INVESTIGATION OF THE MICROSOLVATION OF SECONDARY ORGANIC AEROSOL PRECUSORS: MICROWAVE SPECTROSCOPY OF NITROMETHOXYPHENOLS HYDRATES

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Atmospheric aerosol particles strongly influence the Earth´s atmosphere, and their contribution to climate change is versatile. Especially, Secondary Organic Aerosols (SOAs) play a major role in the radiative budget and the clouds formation through their hygroscopic properties and atmospheric chemistry.[1] Methoxyphenols (lignin´s monomer) represent a significant part of biomass burning emissions. Recent works have shown that SOAs are formed by oxidation of methoxyphenols such as guaiacol and nitro-guaiacols (NG) are the main oxydation products yielding to SOAs with an hydrophobic character.[2]

We present here the rotational spectroscopy of 4- and 5-NG isomers studied using a free jet Fabry-Perot Fourier-transform microwave (FP-FTMW) spectrometer (2 to 20 GHz) with the support of quantum chemistry calculations. The observation of the hyperfine structure induced by the presence of a ^{14}N nucleus allowed us to simulate the nuclear quadrupole coupling constants in addition to the Watsonian rotationnal parameters. Each isomer shows only one planar conformer stabilized by an intramolecular hydrogen bond as already observed for guaiacol.[3] However, the position of the nitro-group seems to influence the global stability of the molecule. The microsolvation of 4-NG with water has been investigated, unveiling only one monohydrate complex in agreement with the demonstrated hydrophobic character of 4-NG aerosols.[3] The study of the hydration of 5-NG is ongoing as well as the study of the less volatile 4-nitro-syringol, a precursor with more hydrophilic SOAs than NG.[4]

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[2] doi:10.1364/AO.56.00E116, W. Ahmad *et al.*, Infrared spectroscopy of secondary organic aerosol precursors and investigation of the hygroscopicity of SOA formed from the OH reaction with guaiacol and syringol, *Applied Optics*, **56**, E116-E122 (2017)

[3] doi:10.1063/1.5089426, A. Jabri *et al.*, Conformational landscape and inertial defect of methoxyphenol isomers studied by mm-wave spectroscopy and quantum chemistry calculations, *The Journal of Chemical Physics*, **150**,10, 104303 (2019)

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