Solvent effects on chiroptical properties of carbonyl functional group molecules WATHEQ AL-BASHEER, RICHARD PAGNI, ROBERT COMPTON, The University of Tennessee — Solvent effects on Optical Rotatory Dispersion (ORD) and Circular Dichroism CD of carvone enantiomers and R-(+)-3-methylcyclopentanone (R3MCP) are studied for 35 common solvents. Solvent effects are significantly attributed to the solute-solvent electrostatic and Van der waals interactions. Hartree-Fock and Density Function theoretical calculations of R3MCP CD and ORD in solvation are also employed to support the experimental findings and observed to have good agreement with experimental results. Enantiomers (R,S) of chiral molecules are known to exhibit optical activity effects which are equal in magnitude and opposite in sign. For some carbonyl molecules (possessing C=O) the equatorial and axial conformers also exhibit CD and ORD of opposite sign but not necessarily the same absolute magnitude for the $n \rightarrow \pi^*$ ($n \rightarrow 3s$) molecular transition. Temperature dependent variations of CD and Raman spectra are shown to be a useful technique to study the conformer’s populations and energy difference of R3MCP. Thermodynamic constants of R3MCP in 35 solvents, will be presented and related to solvent polarity parameters.