Hydrogen bond: Second order effects on potentials calculated by CNDO/2 method

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Second order perturbation theory (SOP) has been used to introduce electronic correlation effects on CNDP/2 calculated quantities like stabilization energy, proton potential curves, intermolecular dependence on distance and orientation. The HCHO...H2O' model has been studied. The SOP energy as a function of the RO...O' distance introduces changes in the potential minima which amount to 14% of the CNDO/2 value and in the asymmetry of the potential energy curve. For the proton curve, an extra stabilization energy of 4 kcal/mole at the minimum is found as well as changes in the shape of the potential curve. Effects on orientation dependence are also reported. © 1974.