

A BROADBAND ROTATIONAL SPECTROSCOPIC AND THEORETICAL STUDY OF CIS AND TRANS (-)-CARVEOL

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Carveol, a primary constituent in spearmint and peppermint oil, is a monocyclic monoterpene alcohol that is produced in nature by the photooxidation of limonene.¹ Structurally, carveol contains two chiral centers with three substituents (methyl group, hydroxyl group, and propylene group) attached to its cyclohexane ring. The combination of the three flexible substituents, ring puckering, and two chiral centers introduce a complex conformational topography that is non-trivial to elucidate. However, a thorough study of the topology of chiral carveol may provide valuable insights into complex conformational dynamics, as well as chirality recognition studies. We believe chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW) is an excellent tool for this investigation as it is able to unambiguously distinguish structural conformers within a complex mixture.² The broadband rotational spectrum of cis and trans (-)-carveol was recorded using a chirped pulse Fourier Transform microwave spectrometer in the 2-6 GHz region.³ To aid in experimental assignment, a theoretical conformational search was carried out using a combination of a two dimensional potential energy scan, which scans over the propylene group and hydroxyl group, and the Conformer–Rotamer Ensemble Sampling Tool (CREST).⁴ The theoretical results yielded a total of 23 conformers for the trans and 19 for the cis. Utilizing these results, a total of five experimental conformers were then assigned: two for the trans conformer and three for the cis conformer. For trans, it was determined both experimental conformers occupy the equatorial position. For the cis conformer, two equatorial and one axial conformer was experimentally assigned. The conformational cooling pathways and intermolecular interactions within each conformer were also analyzed to further understand the conformational landscape of cis and trans (-)-carveol.

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