Abstract Submitted
for the DAMOP07 Meeting of
The American Physical Society

Molecular Conformation of Optically Active Five and Six-Membered-Ring Ketones WATHEQ AL-BASHEER, The Hashemite University, Zarqa 13115, Jordan, RICHARD PAGNI, ROBERT COMPTON, The University of Tennessee, Knoxville — Conformational analysis of chiral five and six – membered - ring ketones will be presented. Electronic circular dichroism (CD) and vibrational circular dichroism (VCD) spectra for both *R*- and *S*- enantiomers of optically active carvone ($C_{10}H_{14}O$) exhibit marked temperature dependences. Theoretical calculations, using density functional theory (B3LYP with aug-cc-pVDZ basis set), show an equal magnitude but opposite *sign* for the CD and VCD for the two conformers of each *R*- and *S*- enantiomer. The Temperature dependent circular dichroism (CD) measurements of *R*-(+)-3-methylcyclopentanone *R*3MCP in 36 different common solvents is being employed to determine the conformers energy between the equatorial methyl and axial methyl of *R*3MCP and carvone. The results will be compared to the CD in the gas phase, solvent effect on optical rotation of *R*3MCP and carvone will be demonstrated and supported by DFT calculations. Temperature dependent vibrational Raman spectroscopy in the C-H stretch region is used to study conformation over a wide range of temperature (-15-135 $^{\circ}$C) and at liquid nitrogen temperature. Temperature dependent variations of CD and Raman spectra are shown to be a useful technique to study the conformer's populations and energy difference.

Watheq Al-Basheer
The Hashemite University, Zarqa 13115, Jordan

Date submitted: 29 Jan 2007 Electronic form version 1.4