GAS-PHASE STRUCTURES OF LINALOOL AND COUMARIN STUDIED BY MICROWAVE SPECTROSCOPY

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The microwave spectra of two natural substances, linalool and coumarin, were recorded in the microwave range from 9 to 16 GHz and 8.5 to 10.5 GHz, respectively.

Linalool is an acyclic monoterpene and the main component of lavender oil. It has a structure with many possible conformations. The geometry of the lowest energy conformer has been determined by a combination of microwave spectroscopy and quantum chemical calculations. Surprisingly, a globular rather than a prolate shape was found. This structure is probably stabilized by a π interaction between two double bonds which are arranged in two stacked layers of atoms within the molecule. A-E splittings due to the internal rotation of one methyl group could be resolved and the barrier to internal rotation was determined to be 400.20(64) cm^{-1}. The standard deviation of the fit was close to experimental accuracy. For an identification of the observed conformer not only the rotational constants but also the internal rotation parameters of one of the methyl groups were needed.

Coumarin is a widely used flavor in perfumery as sweet woodruff scent. The aromatic structure allows solely for one planar conformer, which was found under molecular beam conditions and compared to other molecules with similar structures. Here, the rotational spectrum could be described by a set of parameters including the rotational constants and the centrifugal distortion constants using a semi-rigid molecule Hamiltonian. Furthermore, the rotational transitions of all nine ^{13}C isotopologues were measured in natural abundance. As a consequence, the microwave structure of coumarin could be almost completely determined.