



Theoretical investigation of tautomeric equilibrium in *ortho*-hydroxy phenyl Schiff bases.

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This Letter presents a study of the tautomeric equilibrium in *ortho*-hydroxy phenyl Schiff bases. The influence of substitution and solvent (simulated by the self-consistent reaction field model, SCRF) on the energy barrier of the transition state and on proton transfer is investigated. Dependencies of the HOMA and HOSE aromaticity indices on the molecular, transition state, and proton transfer forms were obtained. The state of chelate chain and phenyl ring aromaticity depending on the tautomeric equilibrium is studied.

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