Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

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 (*R*3MCP) 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 *R*3MCP 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 *R*3MCP. Thermodynamic constants of *R*3MCP in 35 solvents, will be presented and related to solvent polarity parameters.

Watheq Al-Basheer
The University of Tennessee

Date submitted: 28 Nov 2006 Electronic form version 1.4