

A BROADBAND ROTATIONAL SPECTROSCOPIC STUDY OF TETRAHYDRO-2H-PYRAN-2-OL

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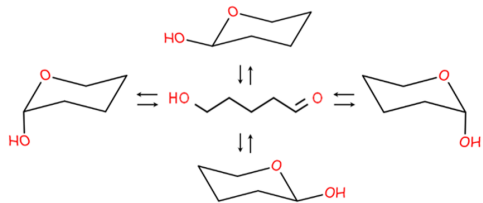


Figure 1: Tetrahydro-2H-pyran-2-ol molecule.

Tetrahydro-2H-pyran-2-ol (THP) is an alcohol containing pyranose ring. The lack of substituents in THP minimizes the conformational flexibility and the non-covalent interactions within the structure, drastically simplifying the system in relation to physiologically relevant carbohydrates, such as glucose. This makes THP a prototypical system to study various phenomena and dynamics of carbohydrate chemistry. Such phenomena include the anomeric effect, which describes the preference for the axial conformation over the less hindered and more energetically favoured equatorial conformation. When in solution, THP is in equilibrium with its linear counterpart, 5-hydroxypentanal, and readily interconverts between its two chiral forms. A high resolution gas phase study of THP may not

only confirm phenomena such as the anomeric effect, but also allow for the study of chiral interconversion in the gas phase. An in-depth study of THP will also lay a foundation for future gas phase carbohydrate systems with more physiological relevance. However, before we can study the various phenomena and dynamics, it is first beneficial to study the structure of THP in great detail. To elucidate the THP structure we analyzed rotational spectra measured with a chirped-pulse Fourier transform microwave spectrometer, operating in the 2-6 GHz range. In addition to the monomers, some dimer conformations were assigned to the rotational spectrum. The intermolecular interactions within the dimers were then visualized using a non-covalent interactions (NCI) analysis.