

Accepted Manuscript

Oxidation of hydro–silamine, phosphasilene, and arsilene structures $(\text{CH}_3)_2\text{HSi}=\text{E}(\text{CH}_3)$ (E: N, P, or As) via concerted 1,3-dipolar cycloaddition of nitrous oxide: A DFT study

Cem Burak Yildiz

PII: S2210-271X(18)30163-4
DOI: <https://doi.org/10.1016/j.comptc.2018.05.003>
Reference: COMPTC 2789

To appear in: *Computational & Theoretical Chemistry*

Received Date: 20 March 2018
Revised Date: 2 May 2018
Accepted Date: 2 May 2018

Please cite this article as: C. Burak Yildiz, Oxidation of hydro–silamine, phosphasilene, and arsilene structures $(\text{CH}_3)_2\text{HSi}=\text{E}(\text{CH}_3)$ (E: N, P, or As) via concerted 1,3-dipolar cycloaddition of nitrous oxide: A DFT study, *Computational & Theoretical Chemistry* (2018), doi: <https://doi.org/10.1016/j.comptc.2018.05.003>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Oxidation of hydro–silaimine, phosphasilene, and arsilene structures (CH₃)HSi=E(CH₃) (E: N, P, or As) via concerted 1,3-dipolar cycloaddition of nitrous oxide: A DFT study

Cem Burak Yildiz*

Department of Aromatic and Medicinal Plants, University of Aksaray, Aksaray, Turkey.

* Corresponding author.

Dr. Cem Burak Yildiz

E-mail address: cemburakyildiz@aksaray.edu.tr

Phone: +90 382 288 2011

Abstract

Possible concerted 1,3-dipolar cycloaddition reactions of element–hydrogen containing silaimine, phosphasilene, and arsilene structures (CH₃)HSi=E(CH₃) (denoted as **SiE**, E = N, P, As) with nitrous oxide (N₂O) 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 N₂O was observed to be **SiAs>SiP>SiN**, as it is evident from the calculated energy barriers. All the potential products (**3_{SiE}**–**9_{SiE}**) were found to have exergonic formation energies. Among them, the pathways to generate the heavier ketones (**3_{SiE}**) are more likely to appear due to lower energy barriers.

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

Download English Version:

<https://daneshyari.com/en/article/7838816>

Download Persian Version:

<https://daneshyari.com/article/7838816>

[Daneshyari.com](https://daneshyari.com)