Abstract Submitted
for the DAMOP06 Meeting of
The American Physical Society

An investigation of electron helicity density in bromocamphor and dibromocamphor as a source of electron circular dichroism[1] ADAM SCHEER, GORDON GALLUP, TIMOTHY GAY, University of Nebraska — Using electron transmission spectroscopy (ETS), we have measured the vertical attachment energies (VAEs) of bromocamphor and dibromocamphor. We have also performed quantum chemical calculations to obtain the virtual orbital energies (VOEs) of camphor, bromocamphor and dibromocamphor. With scaling based on the trend between VAEs and VOEs of previously studied chloroalkanes, we have assigned the resonances observed in ETS to temporary occupation of specific normally empty orbitals. Further calculations were conducted to determine the helicity densities of bromocamphor and dibromocamphor. We find large helicity densities in the regions of large wave function amplitude of the normally unoccupied orbitals responsible for resonances in the scattering cross sections. Our ETS assignments and helicity density results are compared with the chiral asymmetry data observed in electron-circular dichroism experiments by the Münster group [1]. Evidence is seen to support helicity density as a source for chiral asymmetry at certain resonance positions in bromocamphor and dibromocamphor. [1] C. Nolting, S. Mayer, and J. Kessler, J. Phys. B **30**, 5491 (1997).

[1]This work was supported by the NSF under grant PHY-0354946.

Adam Scheer
University of Nebraska

Date submitted: 01 Feb 2006 Electronic form version 1.4