Photoactivation of CF_3I in the presence of photoexcited $Ru(bpy)_3^+$ and the Subsequent Cu-Catalyzed Trifluoromethylation of Boronic Acids

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In a recent work[1], Ye and Stanford proposed a mechanism for the trifluoromethylation of boronic acids by using photoredox and copper catalysis. If visible light can be used in the process of catalysis, it would greatly benefit society both economically and environmentally. Our goal is to gain a better, more detailed understanding of this process by using computational methods. The first step in the reaction mechanism is the photoactivation of CF_3I, which will yield the CF_3 radical necessary for the second part of the reaction mechanism. Here, we study the photoactivation of CF_3I in the presence of the photoexcited $Ru(bpy)_3^+$ complex. Calculations for excited states for the molecule $Ru(bpy)_3^+$ were performed successfully using the basis set def2-TZVP and functional B3-LYP. By placing a CF_3I molecule in various locations near $Ru(bpy)_3^+$, we were also able to examine the ways in which CF_3I interacts with $Ru(bpy)_3^+$. The second part of the mechanism involves the copper-catalyzed trifluoromethylation of the boronic acid to yield a CF_3-aryl. Using an IRC (internal reaction coordinate) technique, a path from reactant to product was made for each step in the mechanism with the hope of finding each transition state. These results provide a better understanding of the mechanism proposed by Ye and Stanford, though there is still much to be examined.

References

[1] Merging Visible-Light Photocatalysis and Transition-Metal Catalysis in the Copper-Catalyzed Trifluoromethylation of Boronic Acids with CF_3I
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