INVESTIGATION OF INTERMOLECULAR HYDROGEN BONDING IN THE 2-PYRIDONE DIMER VIA PULSED TERAHERTZ SPECTROSCOPY

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The terahertz spectrum (10 - 140cm-1) of 2-pyridone (2PD) in a carbon tetrachloride solution was obtained. Theoretical structures, spectra, and binding energies were calculated using both MP2 and DFT methods and reveal that the strong absorption at 115 cm-1 arises from an intermolecular in-plane rocking of 2PD dimer. However, there is additional intensity in the 2PD experimental spectrum that is not accounted for by theoretical predictions of the dimer alone. A hydrogen-bonded 2PD tetramer could be the source of this anomalous intensity and calculations of the proposed structure and vibrations will be presented.