MINDO-Forces Study on the Substituent Effect in the Keto-Enol Tautomerism of Acetyl Derivatives

Wasim F. Al-Halasah, Ali Mahasnah, and Salim M. Khalil

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

Reprint requests to Prof. S.M.K.; E-mail: qukhalil@mutah.edu.jo

Z. Naturforsch. **59a,** 299 – 308 (2004); received February 11, 2004

MINDO-Forces calculations with complete geometry optimization have been performed on acetaldehyde, vinyl alcohol and acetyl derivatives CH_3COX(X=H, F, OH, CN, NH_2, NO_2, CH_3, CF_3,OCH_3). It was found that acetaldehyde is more stable than vinyl alcohol by 10.451 kcal/mol. Thermodynamically, keto tautomers are more stable than their enol counterparts. This agrees with theoretical calculations. The electron releasing substituents tend to stabilize keto tautomers, while the electron withdrawing substituents tend to destabilize the keto tautomers, relative to the parent. Geometrical parameters, heats of formation, electron densities, Gibbs free energies and orbital energies (HOMO-LUMO) are reported.

Key words: Acetaldehyde; Vinyl Alcohol; Keto-Enol Tautomerism; Acetyl Derivative.