THE DELICATE BALANCE OF HYDROGEN BOND FORCES IN D-THREONINOL

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The molecule of D-threoninol has been studied using CP-FTMW spectroscopy. Despite the small size of this molecule, a great variety of conformations have been observed in the molecular expansion. With 2 OH groups and one NH_2 group, many possibilities for hydrogen bonding are anticipated. The multiple ways they can interact with each other make the analysis of its rotational spectrum challenging and only through an exhaustive conformational search and the comparison with the experimental rotational parameters and line strengths are we able to understand the complex nature of these interactions. In the 7 conformations already assigned, evidences for hydrogen bonded cycles and chains are revealed with dipole moment very sensitive to the configuration of the hydrogen bond.