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.