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Isotopomeric Conformational Changes in the Anisole−Water Complex: New Insights from HR-UV Spectroscopy and Theoretical Studies

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Streszczenie

Resonance enhanced multiphoton ionization and rotationally resolved $S_1 \leftarrow S_0$ electronic spectra of the anisole–^2H_2O complex have been obtained. The experimental results are compared with high level quantum mechanical calculations and with data already available in the literature. Quite surprisingly, the equilibrium structure of the anisole–^2H_2O complex in the S_0 state shows some non-negligible differences from that of the isotopomer anisole– ^1H_2O complex. Actually, the structure of the deuterated complex is more similar to the corresponding structure of the anisole–^1H_2O complex in the S_1 state. In anisole−water, two equivalent H(D) atoms exist as revealed by line splitting in the rotationally resolved spectra. It is possible to suggest a mechanism for the proton/deuteron exchange ruled by a bifurcated transition state for the exchange reaction, with both water hydrogen atoms interacting with the anisole oxygen atom. From the analysis of all of the available experimental data and of computational results, we can demonstrate that in the S_1 excited state the hydrogen bond in which the water molecule acts as an acid is weaker than in the electronic ground state but is still the principal interaction between water and the anisole molecules.

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