VIBRATIONAL SPECTRA AND THEORETICAL CALCULATIONS FOR 2-METHYLCYCLOPENTANONE

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The liquid and vapor phase far-infrared, mid-infrared and Raman spectra of 2-methylcyclopentanone have been recorded and analyzed. Semi-empirical (MM3) and ab-initio (Gaussian 94) calculations have also been performed to help assign the ground state spectra and predict ground state conformations. The low frequency modes were of special interest: the ring bending (75 cm^{-1}), the ring twisting (251 cm^{-1}), and the methyl torsion (209 cm^{-1}). Preliminary fluorescence studies of the C=O inversion in the $S_1(n,\pi^*)$ state have been carried out.