Abstract Submitted
for the DAMOP06 Meeting of
The American Physical Society

Temperature Dependent Electronic and Vibrational Circular Dichroism of Carvone and Limonene WATHEQ AL-BASHEER, The University of Tennessee, JIANGTAO HE, PRASAD POLAVARAPU, Vanderbilt University, RICHARD PAGNI, ROBERT COMPTON, The University of Tennessee — Circular dichroism (CD) involves the differential absorption of right –and left-circularly polarized light by chiral molecules. Electronic circular dichroism (CD) and vibrational circular dichroism (VCD) spectra for both R- and S- enantiomers of optically active carvone ($C_{10}H_{14}O$) and limonene ($C_{10}H_{16}$) exhibit marked temperature dependences. The temperature dependence is due to the presence of both axial and equatorial conformations. Theoretical calculations, using density function 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 energy difference between the two conformers is also determined from these data (van t'Hoff plot) which show good agreement with values obtained by other spectroscopic methods. In addition, temperature dependent infrared absorption and Raman spectra for carvone and limonene will be used to further strengthen the conclusions from of the CD and VCD methods.

Watheq Al-basheer
The University of Tennessee

Date submitted: 27 Jan 2006 Electronic form version 1.4