INTERACTIONS OF ATMOSPHERIC POLLUTANTS WITH WATER: 4-METHYL-2-NITROPHENOL AND ITS WATER COMPLEX STUDIED BY MICROWAVE SPECTROSCOPY AND QUANTUM CHEMISTRY

E. ANTONELLI,[1] **S. BAWEJA,**[2] **S. HUSSAIN,**[2] **A. FERNANDEZ-RAMOS,**[3] **I. KLEINER,**[4] **H. V. L. NGUYEN,**[1,5] **M. E. SANZ**[2], [1]*Univ Paris Est Créteil and Université Paris Cité, CNRS, LISA, F-94010 Créteil, France,* [2]*Department of Chemistry, King's College London, Britannia House, 7 Trinity Street, London SE1 1DB, UK,* [3]*Departamento de Química Física and Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS), Jenaro de la Fuente s/n, Universidad de Santiago de Compostela, 15782 Santiago de Compostela, Spain,* [4]*Université Paris Cité and Univ Paris Est Créteil, CNRS, LISA, F-75013 Paris, France,* [5]*Institut Universitaire de France (IUF), F-75231 Paris, France*

The microwave spectrum of 4-methyl-2-nitrophenol (4MNP) and its complex with one water molecule was measured by a molecular jet chirped-pulse Fourier transform microwave (FTMW) spectrometer working in the frequency range from 2 to 8 GHz and for the monomer, a resonator FTMW spectrometer from 2 to 26.5 GHz in addition. Quantum chemical calculations were performed at the B3LYP-D3BJ/6-311++G(d,p) and MP2/6-311++G(d,p) levels of theory to obtain optimized molecular geometries. One conformer for 4MNP and two different isomers for 4MNP-H_2O were identified in the rotational spectrum. Large tunneling splittings arising from the low barrier to internal rotation of the methyl group and hyperfine structures from the quadrupole coupling of the ^{14}N nucleus were observed for all species. The spectra were analyzed and fitted using the *XIAM*[1] and *BELGI-C_s-hyperfine*[2] codes. The standard deviations of the fits achieve measurement accuracy of 4 kHz for the monomer and 10 kHz for the water complexes. The deduced V_3 potential values of 106 cm^{-1} for the monomer and the more stable water complex as well as 158 cm^{-1} for the second water complex are in reasonable agreement with the values predicted by quantum chemistry.

[1] doi:10.1515/zna-1996-0807, H. Hartwig, H. Dreizler, *Z. Naturforsch.*, **51**, 923-932 (1996).

[2] doi:10.1021/acs.jpca.6b02111, R. Kannengießer, W. Stahl, H.V.L. Nguyen, I. Kleiner, *J. Phys. Chem. A*, **120**, 3992-3997 (2016).