Abstract Submitted
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**Spectroscopic and *ab initio* studies on the conformations and intramolecular hydrogen bonding of 2-indanol**[1] ABDULAZIZ A. AL-SAADI, MARTIN WAGNER, JAAN LAANE, Department of Chemistry, Texas A&M University, College Station, TX 77843-3255 — Infrared, Raman, ultraviolet absorption, and laser induced fluorescence (LIF) spectroscopies have been used along with theoretical calculations to study the structure and conformations of 2-indanol in its ground and excited electronic states. This molecule possesses an alcoholic OH group which can weakly hydrogen bond to its benzene ring. Both the calculations and the LIF of the jet-cooled molecules show that there are four stable conformers of this molecule which can interconnect through the ring-puckering and internal rotation vibrations. A two-dimensional potential energy surface was generated from the MP2 *ab initio* calculations to depict the energetics of the conformational changes. The conformer with the intramolecular hydrogen bonding has the lowest energy by about 500 $cm^{-1}$ (1.4 kcal/mole) in the $S_0$ state. The ring-puckering frequencies for the different conformers range from 80 to 92 $cm^{-1}$.

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