Theoretical Characterization of Chemical Processes Involving Charge Transfer

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Nowadays, variety of phosphorus-containing compounds is widely used as nerve agents, pesticides, fire retardants etc. The mechanism of decomposition, reactivity and toxicity of these compounds are extensively studied experimentally but there is a lack of theoretical characterization of these processes and the structures involved. Theoretical elucidation of the mechanism of the reactions of $POCl_3^-$ with O_2 and O_3 was attempted in this study. The experimental work indicates that various charge transfer steps are involved in the mechanism of these reactions. It is believed that the reaction channels studied here are ground state processes which made them excellent candidates for theoretical characterization using DFT and high level ab initio methods. In order to provide theoretical insights into the mechanisms of the reactions of $POCl_3^-$ with O_2 and O_3, we determined structures and energies of reactant and product states as well as for intermediate and transition states. Density functional calculations were used as starting point because they allow to explore quickly different pathways leading to various products. However, for more accurate energetics, MP2 and CCSD(T) calculations were performed as well.