**Effect of CH/P exchange on tandem Cope rearrangement and [2 +2] cycloaddition of *cis*-1,2diethynylcyclopropane and its mono-hetero analogues: A DFT investigation.**

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**Abstract:** An almost explosive growth in the field of low-coordination phosphorus compounds during the last three decades of the 20th century led the chemists realize that a remarkable analogy existed between these compounds and their carbon-analogues [1]. The analogy was so overwhelming that a new phrase “Phosphorus: The Carbon Copy” [2] was coined.

We recently reported tandem Cope rearrangement and [2+2] cycloaddition of cis-1,2-diethynylcyclopropane and its mono-hetero analogues [3] We thought it interesting to study theoretically the effect of CH/P exchange on the activation and reaction enthalpies of tandem Cope rearrangement and [2+2] cycloaddition. We report herewith the results of tandem Cope rearrangement and [2 +2] cycloaddition of cis-1-ethynyl, 2-monophosphaethynylcyclopropane and its mono-hetero analogues (Scheme 1) investigated in the gas phase at the B3LYP/6-31+G(d) level.



Reactant TS1  **Intermediate** TS2 Product

**Scheme 1 ( X = CH2, O, PH, NH )**

**References**

1. F. Mathey. *Acc. Chem. Res.* **25**, 90 (1992).

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3. Kaur,M.; Gupta, R.; Bansal, R. K.*Comp. Theo. Chem.* **2018**, *1123*, 142.