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Title:	Non-Covalent Interactions in N-Bromosuccinimide (NBS) & N-Iodosuccinimide (NIS) and their Role in Chemical Reactivity: A Matrix Isolation and Ab Initio Study
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Abstract:	<p>The halogenation reactions have been extensively studied for many decades now. One of the oft used reagent for this reaction is N-Bromosuccinimide (NBS). For example, ethylene with NBS will yield a haloalkane. The mechanism of this was well known and is believed to proceed through the formation of a Bromonium ion as an intermediate. The question arises as to what is the driving force for the formation of the intermediate and in this thesis we explore the possibility of non-covalent interactions playing a role as a gateway for this intermediate. We first studied the NBS-water interaction and followed it up with studies on the N- Iodosuccinimide (NIS)-water interaction. Our computations yielded five different complexes. While four of these were hydrogen bonded interactions, of these involved an oxygen-halogen interaction, which in the literature has been referred to as the halogen bond. All ab initio computations were performed using M06-2X and MP2 methods with DGDZVP basis sets, using Gaussian-09 software. Interaction energies of the complexes were also computed using the same level of theory. Frequency calculations were performed to confirm if the structure corresponding to a stationary point is a minimum and to assign our experimental features. AIM and NBO calculations were done to understand the nature of the interactions in the complexes. At the MP2/DGDZVP level, BSSE corrected interaction energies shows that the halogen bonded complex was the most strongly bound complex among all the minima in the NIS- water system. In the NBS-water system, the halogen bonded complex was only marginally less bound than the hydrogen bonded complex, indicating that this interaction could well play a role in the reaction mechanism. This work has therefore highlighted the important role of the halogen bonding complexes and its role in the halogenation reaction mechanism.</p>
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