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Title:	Computational and Matrix Isolation Infrared Spectroscopic Studies of 2-Dehydroacetophenone Radical
Authors:	Bhagat, Virinder (/jspui/browse?type=author&value=Bhagat%2C+Virinder)
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Abstract:	Intramolecular sensitization is one of the important photochemical phenomena, by which the structural and reactivity pattern of the excited state of the molecules can be tuned. The introduction of aryl ketones or the incorporation of heavy atoms such as iodine is some of the popular strategies through which triplet excited states can be accessible that can tune the photoreactivity. This is well known in reactive intermediates like carbenes, nitrenes, etc. but has not been explored in case of radicals. In this respect, we decided to investigate the o-iodoacetophenone, which has both aryl ketone as well as iodine atom that can trigger the triplet excitation upon irradiation. Now the question will be related to the C-I bond, whether we can able to cleave it at triplet excited state to generate the 2-dehydroacetophenone radical. For examining this, we utilized nitrogen gas matrix isolation in combination with infrared spectroscopy. For further understanding the structural reactivity aspects of the resulting dehydroacetophenone radical, we have performed DFT and ab-initio computations. For comparison, we have investigated the 3- and 4-dehydroacetophenone radical isomers as well.
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