Theoretical Study of the Effect of Different α-Substituents on the Acetaldimine-Vinylamine Tautomeric System

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The Acetaldimine-Vinylamine tautomeric system has been studied by employing the MNDO semi-empirical method. The imine structure was found to be energetically favorable, as indicated by the calculated heats of formation, Gibbs free energy, LUMO and HOMO, and charges. The substitution of F, Cl, CN, CH_3, CF_3, NO_2 and BH_2 at the α-position was found to affect the geometrical parameters. F and Cl substituents are found to favor the imine formation, while CF_3, NO_2, CN_2 and BH_2 favor the amine formation. The proton transfer in this tautomeric system is found to be easier ($\Delta H =$ 5.224 kcal/mol) than that in the keto-enol tautomeric system ($\Delta H = 11.1$ kcal/mol).

Key words: Imine-enamine; Tautomerization; Acetaldimine; Vinylamine; MNDO.