

Nitration of Phenylacetylene; Synthesis of β -nitrostyrene

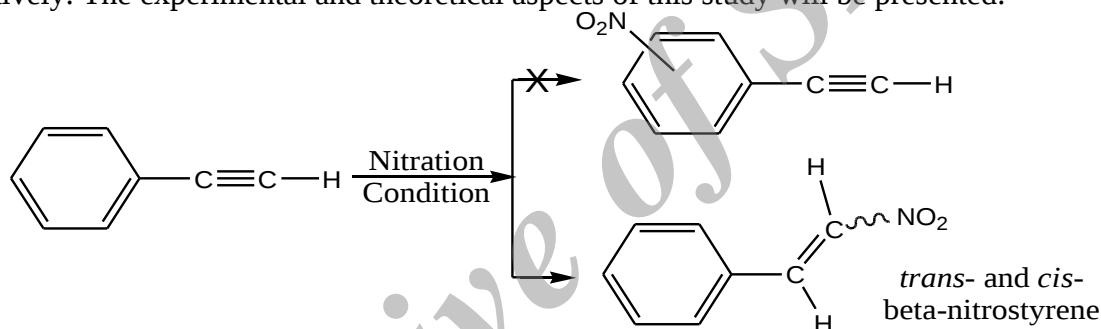
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In this study, the nitration of phenylacetylene (H-C≡C-Ph) was investigated. The investigation of the product has shown that the triple bond of the acetylenic part of phenylacetylene has participated in the nitration process.[1,2] It means that in the reaction condition the additional reaction on the -C≡C- of phenylacetylene is much better than the substitution reaction on Ph- group.[1-3] The structures of the products were analyzed by the data of IR, ¹H-NMR, ¹³C-NMR and MS spectroscopy. The B3LYP/6-31G* shows that the trans- β -nitrostyrene is more stable than its cis-form. The HOMO level of the trans- and cis- isomers of β -nitrostyrene are -6.95 and -6.90eV, respectively. The experimental and theoretical aspects of this study will be presented.



References:

- [1] K. N. Campbell and B. K. Campbell, *Org. Synth. Coll.*,1963, 4, 763.
[2] J. C. Hessler, *Org. Synth.Coll*, 1941, **1**, 438.
[3] G. Hilt , T. Vogler, W. Hess, F. Galbiati (2005). *Chemical Communications*, 2005, 11, 1474–1475.