A Theoretical Study of Substituted Cyclobutanones and Their Enols

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MINDO-Forces calculations have been performed with complete optimization of the geometry on cyclobutanone and its enol counterpart, perfluorination of cyclobutanones and enol counterparts, and X-cycolobutanones and their X-enols, where X is NO_2, CF_3, CN, OH, NH_2 and F. It was found that ketone is more stable than its enol counterpart. Perfluorination destabilizes ketone on the expense of enol. These results agree with experimental and theoretical calculations. Electron releasing substituents (NH_2, OH, F) stabilize cyclobutanone, while electron withdrawing substituents (CF_3, NO_2) destabilize it. CN substituents have almost no effect on the stabilization of this keto-enol system.

Geometrical parameters, heats of formation, electron densities and Gibbs free energy are reported.

Key words: Perfluorocyclobutanones; Substituted Cyclobutanones; Keto-enol Equilibria.