CHIRAL ANALYSIS OF MOLECULES WITH MULTIPLE CHIRAL CENTERS USING CHIRAL TAG ROTATIONAL SPECTROSCOPY

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One major challenge in analytical chemistry is the quantitative determination of the ratio of all stereoisomers in a molecule with multiple chiral centers. The analysis is especially challenging if there are no reference samples available for calibration. In general, a molecule with N chiral centers has 2^N stereoisomers. There are 2N-1 distinct structures, the diastereomers, that can be distinguished by traditional rotational spectroscopy. Each diastereomer exists in two non-superimposable mirror images – the enantiomers. Menthone is a simple case of a molecule with two asymmetric carbons. The two diastereomers are known as menthone and isomenthone and each is chiral. The full analysis of the stereoisomers of several commercial samples has been performed using chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW). To determine the diastereomer ratio it is necessary to determine all conformers of the molecule with appreciable population in the pulsed jet sample. The present work expands on previous efforts to assign the lowest conformers of the menthone and isomenthone by analyzing two additional conformers of isomenthone.[1] For a commercial sample where the diastereomer ratio was reported in the Certificate of Analysis, we obtained a menthone and isomenthone composition of 82.8+/-0.9

[1] Schmitz, D.; Shubert, V.A.; Betz, T.; Schnell, M., "Exploring the conformational landscape of menthol, menthone, and isomenthone: a microwave study", Frontiers in Chemistry 3, 1-13 (2015). [2] Shubert, V.A., Schmitz, D, Schnell, M., "Enantiomer-sensitive spectroscopy and mixture analysis of chiral molecules containing two stereogenic centers – Microwave three-wave mixing of menthone", J. Mol. Spectrosc. 300, 31-36 (2014).