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Authors:	Lincoln
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Abstract:	Benzyloxyl radical is an important reactive intermediate in the oxidation of toluene and other substituted aromatic hydrocarbons. The benzyloxyl radical is expected to promptly decompose to new products like benzaldehyde and benzene. Despite the experimental exploration of kinetics and product branching ratios of decomposition channel of benzyloxy radical, the isomerization pathways of benzyloxyl to other radical isomers and its unimolecular decomposition pathways have not been well investigated. In this work, we explore the isomerization and decomposition pathways of benzyloxyl radical using computational methods. To get additional insights into the effect of replacement of sulfur with oxygen, we have also explored the benzylthiyl radical isomers as well as their isomeric phenyl radical isomers. Furthermore, the target benzyloxy radical was intended to generate under photochemical conditions using 2-iodobenzylacohol as a precursor isolated in argon matrix at 4 K. A possible isomerization of the 2-dehydrobenzylalcohol (formed from photo irradiation) to benzyloxyl radical through 1,4-H shift was expected in the further photochemistry of the benzyloxyl radical. Surprisingly, our experimental investigations led to light-induced conformational changes of 2- iodobenzylalcohol instead of the radical in argon matrix. Both these computational and experimental results are discussed in the thesis in detail.
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