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Ultraviolet Absorption Spectra and the Quasi-planarity of Pyridine and its d_5 Isotopomer in its $S_1(\pi,\pi^*)$ Excited State[1] PRAVEEN BOOPALACHANDRAN, KATHLEEN MCCANN, JAAN LAANE, Texas A&M University, College Station, Texas — The ultraviolet absorption spectra of pyridine-d_0 and $-d_5$ vapor have been recorded and analyzed in the 32,000 to 38,000 cm^{-1} region. The electronic band origins are at 34,767 (d_0) and 34,945 cm^{-1} (d_5) for the two isotopomers. For both molecules series of transitions for ν_{18}, the out-of-plane ring-bending vibration, in the excited electronic state can be observed, and a one-dimensional potential energy function of the form $V = ax^4 - bx^2$ can be determined, where x is the out-of-plane vibrational coordinate. In the S_0 electronic ground state pyridine is rigid and planar with ν_{18} at 403 cm^{-1}. In the $S_1(\pi,\pi^*)$ excited state ν_{18} drops to 59.5 cm^{-1} and the molecule becomes floppy with a tiny barrier to planarity of 3 cm^{-1} resulting in a quasi-planar structure.

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