Research Article

Theoretical study of keto–enol tautomerism by quantum mechanical calculations (the QM/MC/FEP method)

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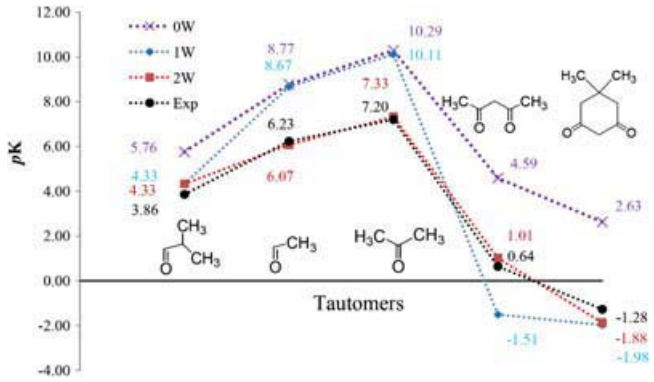

The tautomeric equilibrium between the keto and enol forms has been studied for five typical ketones and aldehydes. The free energies of solvation were included in the calculation by using quantum mechanical/Monte Carlo/free-energy perturbation method. The two-water model using quantum mechanical/Monte Carlo/free-energy perturbation method produced values that were very consistent with the experimental data for all of the tautomers.