

Spectroscopic and Computational Studies of the Intramolecular Hydrogen Bonding of 2-Indanol

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Abstract

2-Indanol in its most stable form is stabilized by internal hydrogen bonding, which exists between the hydroxyl hydrogen atom and the π -cloud of the benzene ring. A comprehensive *ab initio* calculation using the MP2/cc-pVTZ level of theory showed that 2-indanol can exist in four possible conformations, which can interchange through the ring-puckering vibration and the internal rotation of the OH group on the five-membered ring. A potential energy surface in terms of these two vibrational coordinates was calculated. Density functional theory calculations were used to predict the vibrational frequencies and to help in normal mode assignments. Fluorescence excitation spectra of 2-indanol confirm the presence of the four conformers in the electronic ground and excited states. The spectral intensities indicate that 82% of the molecules exist in its most stable form with the intramolecular hydrogen bonding. The other isomers are present at approximately 11, 5, and 3%. The MP2/6-311++G(d,p) calculation predicts a distribution of 70, 13, 9, and 8% at 90°C, the experimental sample temperature.

Keywords: 2-indanol, intramolecular hydrogen bonding, *ab initio* calculations, internal rotation, vibrational spectra, fluorescence spectra, ring-puckering