

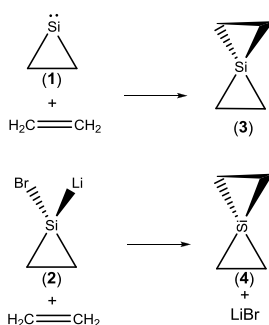
Theoretical Study on Silaspiropentation Reactions of Silacyclopropylidene and Silacyclopropylidenoid

Cem Burak Yıldız^{a,b} and Akın Azizoglu^b

^aDepartment of Chemistry, Faculty of Arts and Sciences, University of Aksaray, TR-68100, Aksaray, Turkey.

^bLaboratory of Computational Chemistry, Department of Chemistry, Faculty of Arts and Sciences, University of Balıkesir, TR-10145, Balıkesir, Turkey.
cbyildiz@gmail.com

Spiropentanes are remarkable strained compounds and they are not easily accessible. Several synthesis methods are available to produce spiropentanes. More recently, Brinker et al have investigated the spiropentation reactions via addition of *gem*-dibromocyclopropane to double bond experimentally and computationally. The synthesized spiropentane was prepared in only three steps from commercially available 1,2,4,5-tetrabromobenzene [1]. The chemistry of heterospiropentanes, compounds in which spiro carbon atom of a spiropentane has been replaced by heavier element of Si have constituted a new challenge in organometallic chemistry [2,3]. Herein, we would like to investigate the concerted silaspiropentation reactions between singlet silacyclopropylidene(1)/silacyclopropylidenoid(2) and ethylene with the help of the Gaussian 09 program using the B3LYP theory and the cc-pVTZ basis set. The concerted reaction of silacyclopropylidenoid (2) with ethylene is examined. We obtained a van der Waals complex for silacyclopropylidenoid (2), whereas not for silacyclopropylidene (1). Moreover, the calculated reaction barrier for the concerted silaspiropentation reaction mechanism of silacyclopropylidenoid is found to be 16.2 kcal/mol, but in this case the reaction is moderately endothermic, by 4.4 kcal/mol. Moreover, the calculated energy barrier of silaspiropentation reaction between silacyclopropylidene and ethylene determined to be 3.9 kcal/mol to overcome.



Scheme 1

[1] K.-J. Su, J.-L. Mieusset, V.B. Arion, W. Knoll, L. Brecker, U.H. Brinker, *J. Org. Chem.*, **2010**, *75*, 7494 – 7497

[2] M. Zielinski, M. Trommer, W. Sander, *Organometallics*, **1999**, *18*, 2791 – 2800

[3] P.N. Skancke, *J. Phys. Chem.*, **1994**, *94*, 3154 – 3160.

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