CONFORMATIONAL FLEXIBILITY IN HYDRATED SUGARS: THE GLYCOLALDEHYDE-WATER COMPLEX

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Conformational flexibility in the smallest hydrated sugar - the glycolaldehyde-water complex - has been investigated in the gas phase by means of a combination of a microwave Fourier transform spectroscopy experiment in a supersonic molecular beam, and ab initio quantum chemistry calculations. The water molecules inserts into glycolaldehyde using H-bonding selectivity: the two lowest energy conformations are stabilized by two intermolecular hydrogen bondings, and the next two ones by one intra- plus one inter-molecular hydrogen bondings. A dynamical flexibility associated with the two lowest ennergy conformations has been experimentally observed, and accurately modeled with a two dimensional landscape involving the hydroxyl group and the free OH water group coordinates. The conclusions drawn from the role played in the conformational flexibility by the hydroxyl and carbonyl groups are extended to other carbohydrates and molecules.