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Sugars in the gas phase

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The functional importance of carbohydrates in biological processes, particularly those involving specific molecular recognition is immense. Characterizing the three-dimensional structures of carbohydrates and glycoconjugates and their interactions with other molecules, particularly the ubiquitous solvent, water, are key starting points on the road towards the understanding of these processes. A new strategy, combining electronic and vibrational spectroscopy of mass-selected carbohydrate molecules and their hydrated complexes, conducted under molecular beam conditions, with ab initio computation is being exploited to characterize carbohydrate conformations and hydrated structures, the hydrogen-bonded networks they support (or which support them) and the specificity of their interactions with other molecules. The spectral features of monosaccharide residues can be used to refine the assignment of larger, oligosaccharide structures - a supplementary 'building-block' approach to the study of complex structures based upon an 'alphabet' of established IR spectral signatures of different conformations of the monosaccharide units - when their spectroscopic patterns are retained. When their patterns are altered the changes may be understood by analyzing the modification of the hydrogen-bonded networks, eg., the retention (or disruption) of the secondary structural motifs generated by intra-residue hydrogen-bonding. Feedback from the increasing body of experimental data will also help to inform and guide future theoretical conformational searches.