

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Proton transfer induced by receding water in Glycine—(Water)₂ Complex RAJEEV PATHAK, Department of Physics, University of Pune, India — We investigate molecular co-operativity in the zwitterionic configuration of Glycine (Gly) with two proximal water molecules, Gly—(Water)₂, by deliberately making one of the water molecules recede from the remaining complex. The consequent intra-molecular proton transfer that renders the zwitterionic configuration into a neutral one is viewed under two scalar field descriptors: Molecular Electrostatic Potential (MESP), reflecting the modifications in the environment and the HOMO (highest occupied molecular orbital) electron density. We quantify the process further by energetics, through a many-body analysis of the interaction energy as well as salient IR spectral signatures associated with the proton-transfer. While we employ the decent MP2/aug-cc-pvDZ level of theory to seek optimal structures, it is gratifying that a prescription within density functional theory (DFT) also provides a reliable description of this process.

Rajeev Pathak
Department of Physics, University of Pune, India

Date submitted: 22 Oct 2010

Electronic form version 1.4