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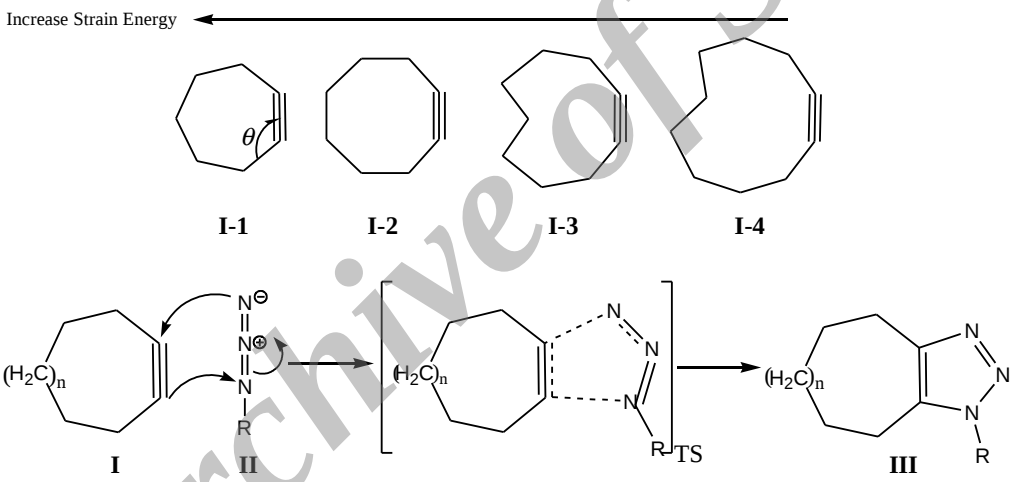
Theoretical Studies of 1,3-Dipolar Cycloaddition Reactions Between 7-10 Membered Simple Cycloalkynes and Triazoles R-N_3 (R= H, CH_3, Ph)

Avat (Arman) Taherpour, Elahe Rajaeian, Hadi Shafiei and Maryam Malekdar*
Chemistry Department, Science Faculty, Islamic Azad University, P.O.Box 38135-567, Arak, Iran.
**E-mail: avatarman.taherpour@gmail.com and a.taherpour@iau-arak.ac.ir*

The energy content in alkynes may be increased further by bending the normally linear triple bond, as in the small cycloalkynes. The strain energy in the cycloalkynes increases as the size of the ring decreases. Cycloadditions of 1,3-dipoles with alkynes may occur by concerted mechanisms. In this study, the reactivity and strain energy effect of the cycloalkynes with substituted triazoles R-N_3 (R= H, CH_3 and Ph) by the use of B3LYP/6-31G* level method will be discussed. The investigation of the structured properties, theoretical thermodynamic and kinetic data i.e. ΔrG, ΔG* and rate constants of the reactions in 298K will be presented.



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