

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

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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-H₂O 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 ¹⁴N nucleus were observed for all species. The spectra were analyzed and fitted using the XIAM¹ and BELGI-C_s-hyperfine² 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 V₃ 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](https://doi.org/10.1515/zna-1996-0807), H. Hartwig, H. Dreizler, Z. Naturforsch., **51**, 923-932 (1996).

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