Theoretical study of the internal rotation of the hydroxylic group of the enol form of guanine

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Emphasis was placed in the present work on a density functional theory and Hartree-Fock study of the internal rotation of the hydroxylic group of the enol form of guanine. This was achieved by monitoring the behavior of energy, chemical potential, hardness, electrophilicity, and polarizability along the torsional coordinate. An energy barrier of about 9.5 kcal/mol was found about midway between two stable planar conformations. The analysis of the behavior of reactivity descriptors shows that the principles of maximum hardness and minimum polarizability are satisfied. Very good linear relations have been established between energy, chemical potential, hardness, and electrophilicity power allowing the characterization of the rotational process in terms of the simultaneous change of these global properties.