## LASER SPECTROSCOPY, *AB INITIO* CALCULATIONS AND VIBRATIONAL ASSIGNMENTS OF SOME DERIVATIVES OF 2-OXAZOLIN-5-ONES

<u>V. B. SINGH</u>, Department of Physics, Udai Pratap Autonomous College, Varanasi 221002; A. K. RAI, S. B. RAI, Department of Physics, Banaras Hindu University, Varanasi-221005; K. N. SINGH, Department of Chemistry, Banaras Hindu University, Varanasi-221005.

The spectroscopic properties of some derivatives of 2-oxazolin-5-ones have been investigated by a combination of experimental spectroscopic methods and *ab initio* calculations. Vibrational assignments for the ground state of some of these organic molecules have been carried out using Raman spectra and ab initio calculations. A splitting in the carbonyl group (C=O stretching) frequency observed in the vibrational spectra, is explained as Fermi-resonance. Conformational studies regarding the effect of moving the methoxy group in the 2-phenyl-4-(4-methoxy benzylidene)-2-oxazolin-5- one molecule to a different position on the ring has been carried out. The strong fluorescence and the observation of a circular ring around the incident laser radiation indicate some probable stimulated process in the above organic derivative. Laser spectroscopic study of some of these molecules is presently in progress.