MINDO-Forces Study on Substituted Nitromethane $\rightleftharpoons$ *aci*-Nitromethane Tautomerism

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MINDO-Forces calculations with complete geometry optimization have been performed on nitromethane, *aci*-nitromethane and X-substituted nitromethane and *aci*-nitromethane (X = F, OH, NH_2, CH_3, CN, CF_3, NO_2, CHO). It is found that nitromethane is more stable than *aci*-nitromethane by 9.337 kcal/mol. This agrees with theoretical calculations. Thermodynamically, substituted *aci*-nitro tautomers are more stable than the corresponding nitromethane, except in case of the substituent F. Geometrical parameters, heats of formation, electron densities, Gibbs free energies and isodesmic reactions are reported.

Key words: Nitromethane; *aci*-Nitromethane; Tautomerism.