

URONIC ACIDS IN GAS PHASE

ARAN INSAUSTI, *Departamento de Química Física, Universidad del País Vasco (UPV-EHU), Bilbao, Spain*; ELENA R. ALONSO, *Grupo de Espectroscopia Molecular, Lab. de Espectroscopia y Bioespectroscopia, Unidad Asociada CSIC, Universidad de Valladolid, Valladolid, Spain*; ANDER CAMIRUAGA, PIERRE ÇARÇABAL, *Institut des Sciences Moléculaires d'Orsay, Université Paris-Saclay, CNRS, Orsay, France*; EMILIO J. COCINERO, *Departamento de Química Física, Universidad del País Vasco (UPV-EHU), Bilbao, Spain*.

Sugars are versatile molecules that play a variety of roles in the organism. For example, they are important in energy storage processes, cellular recognition or as structural scaffolds. Here, we focus on uronic acids derivatives of the most abundant monosaccharides in the nature, concretely in glucuronic acid (GlcA) and galacturonic acid (GalA). By the combination of high resolution spectroscopy, supersonic expansions and laser ablation as vaporization technique with quantum chemistry calculations we are able to obtain valuable information in gas phase about the bare structures of both anomers of GlcA and GalA (with rotational spectroscopy) and water clusters of the 1-O-phenylated derivative of GlcA (using ion-dip spectroscopy (IR-UV)). Previous studies in the gas phase had been performed on α/β -Glucose^{1,2} and β -Galactose^{2,3} where the importance of $-\text{CH}_2\text{OH}$ backbone in H-bond orientation and hydration was reported. In this work, we focus on how the characteristic $-\text{COOH}$ group of uronic acids and their anomeric hydroxyl group configuration have effect in the H-bond network cooperativity/orientation and microsolvation process.

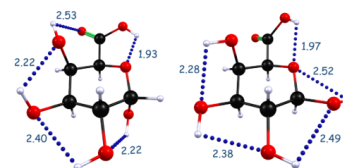


Figure 1: Observed conformers of both anomers of GalA