

Gas Phase Anion Chemistry via Direct Chemical Dynamics Simulations

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Chemistry of anions has received a great attention in the literature due to their wide applicability in synthetic chemistry. Studying the anions in the gas phase eliminates the complexities posed by solvation, counterion, etc., and provides a platform to understand intrinsic reactivity. In our research group, electronic structure theory calculations and direct chemical dynamics simulations are used to study interesting anion chemistry in the gas phase. In this talk, studies of two important reactions involving anions will be discussed. The first one is the collision induced dissociation (CID) of isoxazole and one of its substituents in the anionic form. They can be deprotonated at various positions resulting in different isomers. Dissociation chemistry of these isomers were simulated under CID conditions. The results are in fairly good agreement with mass spectrometry experiments and an interesting *non-statistical* reaction pathway identified in the simulations. The second one is a bimolecular nucleophilic substitution (S_N2) reaction between CH_3I and the CN^- anion. This reaction is particularly interesting because it can result in two different substitution products (CH_3CN and CH_3NC). Simulations were performed to model a velocity map imaging experiment of the same reaction and detailed mechanisms, branching ratios, product energy distributions, etc., were investigated. Simulations show that the mechanism is primarily *direct* with dominant *backward scattering*.