FAR-INFRARED SPECTRA AND TWO-DIMENSIONAL POTENTIAL ENERGY SURFACES FOR THE OUT-OF-PLANE RING VIBRATIONS OF TETRAHYDROFURAN-3-ONE IN ITS S0 AND $S_1(n,\pi^*)$ ELECTRONIC STATES

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The far-infrared spectra of tetrahydrofuran-3-one show ring-bending (100 - 120 cm^{-1}), ring-twisting (227 - 237 cm^{-1}), difference (115 - 137 cm^{-1}), sum (320 - 350 cm^{-1}) and overtone (200 - 225 cm^{-1}) bands. A two-dimensional potential energy surface for the twisting and bending was determined and this has minima corresponding to twisted conformations. A potential energy surface for the $S_1(n,\pi^*)$ excited state, based on previous fluorescence excitation data, was also calculated.