THE STRUCTURE AND MOLECULAR PARAMETERS OF CAMPHENE DETERMINED BY FOURIER TRANSFORM MICROWAVE SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS

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The emission of volatile organic compounds, from plants has strong revelance for plant physiology, plant ecology and atmospheric chemistry.[a] Camphene ($C_{10}H_{16}$) is a bicyclic monoterpene which is emitted in the atmosphere by biogenic sources.[bc] The structure of the unique stable conformer was optimized using density functional theory and *ab initio* calculations. The rotational spectrum of camphene was recorded in a supersonic jet expansion with a Fourier transform microwave spectrometer over the range 2-20 GHz. Signals from the parent species and from the ten ^{13}C isotopomers were observed in natural abundance. The rotational and centrifugal distortion parameters were fitted to a Watson's Hamiltonian in the A-reduction. A magnetic hyperfine structure associated with the pairs of hydrogen nuclei in the methylene groups was observed and modeled.

The rotational constants coupled to the equilibrium structure calculations were used to determine the r_0 and the $r_m^{(1)}$ gas-phase geometries of the carbon skeleton. The present work provides the first spectroscopic characterization of camphene in the gas phase and these results are also relevant for ozonolysis kinetics study through Criegee intermediates.[d]

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