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A study of the chiro-optical properties of Carvone JASON LAMBERT, University of Tennessee — The intrinsic optical rotatory dispersion (IORD) and circular dichroism (CD) of the conformationally flexible carvone molecule has been investigated in 17 solvents and compared with results from calculations for the "free" (gas phase) molecule. The G3 method was used to determine the relative energies of the six conformers. The ORD of (*R*)-(-)-carvone at 589 nm was calculated using coupled cluster and density-functional methods, including temperature-dependent vibrational corrections. Vibrational corrections are significant and are primarily associated with normal modes involving the stereogenic carbon atom and the carbonyl group, whose $n \rightarrow \pi^*$ excitation plays a significant role in the chiroptical response of carvone. However, without the vibrational correction the calculated ORD is of opposite sign to that of the experiment for the CCSD and B3LYP methods. Calculations performed in solution using the PCM model were also opposite in sign to of the experiment when using the B3LYP density functional.

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