

Abstract Submitted
for the TSF13 Meeting of
The American Physical Society

Spectroscopic and Theoretical Determination of the Structure of 2,6-Difluoropyridine in Its Ground and Excited Electronic States JAAN LAANE, HONG-LI SHEU, Texas A&M Univ, SUNGHWAN KIM, Hanyang University — The infrared and Raman spectra of 2,6-difluoropyridine (26DFPy) along with *ab initio* and DFT computations have been used to assign the vibrations of the molecule in its S_0 electronic ground state and to calculate its structure. The ultraviolet absorption spectrum showed the electronic transition to the $S_1(\pi,\pi^*)$ state to be at $37,820.2\text{ cm}^{-1}$. With the aid of *ab initio* computations the vibrational frequencies for this excited state were also determined. TD-B3LYP and CASSCF computations for the excited states were carried out to calculate the structures for the $S_1(\pi,\pi^*)$ and $S_2(n,\pi^*)$ excited states. The CASSCF results predict that the $S_1(\pi,\pi^*)$ state is planar and the $S_2(n,\pi^*)$ state has a barrier to planarity of 256 cm^{-1} . The TD-B3LYP computations predict a barrier of 124 cm^{-1} for the $S_1(\pi,\pi^*)$ states, but the experimental results support the planar structure. Hypothetical models for the ring-puckering potential energy function were calculated for both electronic excited states to show the predicted quantum states. The changes in the vibrational frequencies in the two excited states reflect the weaker π bonding within the pyridine ring.

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Date submitted: 05 Sep 2013

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