A COMPARATIVE STUDY OF CHIRAL ANALYSIS OF FENCHYL ALCOHOL USING NUCLEAR MAGNETIC RESONANCE, INFRARED, AND ROTATIONAL SPECTROSCOPY

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The analysis of chiral molecules with multiple chiral centers is a challenging problem in analytical chemistry. The goal of the analysis is to determine the fractional composition for each unique stereoisomer. In the most general case, a molecule with N chiral centers will have 2^N distinct stereoisomers. Half of these, 2^{N-1}, will be molecules with distinct molecular structures (the diastereomers). The diasteormer composition can be analyzed by normal spectroscopy methods because they have distinct spectra. For each diastereomer, there are the two non-superimposable mirror images (the enantiomers) and additional measurement methodology is required to determine the enantiomeric ratio using spectroscopy. Furthermore, in many applications the "unwanted" isomers (diastereomers and/or enantiomers) will be present as low-abundance impurities placing strong demands on the dynamic range of the spectroscopic technique. A commercial sample of (1R)-endo-(+)-Fenchyl alcohol (C10H18O, four stereoisomers) has been analyzed using nuclear magnetic resonance (NMR), infrared (IR), and rotational spectroscopy. The commercial sample has a small amount (3%) of the diastereomer as an impurity. The ability to quantitatively identify the diastereomer impurity using quantum chemistry estimates of the NMR, IR, and rotational spectrum parameters will be discussed. The enantiomer analysis uses chiral resolving agents for NMR spectroscopy, vibrational circular dichroism (VCD) for IR spectroscopy, and chiral tag rotational spectroscopy. The ability of these techniques to verify the stereochemistry of the dominant (1R)-endo-(+)-Fenchyl alcohol will be discussed. The ability to identify the enantiomeric excess of fenchyl alcohol and the possibility of performing enantiomer analysis on the low abundance diastereomer using the direct sample without purification will also be presented.