models, based on density functional, many body second order perturbation, and coupled cluster theories. In the most stable nonplanar structure of the complex, the ammonia interacts with the delocalized π electron density of the anisole ring: hydrogen bonding and dispersive forces provide a comparable stabilization energy in the ground state, whereas in the excited state the dispersion term is negligible because of electron density transfer from the oxygen to the aromatic ring. Ground and excited state geometrical parameters deduced from experimental data and computed by quantum mechanical methods are in very good agreement and allow us to unambiguously determine the molecular structure of the anisole-ammonia complex.

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