Application of DFT and MP2 Calculations on Structural and Water-assisted Proton Transfer in 3-Amino-4-nitrofurazan[1]

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Received November 4, 2014

Abstract—Density functional theory (DFT) and MP2 calculations have been employed to study of 3-amino-4-nitrofurazan molecule using the standard 6-311++G(*d*,*p*) basis set. The chemical properties of the 3-amino-4-nitrofurazan have been extensively studied. The geometries of molecules in the gas phase were optimized and compared with the crystallography of this substance. The results suggest that **A** form is the most stable form in the gas phase and it is the predominant tautomer in solution according to the DFT and MP2 calculations, respectively. In addition, variation of dipole moments in the gas phase, the specific solvent effects with addition of one molecule of water near the electrophilic centers of tautomers, the transition state of proton transfer assisted by a water molecule, the NBO charges of atoms and the potential energy surface were investigated. The calculated highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are presented.

Keywords: 3-amino-4-nitrofurazan, tautomerism, solvent effect, transition state, DFT, MP2.

DOI: 10.1134/S0036024415130038