

## Urea and Thiourea Hydrolysis: (Re)visiting an Old Friend

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The proficiency of the Ni(II) metalloenzyme urease to hydrolyze urea is established by comparison to the uncatalyzed reaction in water. In a previous study two principal reaction profiles of uncatalyzed urea decomposition into ammonia and isocyanic acid (or ammonium and isocyanate) were considered using MP2/6-311++G(d,p) calculations: i) a direct and ii) a water assisted proton transfer [1]. Both processes were evaluated in the gas-phase and in the aqueous phase using the IPCM solvent model.

In the current work the same level of calculation was employed and the reaction profiles were revisited with the ability to optimize the geometry not only in gas phase, but also in solution using the PCM method as implemented in the G09 program. In addition the effect of using the dimer of urea as a new starting point as well as the change of the carbonyl oxygen to sulfur were also investigated. Full mechanistic details will be highlighted and discussed.

1 – G. Estiu and K. M. Merz Jr., J. Am. Chem. Soc. **126**, 6932-6944(2004).