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Encaged molecules in external electric fields: a molecular 'tug-of-war'[1] RAJEEV PATHAK, NALINI GURAV, SHRIDHAR GEJJI, University of Pune, LIBERO BARTOLOTTI, East Carolina University — We investigate applying ab initio theoretical methods, the molecules Hydrogen peroxide, H_2O_2, and Methanol, CH_3OH, encaged in hydrogen-bonded water "buckyballs" $(H_2O)_{20}$, subjected to an externally applied electric field. While the water-cage (host) tends to confine the guest-molecule, the external electric field tends to stretch it along with its labile hydrogen-bonded host, resulting into a molecular 'tug-of-war'. We appraise these two competing effects in terms of the extent of 'screening' of the host by the cage and compare the response of the composite system in the form of the consequent structural mutations, redistributions in the electron density and the electrostatic potential leading to emergence and suppression of the covalent O-H characteristic frequency shifts in the infra-red vibrational spectrum. This study brings forth the cooperative effect of hydrogen-bonding up to a maximally sustainable threshold electric field, beyond which fragmentation of the water cage occurs.

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