Molecular orbital calculations of hydrogen bonding in ammonia - Formic acid system in the presence of electric fields

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The effects of electric fields on hydrogen bonding in ammonia - formic acid system, are examined with STO-3G and 6-31 G(d) wavefunctions. This system was used in a previous work to model hydrogen bonding in crystalline amino acids and the calculations were performed at HF / STO-3G level. The results on the relative position of the tautomeric equilibrium between the neutral and zwitterionic forms were explained in terms of the relative stabilization of the ionic partners as a function of their placement in positive and negative wells created by the external electric field. In order to rationalize those results at electronic structure level, in this paper we analyze the response of the molecular orbitals implicated in the hydrogen bridge, N..H..O, to various imposed external fields. It is found that the stabilization of the zwitterionic structure occurs due to the destabilization of the MO localized essentially at the nitrogen electron lone pair, n-orbital, and concomitant with the stabi