Semiempirical Method MNDO for the Evaluation of the Effect of Different Substituents at the Imine-Carbon Position on the Acetaldemine-Vinylamine Tauotomerization and Comparison to the Substitution at α-Position

Hamzeh S. M. Al-Omari

Chemistry Department, College of Science, University of Mutah, Karak, Jordan

Reprint requests to Dr. H. S. M. Al-O. E-mail: hamzehs@mutah.edu.jo

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MNDO calculations have been employed to study the effect of some substituents of the acetaldemine-vinylamine tautomeric system at the imine-carbon position of CH_3CXNH, where X = H, F, CN, NH_2, NO_2, BH_2, CH_3 and CF_3. It is found that the substitutents F, NH_2 and NO_2 encourage the formation of the enamine tautomer. The substitutents CN, CH_3, CF_3 and BH_2 encourage the formation of the imine tautomer. Isodesmic reactions, free energy change (ΔG), charge distribution and energy gap (E_g) between HOMO and LUMO were used to prove these findings. Resonance stabilization was a major factor in the determination of the most stable tautomer. These results were compared with previous work on the substitution at the σ-carbon position.

Key words: Acetaldemine; Vinylamine; Tautomerism; Imine/enamine; Resonance; MNDO.