

## عنوان مقاله:

Di-Heteroatom effects on divalent five-membered ring carbene  $X_2C_2H_4C$ : DFT calculations

## محل انتشار:

همایش منطقه ای شیمی (سال: ۱۳۸۹)

تعداد صفحات اصل مقاله: ۱

## نویسندگان:

E. Vessally - Islamic Azad University, Miyaneh Branch, Miyaneh, Iran

M. Zargham - Payame Noor University (PNU), Zanjan, Iran

## خلاصه مقاله:

Divalent carbenes and their analogues are interesting intermediates in organic synthesis [1]. The cyclic completely conjugated species are important in the chemistry of the divalent carbene intermediates [2]. In this research work, the energy differences,  $\Delta X_s-t$  ( $\Delta X_s-t=X(\text{singlet})-X(\text{triplet})$ ) between the singlet (s) and triplet (t) states on  $X_2C_2H_4C$  ( $X=NH, PH, AsH, O, S, Se$ ) were calculated at DFT/B3LYP/6-311++G\*\* level of theory. The DFT calculations show that the triplet state of  $X_2C_2H_4C$  is ground state with planar conformer respect to its corresponding nonplanar singlet state. Also, DFT calculations indicate that the heavier heteroatoms at  $\alpha$  position decrease the stability of the singlet state. However, the light heteroatoms at  $\alpha$  position increase the stability of the singlet state. The results will be presented and discussed.

## کلمات کلیدی:

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