

MICROWAVE SPECTROSCOPY OF MONOTERPENES OF ATMOSPHERIC INTEREST: α -PINENE, β -PINENE, AND NOPINONE

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Several monoterpenes and terpenoids are biogenic volatile organic compounds which are emitted in the atmosphere, and react with OH, O₃, NO_x, etc. to give rise to several oxydation and degradation products. Spectroscopic information on these atmospheric species are still very scarce. Meanwhile we have demonstrated that combining quantum calculations to microwave spectroscopy led to the unambiguous characterization of the most stable conformers for perillaldehyde,^a limonene and carvone.^b This information can be used to subsequently model accurately the vibrational signature for atmospheric purposes.^c

We have recorded the pure rotational spectra of α -pinene and β -pinene (C₁₀H₁₆), and of nopinone (C₉H₁₄O), using the MB-FTMW spectrometer of Lille, in the 2-20 GHz range at temperatures varying between 340 and 380 K. For these three bicyclic molecules only one conformer can be observed, and the rotational structure was observed up to J, K_a = 8, 3 ; 8, 4 ; 8, 5, respectively. All the spectra were modeled with a semi-rigid rotor Hamiltonian and fitted to obtain a rms value better than 5 kHz using a-, b- and c- type transitions.

All the experimental results were supported by several quantum calculations performed at different levels of theory (DFT and ab initio). In particular no experimental evidence of internal rotation motion was found (methyl groups), in good agreement with the calculated barriers.

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