PROBING VITAMINE C, ASPIRIN AND PARACETAMOL IN THE GAS PHASE: HIGH RESOLUTION ROTATIONAL STUDIES

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A solid sample of Vitamin C (m.p. 190 °C) vaporized by laser ablation has been investigated in gas phase and characterized through their rotational spectra. Two spectroscopy techniques has been used to obtain the spectra: a new design of broadband chirped pulse Fourier transform microwave spectroscopy with in-phase/quadrature-phase-modulation passage-acquired-coherence technique (IMPACT) and conventional laser ablation molecular beam Fourier transform microwave spectroscopy (LA-MB-FTMW).[a] Up to now, two low-energy conformer have been observed and their rotational constants determined. Ab initio calculations at the MP2/6-311++G (d,p) level of theory predicted rotational constants which helped us to identify these conformers unequivocally.
Among the molecules to benefit from the LA-MB-FTMW technique there are common important drugs never observed in the gas phase through rotational spectroscopy. We present here the results on acetyl salicylic acid and acetaminophen (m.p. 136 °C), commonly known as aspirin and paracetamol respectively. We have observed two stable conformers of aspirin and two for paracetamol. The internal rotation barrier of the methyl group in aspirin has been determined for both conformers from the analysis of the A-E splittings due to the coupling of internal and overall rotation.

[a] J. L. Alonso, C. Pérez, M. E. Sanz, J. C. López, S. Blanco, *Phys. Chem. Chem. Phys.* **11**,617-627 (2009)and references therein