AB INITIO CHARACTERISATION OF THE STABLE CONFORMERS OF C_4 SUGARS: ERYTHROSE, ERYTHRULOSE AND THREOSE

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The importance of sugars ($C_n H_2 n O_n$) in biology and exobiology motivates this study (i. e. the detection of glycolaldehyde ($C_2H_4O_2$) in Sgr2(N-LMH) cloud by J.M. HOLLIS et al. Astrophys. J. Lett. 540(2000)L107 and the microwave study of glyceraldehyde ($C_3H_6O_3$) by F.J.LOVAS et al. J.Mol.Spect. 222(2003),263).
To the best of our knowlege, there is no experimental characterisation of C_4 sugars in the gas phase. Therefore we have performed *ab initio* calculations for the C_4 sugars in order to help further identifications. We have calculated equilibrium rotational constants, electric dipole moments and relative energies of different conformations. The expected accuracy is 0.5% on rotational constants and 1.0% kJ/mol on relative energies.
Concerning erythrose, 14 conformations have been found at the B3LYP/6-311++G(2df,p) level of the theory. The relative energy of all conformations has been optimized at the G3MP2B3 level of the theory. A few conformations are found within a small range of energy, under 5 kJ/mol. These most stable structures are stabilized by intra-molecular hydrogen bonds. Results on rotational constants and electric dipole moments performed at the B3LYP and the MP2 levels of the theory with 6-311++G(2df,p) basis sets suggest that a detection in the microwave region could be possible, using for example FTMW spectroscopy coupled to a molecular beam.
Calculations for erythrulose and threose are in progress.
This work is supported by grants IDRIS number 041715 and 051715.