

## Theoretical Study on the Mechanism of 1,3-Dipolar Cycloaddition Reactions between $\alpha,\beta$ -Unsaturated Selenoaldehyde with Nitrene and Nitrile Oxide

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The reaction mechanisms of 1,3-dipolar cycloaddition between the  $\alpha,\beta$ -unsaturated selenoaldehyde with nitrene and nitrile oxide were investigated. It was expected to undergo four pathways in two separate reactions with nitrene and nitrile oxide. The study was conducted using *ab initio* approach at MP2/6-31G(d) level of theory. Potential energy surfaces were generated from the energies of the stationary points involved in the mechanisms and the dominant reaction pathways were identified. It was found that the favourable cycloaddition reaction occurs at the selenium-analogue carbonyl group of selenoaldehyde. The tendency of the reactions to occur at the carbonyl group instead of the alkene moiety in the structure is explained by the spatial orientation of HOMO and LUMO of the reactants.