A Theoretical Study of Substituted Cyclopentanones and their Enols

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MINDO-Forces calculations with complete geometry optimization have been performed on cyclopentanone and its enol counter part, perfluorination of cyclop entanone and its enol counterpart and X-cyclopentanones and their X-enols, where X is NO_2, CF_3, CN, OH, NH_2 and O^-. It was found that ketone is more stable than its enol counterpart. Perfluorination destabilizes ketone on the expense of enol. These results agree with the experimental results and density functional theory calculations. All substituents are destabilizing except O^- in the case of cyclopentanone. It was found that NO_2 and CF_3 behave as strong electron withdrawing groups, CN and NC show amphielectronic behavior, and the substituents OH,NH_2 and O^- behave as electron releasing groups with O^- being strongest. Geometrical parameters, heats of formation, entropies, and Gibbs free energies are reported.

Key words: Perfluorocyclopentanones; Substituted Cyclopentanones; Keto-enol Equilibria.