MINDO-Forces Study on the Keto-Enol Tautomerism of α-Substituted Acetaldehydes $XCH_2CH{=}O$ (X = H, F, OH, CN, NH_2, NO_2, CH_3, CF_3, OCH_3): Comparison with Acetyl Derivatives

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MINDO-Forces calculations with complete geometry optimization have been performed on α-substituted acetaldehydes $XCH_2CH{=}O$ and their enols (X = H, F, OH, CN, NH_2, NO_2, CH_3, CF_3, OCH_3). All substituents were found to decrease the stability of the acetaldehyde and mostly in the case of electron withdrawing capacity (e. g NO_2 and CF_3). This agrees with theoretical calculations, except in the case of F. The substituent effects on the stabilities in this study are compared with results obtained from our previous theoretical calculations on acetyl derivatives. Geometrical parameters, electron densities, and Gibbs free energies are reported.

Key words: α-Substituted Acetaldehyde; Keto – Enol Tautomerism; Acetyl Derivative.