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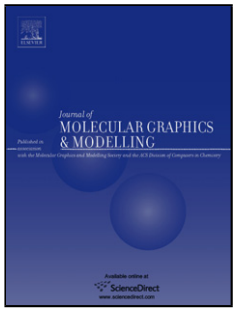

Title: One-step versus two-step mechanism of Diels-Alder reaction of 1-chloro-1-nitroethene with cyclopentadiene and furan

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One-step versus two-step mechanism of Diels-Alder reaction of 1-chloro-1-nitroethene with cyclopentadiene and furan

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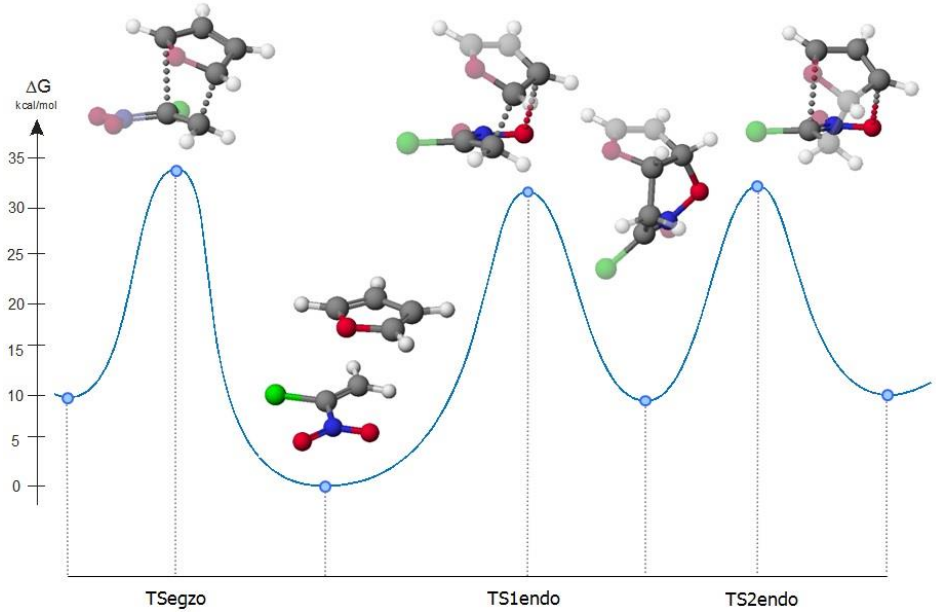
Graphical abstract



Highlights

- Polar nature of Diels-Alder reactions involving 1-chloro-1-nitroethene
- Two-step mechanism for reaction of cyclopentadiene with 1-chloro-1-nitroethene

ABSTRACT

DFT computational study shows that Diels-Alder (DA) reactions of 1-chloro-1-nitroethene with cyclopentadiene and furan have polar nature. However, their mechanism is substantially different. In particular, 1-chloro-1-nitroethene react with cyclopentadiene according to one-step mechanism. In the same time, more favourable channel associated with the P-DA reaction between furan and 1-chloro-1-nitroethene is a domino process, that comprises an initial hetero-Diels-Alder reaction yielding a [2+4] cycloadduct, which experiences a subsequent [3,3] sigmatropic shift to yield the expected formal [4+2] cycloadduct. This is a consequence of more polar nature of reaction, due to higher nucleophilicity of furan in comparison to cyclopentadiene.

KEYWORDS: Diels-Alder reaction, Nitroalkenes, DFT study,Mechanism

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