EXPERIMENTAL EVIDENCE OF LONE PAIRS - π SYSTEM INTERACTION: THE ROTATIONAL SPECTRUM OF CHLOROTRIFLUOROETHYLENE - WATER COMPLEX

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Chemists have always been interested in labeling the interactions between the molecules, i.e. from covalent to ionic bond or van der Waals force. Certainly the most important non-covalent bond is the hydrogen bond, also of fundamental importance in biology. More recently also weak Hbond, sometimes in competion with halogen bonding, have been investigated because they have assumed a fundamental importance. Here, we show the lone pairs - π interaction prevails on the latter ones. We measured the molecular beam Fourier transform microwave spectra of five isotopologues of the 1:1 adduct of chlorotrifluoroethylene with water. Besides the rotational constants, the quadrupole coupling constants of the chlorine atom have been determined. Quantum chemistry calculations, at the MP2/6-311++G(d,p) level, have been carried out in order to obtain information about the structure and relative stability of the conformers under study.