

## CONFORMATIONAL BEHAVIOUR OF m-ANISALDEHYDE AND ITS MICROSOLVATES

ANDRES VERDE, JUAN CARLOS LOPEZ, SUSANA BLANCO, *Departamento de Química Física y Química Inorgánica - I.U. CINQUIMA, Universidad de Valladolid, Valladolid, Spain.*

The rotational spectra of m-anisaldehyde and its microsolvated complexes generated in a supersonic jet have been studied by chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW) in the 2-8 GHz region. Four conformers have been detected for the monomer. The three most intense rotamers have line intensities high enough to allow the observation of the monosubstituted  $^{13}\text{C}$  isotopologues in natural abundance allowing the determination of their  $r_e$ ,  $r_s$  and  $r_m$  structures. When allowing water vapor to expand in the supersonic jet, the spectra of ten new species assigned to microsolvated complexes appear. Seven monohydrated species have been identified reflecting the two possible interactions of water and the aldehyde group. The two dihydrated species observed are related to the most stable m-anisaldehyde conformer. The most abundant dihydrated complex presents a structure with water dimer closing a cycle with the aldehyde and methoxy groups which confers high stability. In the less abundant dihydrate, water dimer closes a cycle with the aldehyde group, a structure of great interest to better understand the solvation of aldehydes. Additionally, one complex of m-anisaldehyde with four molecules of water has been detected. In this species, the most stable conformer of m-anisaldehyde captures the tetramer of water adopting a stacked configuration. Work is in progress.