GAS-PHASE CONFORMATIONAL LANDSCAPE OF THE ANAESTHETICS PROPOFOL, BENZOCAINE AND BENZOCAINE···WATER USING ULTRA-BROADBAND CHIRP-PULSE MICROWAVE SPECTROSCOPY

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We report the investigation of the gas-phase conformational landscape of the anaesthetics propofol (2,6-diisopropylphenol), benzocaine (ethyl 4-aminobenzoate) and benzocaine···water with the ultra-broadband chirp-pulse microwave spectrometer developed at the University of Virginia. Configurations with detection bandwidths of either 2-8 GHz or 7-18 GHz were used in this work. For propofol, two conformers originated by the internal rotation of the two isopropyl groups were detected in the jet-cooled rotational spectrum. The most stable conformer exhibits an inversion tunnelling caused by a large-amplitude motion of the hydroxyl group. Analysis of the rotation-inversion transitions led to the energy difference between the tunnelling states and barrier height. For benzocaine, 2 conformers with *gauche* and *trans* orientation of the ester ethyl group were detected, resolving the small hyperfine effects due to ^{14}N nuclear quadrupole coupling. Microsolvation of benzocaine offers competitive hydrogen bonding sites at the carbonyl and ether oxygens, the amino group atoms and the aromatic π electron system. Preliminary analysis of the rotational spectrum of benzocaine··· water shows evidence of a first conformer, with water acting as proton donor to the carbonyl group of the most stable conformer of benzocaine. Further results and supporting *ab initio* calculations will be presented at the Conference.