STUDY OF THE GLYCOLALDEHYDE AND GLYCOLALDEHYDE-WATER COMPLEX BY AB INITIO CALCULATIONS AND FTMW SPECTROSCOPY IN A SUPERSONIC MOLECULAR BEAM.

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We are interested in studying sugars ($C_nH_2nO_n$) because of their biological role. Also, the spectroscopic characterization of their hydrated complexes could help to better understand in the gas phase the micro-solvation process of biomolecules.
We will present the most recent results on $C_2H_4O_2$ and $C_2H_4O_2$-$H_2O$.
Concerning glycolaldehyde, the microwave spectrum of one conformer was measured by K.M.MARSTOKK and H.MØLLENDAL J.Mol.Struc 16, 259 (1973) and R.A.H.BUTLER et al. The Astrophysical Journal Supplement Series, 134,319-321 (2001). The interstellar detection has been made by J.M.HOLLIS et al. The Astrophysical Journal, 554:L81-L85 (2001).
Meanwhile four stable conformations have been optimized for glycolaldehyde by *ab initio* calculations by T. Ratajczyk et al. J. Chem. Phys.A 108, 2758(2004).
Consequently we have performed additional calculations to obtain rotational constants and electric dipole moments. Our spectrum, recorded in the region 6-20 GHz, revealed news signals that could be assigned to at least one new conformation.
Concerning the glycolaldehyde-water complex, we have performed *ab initio* calculations at the B3LYP/6-311++G(2df,p) and aug-cc-pVTZ levels of the theory. Six stable conformers have been found.
Relative energies have been calculated at the G3MP2B3 level, the most stable structure is stabilized by two inter-molecular hydrogen bonds. The geometry optimization as well as the analysis of the experimental spectrum (6-20GHz) are in progress.
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