GAS-PHASE MOLECULAR STRUCTURE OF NOPINONE AND ITS WATER COMPLEXES STUDIED BY MICROWAVE FOURIER TRANSFORM SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS

ELIAS M. NEEMAN, JUAN-RAMON AVILES MORENO, T. R. HUET, *UMR 8523 CNRS - Universités des Sciences et Technologies de Lille, Laboratoire PhLAM, 59655 Villeneuve d'Ascq, France*.

Several monoterpenes and terpenoids are biogenic volatile organic compounds which are emitted in the atmosphere, where they react with OH, O_3 and NO_x etc. to give rise to several oxidation and degradation products.[a] Their decomposition products are a major source of secondray organic aerosol (SOA).[b] Spectroscopic information on these atmospheric species is still very scarce. The rotational spectrum of nopinone ($C_9H_{14}O$) one of the major oxidation products of β-pinene,[c] [d] and of its water complexes were recorded in a supersonic jet expansion with a Fourier transform microwave spectrometer over the range 2-20 GHz. The structure of the unique stable conformer of the nopinone was optimized using density functional theory and *ab initio* calculations. Signals from the parent species and from the ^{13}C and ^{18}O isotopomers were observed in natural abundance. A magnetic hyperfine structure associated with the pairs of hydrogen nuclei in the methylene groups was observed and modeled.
The structures of several conformers of the nopinone-water complexes with up to three molecules of water were optimized using density functional theory and *ab initio* calculations. The energetically most stable of calculated conformers were observed and anlyzed. The rotational and centrifugal distortion parameters were fitted to a Watson's Hamiltonian in the A-reduction. The present work provides the first spectroscopic characterization of nopinone and its water complexes in the gas phase.

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