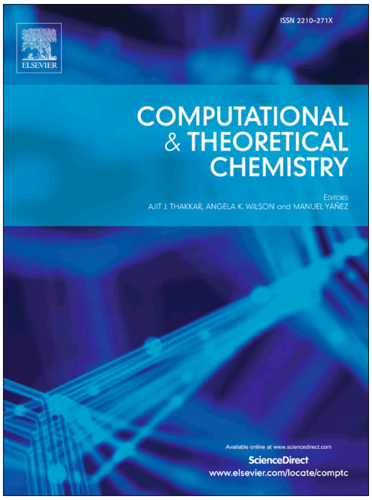

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Oxidation of hydro−silaimine, phosphasilene, and arsasilene structures $(CH_3)HSi=E(CH_3)$ (E: N, P, or As) via concerted 1,3-dipolar cycloaddition of nitrous oxide: A DFT study

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Abstract

Possible concerted 1,3−dipolar cycloaddition reactions of element−hydrogen containing silaimine, phosphasilene, and arsasilene structures $(CH_3)HSi=E(CH_3)$ (denoted as **SiE**, E = N, P, As) with nitrous oxide (N_2O) were investigated at the WB97XD/cc−pVTZ level of theory. In all cases, the nature of E atom determines the kinetic of the reactions. Thereby, the reactivity order of **SiE** structures toward N_2O was observed to be **SiAs**>**SiP**>**SiN**, as it is evident from the calculated energy barriers. All the potential products ($\mathbf{3_{SiE}}$−$\mathbf{9_{SiE}}$) were found to have exergonic formation energies. Among them, the pathways to generate the heavier ketones ($\mathbf{3_{SiE}}$) are more likely to appear due to lower energy barriers.

Keywords: nitrous oxide, DFT, main−group species, reaction mechanism, small molecule activation