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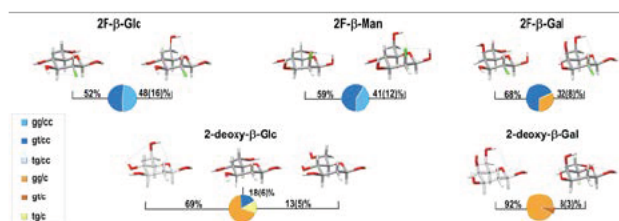


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FLUORINATION AND DEOXYGENATION AS CHEMICAL TOOLS TO STUDY THE CONFORMATIONAL PREFERENCES OF HEXOPYRANOSES: A JOURNEY FROM GAS PHASE TO SOLUTION

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The 3D-arrangement of carbohydrates and, particularly, the orientation of their hydroxymethyl groups are structural features crucial for their biological activities. In this work, we investigate the influence of water on the conformational preferences of model hexopyranoses by performing a comprehensive analysis in the gas phase via microwave spectroscopy^{a,b} of different fluorinated and deoxygenated carbohydrate analogues and comparing the results with those obtained in solution using a combination of NMR data and molecular dynamics simulations. The

gg conformation is stabilized in the gas phase by intramolecular HBs that lock this conformation when oriented clockwise. However, and contrary to previously reported data, the conformation of the hydroxymethyl group in D-glucose and D-mannopyranose series follows a similar tendency in the gas phase and in solution, indicating the importance of steric and electronic and minimizing the importance of competing water molecules against stabilizing intramolecular HBs.

^aC. Calabrese, I. Uriarte, A. Insausti, M. Vallejo-Lopez, F. J. Basterretxea, S. A. Cochrane, B. G. Davis, F. Corzana and E. J. Cocinero *ACS Cent. Sci.*, **6**, 293-303, 2020.

^bE. J. Cocinero, A. Lesarri, P. Ecija, F. J. Basterretxea, J.-U. Grabow, J. A. Fernandez, F. Castaño *Angew. Chem. Int. Ed.*, **51**, 3119, 2012.

UNVEILING THE EIGHT FORMS OF CAFFEIC ACID

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Herein we report a complete conformational analysis of caffeic acid, a relevant polyphenol^[1], and the main hydroxycinnamic acid found in humans' diet using laser ablation chirped-pulse Fourier transform microwave (LA-CP-FTMW) spectroscopy. The entire conformational space consisting of eight distinct rotameric species has been fully deciphered based on a thorough inquiry of the trend of the rotational constants supported by high-level theoretical computations.

^[1]A. M. Boudet, 2007, *Phytochemistry*, **68**, 22-24, 2722-2735

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THE MICROWAVE SPECTRUM OF PIPERONAL: DESIGNING AND TESTING A NEW HEATED NOZZLE ASSEMBLY

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A modular heated nozzle assembly with an open source external temperature control unit was designed for use in a new broadband microwave spectrometer under construction at Missouri University of Science and Technology. The first version of the heated source was tested using MS&T's existing cp-FTMW. As an initial proof of concept, the microwave spectrum of molecular piperonal was collected in the 5.5 to 18.75 GHz region. The parent isotopologues of two conformers, s-cis- and s-trans-piperonal, were observed and an analysis of the ¹³C substituted species are ongoing.