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First principles study on the reaction mechanisms of hydrolysis reaction of PCl_3 and $POCl_3$

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Lethal accidents caused by explosive reactions of toxic chemicals should be prevented and once happened, fast and safe control is of importance. An accurate understanding of thermodynamic properties and kinetic rates is the first step toward accomplishing the purpose Using first principles density functional theory (DFT) and ab-initio molecular dynamic (AIMD) simulations we study hydrolysis reactions of two archetype chemicals, PCl_3 and $POCl_3$, to unveil potential energy surface over reaction cooardinates. By calculating the intermediates and Gibbs free energy diagrams reaction mechanism and activation barriers. Our results indicate that H_2O molecules nearby the chemical species play a key role in catalyzing the hydrolysis reaction as a proton donor or acceptor. The catalytic mechnisms is explained as more water molecules attach the charge separation at the transition state is enhanced, leading to higher polarity and stabilization via hydrogen bonding network. It could dramatically reduce the activation energy of reactant complex. The effect is, however, mitigated by disordering entropic effect resulting in only slight reduction of activation energy upon increasing H_2O molecules. It is noteworthy that PCl_3 react with H_2O molecule by interplay of the proton transfer and dissociation of chlorine, while $POCl_3$ first forms a six-coordinated complex and then, quickly decomposes to HCl. Reaction rate constants are calculated from calculated activation energy using a transition state theory.

Biography

Hyunwook Jung has completed his BS at Department of Chemical & Biomolecular Engieering in Yonsei University. After serving as marine for two years he joined graduate program of Yonsei University. He was invited to the 10th International Conference on Computational Physics (ICCP10) held at Macao in China, January, 2017.

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