PSEUDO JAHN-TELLER ORIGIN OF THE PROTON-TRANSFER ENERGY BARRIER IN THE HYDROGEN-BONDED $[FHF]^-$ SYSTEM

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Abstract. The results of ab initio calculations of the adiabatic potential energy surfaces for the proton-bound $[FHF]^-$ system at different F-F distances have been rationalized in the framework of the vibronic theory. It is shown that the instability of the symmetric $D_{\infty h}$ structure at increased F···F distances and the proton displacement to one of the fluorine atoms are due to the pseudo Jahn–Teller mixing of the ground electronic state $1^1\Sigma_g$ with the lowest excited state of $^1\Sigma_u$ symmetry through the asymmetric σ_u vibrational mode.

Keywords: proton transfer, hydrogen bond, pseudo Jahn–Teller effect, potential energy surfaces, bifluoride anion.