THE CONFORMATIONAL BEHAVIOUR OF THE ODORANT DIHYDROCARVEOL

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The odorant dihydrocarveol ($C_{10}H_{18}O$) has been investigated in the gas phase using a 2-8 GHz chirped-pulse Fourier transform microwave spectrometer. Dihydrocarveol was purchased as a mixture of n-, iso-, neo-, and neoiso- isomers. The sample was placed in a bespoke heating nozzle at about 85°C and seeded in Ne at 5 bar. Three conformers were observed and their rotational constants were determined. By comparing the experimental rotational constants with those calculated ab initio the three conformers were identified as belonging to n-dihydrocarveol. In all three conformers the isopropenyl group is in equatorial position with respect to the six-membered ring, and the OH group maintains the same configuration. The conformers differ in the orientation of the isopropenyl group.