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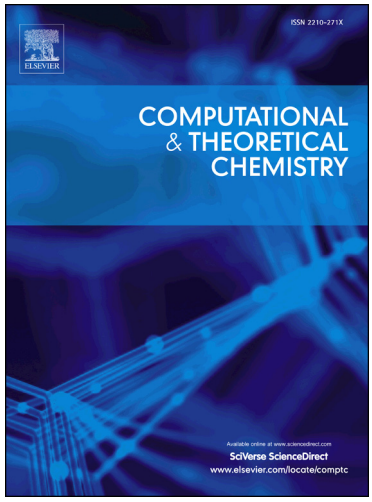

Electron delocalization and relative stabilities for the favored and rare tautomers of hydroxyazines in the gas phase – a comparison with aminoazines

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Electron delocalization and relative stabilities for the favored and rare tautomers of hydroxyazines in the gas phase – a comparison with aminoazines

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ABSTRACT: Quantum-chemical calculations {G2 and/or B3LYP/6-311+G(d,p)} were performed in the gas phase for neutral and ionized hydroxyazines (2- and 4-hydroxy derivatives of pyridine and pyrimidine). For each derivative, all possible tautomeric conversions were considered and all possible prototropic tautomers (OH, NH, and CH) analyzed. Rotational isomerism of the OH group was also taken into account. An interesting change of the relative stabilities takes place when proceeding from the neutral to ionized forms. Positive ionization favors the NH tautomers, and negative ionization the CH ones, except 2-hydroxypyrimidine for which the NH tautomer predominates for both ionized forms. A good relation exists between prototropy and electron delocalization solely for the neutral NH and CH tautomers. The OH forms are separated from the subfamily of the NH and CH tautomers due to significant differences between the stabilities of the tautomeric oxo and hydroxy groups. Intramolecular interactions affect both the geometric and energetic parameters, but the relative stabilities in higher degree. When compared to series of aminoazines, the total geometric effects of the exo −OH/=O and $-NH_2$/=NH groups are similar for neutral azines.

Keywords: Hydroxyazines, Prototropic Tautomers, Effects of ionization, Geometric and energetic parameters, HOMED/Δ*G* relation, DFT, G2

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