Title:	Computational and Matrix Isolation Infrared Spectroscopic Studies of Succinimide Radicals
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Keywords:	Matrix isolation Spectroscopic Succinimide
Issue Date:	28-Jul-2021
Publisher:	IISERM
Abstract:	Substituted derivatives of succinimide are essential components in numerous biological activities and pharmaceutical drug molecules. In order to explore isomerization and decomposition pathways of dehydroradical isomers of succinimide, quantum chemical calculations were carried out. Density functional theory and composite methods have been used throughout the study. Structural optimization and relative stability of the radical isomers are determined at (U)B3LYP, (U)M06-2X, and CBS-QB3 levels of theory using the cc-pVTZ basis set. In addition to that, calculation of first bond dissociation energies, estimation of spin densities and electrostatic potential, and NBO analysis have been performed. Furthermore, reactivity analysis has been done for the radical isomers, including unimolecular decomposition pathways that shed light on their kinetic stabilities. Matrix isolation infrared spectroscopic experiments were carried out to partake in photochemical investigations of succinimide radical isomers.
URI:	http://hdl.handle.net/123456789/3889
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