World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:8, No:06, 2014

A Computational Study on Solvent Effects on the Keto-Enol Tautomeric Equilibrium of Dimedone and Acetylacetone 1,3- Dicabonyls

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Abstract : The solvent effects on the keto-enol tautomeric equilibriums of acetylacetone and dimedone are theoretically investigated at the correlated Becke-3-parameter-Lee-Yang-Parr (B3LYP) and second-order Møller-Plesset (MP2) computational levels. The present study shows that the most stable keto tautomer of acetylacetone corresponds to the trans-diketo, E,Z form; while the most stable enol tautomer corresponds to the closed cis-enol,Z,Z form. The keto tautomer of dimedone prefers the trans diketo, E, E form; while the most stable enol tautomer corresponds to trans-enol form. The calculated free Gibbs enthalpies indicate that, in polar solvents, the keto-enol equilibrium of acetylacetone is shifted toward the keto tautomer; whereas the keto-enol equilibrium of dimedone is shifted towards the enol tautomer. The experimental trends of the change of equilibrium constants with respect to the change of solvent polarity are well reproduced by both B3LYP and MP2 calculations.

Keywords : acetylacetone, dimedone, solvent effects, keto-enol equilibrium, theoretical calculations
Conference Title : ICMCC 2014 : International Conference on Mathematical and Computational Chemistry
Conference Location : Istanbul, Türkiye
Conference Dates : June 19-20, 2014