TORSIONAL POTENTIALS, BARRIER TO INTERNAL ROTATION, MOLECULAR STRUCTURE, VIBRATIONAL PROPERTIES, NLO BEHAVIOUR AND NBO CHARACTERISTICS OF 2-(PHENYLSULFONYL)VINYLBENZENE AND 2-(TOSYL)VINYLBENZENE EMPLOYING FT-IR, FT RAMAN SPECTRAL TECHNIQUES AND DFT APPROACH

K SRISHAILAM, *PHYSICS, SR UNIVERSITY, HANAMKONDA, TELANGANA, INDIA*; BALAKRISHNA AEGURLA, *Department of Chemistry, Indian Institute of Technology , Roorkee, Uttarakhand, India*; BYRU VENKATRAM REDDY, G. RAMANA RAO, *Department of Physics, KAKATIYA UNIVERSITY, WARANGAL, India*.

2-(Phenylsulfonyl)vinylbenzene (2PVB) and 2-(Tosyl)vinylbenzene(2TVB) molecules were characterized, by recording their FT-IR(4000-400 cm^{-1}) and FT Raman(4000-50 cm^{-1}) spectra. Torsional potentials, barrier to internal rotation around phenyl-sulfonyl C-S bond, sulfonyl-vinyl S-C bond, vinyl-benzene C-C bond, and phenyl-methyl C-C bond (this bond is relevant for 2TVB only). Optimized structure parameters, general valence force field, harmonic vibrational fundamentals, potential energy distribution, infrared and Raman intensities, frontier molecular orbital parameters, NLO behaviour and NBO characteristics were determined using density functional theory, employing B3LYP exchange-correlation in conjunction with functional 6-311++G(d,p) basis set. Time dependent DFT was made use of to compute absorption maxima (λmax) and oscillator strengths, for both molecules, in their electronic transitions, in DMSO-d6 solution. Good agreement was found, between measured and computed parameters involving structure parameters, IR and Raman spectra and UV-Vis transitions. The rms error between experimental and theoretical vibrational frequencies was 6.4 and 4.35 cm^{-1}), for 2PVB and 2TVB, respectively. With the help of PED and eigenvectors, all vibrational fundamentals of both the molecules were assigned for the first time. The computations demonstrated that both the molecules were good for NLO applications, that was substantiated by NBO analysis for both 2PVB and 2TVB.