

72nd

INTERNATIONAL
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on

Molecular
Spectroscopy

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WC04

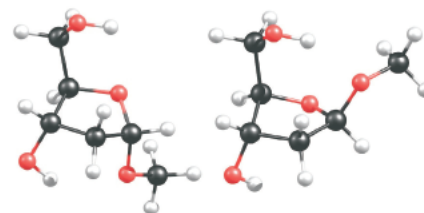
9:21 – 9:36

CONFORMATIONAL STUDY OF DNA SUGARS: FROM THE GAS PHASE TO SOLUTION

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Sugars are versatile molecules that play a variety of roles in the organism. For example, they are important in energy storage processes or as structural scaffolds. Here, we focus on the monosaccharide present in DNA by addressing the conformational and puckering properties in the gas phase of α - and β -methyl-2-deoxy-ribofuranoside and α - and β -methyl-2-deoxy-ribofuranoside. Other sugars have been previously studied in the gas phase^{a,b}.

The work presented here stems from a combination of chemical synthesis, ultrafast vaporization methods, supersonic expansions, microwave spectroscopy (both chirped-pulsed and Balle-Flygare cavity-based spectrometers) and NMR spectroscopy. Previous studies in the gas phase had been performed on 2-deoxyribose^c, but only piranose forms were detected. However, thanks to the combination of these techniques, we have isolated and characterized for the first time the conformational landscape of the sugar present in DNA in its biologically relevant furanose form. Our gas phase study serves as a probe of the conformational preferences of these biomolecules under isolation conditions. Thanks to the NMR experiments, we can characterize the favored conformations in solution and extract the role of the solvent in the structure and puckering of the monosaccharides.



^aE. J. Cocinero, A. Lesarri, P. Écija, F. J. Basterretxea, J.-U. Grabow, J. A. Fernández, F. Castaño, *Angew. Chem. Int. Edit.* 2012, **51**, 3119.

^bP. Écija, I. Uriarte, L. Spada, B. G. Davis, W. Caminati, F. J. Basterretxea, A. Lesarri, E. J. Cocinero, *Chem. Commun.* 2016, **52**, 6241.

^cI. Peña, E. J. Cocinero, C. Cabezas, A. Lesarri, S. Mata, P. Écija, A. M. Daly, Á. Cimas, C. Bermúdez, F. J. Basterretxea, S. Blanco, J. A. Fernández, J. C. López, F. Castaño, J. L. Alonso, *Angew. Chem. Int. Edit.* 2013, **52**, 11840.

WC05

9:38 – 9:53

FOUR STRUCTURES OF TARTARIC ACID REVEALED IN THE GAS PHASE

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The tartaric acid, one of the most important organic compounds, has been transferred into the gas phase by laser ablation of its natural crystalline form (m.p.174°C) and probed in a supersonic expansion by chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW). Four stable structures, two with an extended (trans) disposition of the carbon chain and two with a bent (gauche) disposition, have been unequivocally identified on the basis of the experimental rotational constants in conjunction with ab initio predictions. The intramolecular interactions that govern the conformational preferences are dominated by cooperative O-H...O=C type and O-H...O hydrogen bonds extended along the entire molecule. The observation of only μ_c -type spectra for one “trans” and one “gauche” conformers, support the existence of a C2 symmetry for each structure.

Intermission