Research Article

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Switching behavior of an actuator containing germanium, silicon-decorated and normal C_{20} fullerene

Seyyed Amir Siadati,[a,b,*] Solmaz Rezazadeh[c]

[a] *Department of Chemistry, Tofigh Daru Research and Engineering Pharmaceutical Company, Tehran, Iran*
[b] *Department of Chemistry, Qaemshahr Branch, Islamic Azad University, Qaemshahr, Iran*
[c] *Department of Chemistry, Payambar-e-Azam Educational Complex, Islamic Azad University, Tehran, Iran*

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ABSTRACT

NANO MACHINES which are of the capital aims of many advanced research projects are complexes of different devices and actuators that each of them plays a pre-defined role in the overall unit. Nano sensors, nano batteries, nano engines, and nano switches, which contain the most interesting devices for researchers in the related field, are being under consideration for the advance research projects of nano technology. Therefore, in the present project, we have made attempts to reveal the switching behavior of the benzene-C_{20} fullerene system *via* a 1,5-sigmatropic shift of the germanium, and silicon-decorated C_{20} fullerene carbon atoms on the benzene ring.
The results showed that in the case of the silicon-decorated C_{20} fullerene, changing the system from state A to state B *via* changing the temperature (24.7 kcal mol^{-1}) is much easier than that of germanium-decorated (27.5 kcal mol^{-1}) or normal C_{20} fullerene (37.8 kcal mol^{-1}). It seems that further studies on this phenomenon, might be beneficial for designing the thermal sensor systems, and energy storage devices.

1. Introduction

The alkyl and hydride shifts are types of the sigmatropic shifts which have been discovered and used in synthesizing of many natural products during daces [1,2]. The sigmatropic is also a branch of pericyclic reactions which are of the most interested organic reactions [3]. In fact, the sigmatropic is a reaction which results in breaking a one σ-bond and forming another in an uncatalyzed or recently catalyst assisted intramolecular process [4]. A wide range of different types sigmatropic reactions were found and then used for further application, which carbon shifts and hydride shifts are of those sigmatropics [1]. These intramolecular reactions may proceed under thermal or light irradiation conditions and they are allowed or forbidden for passing of the certain reaction channels [5,6]. Being allowed or forbidden in passing the certain reaction channels could be determined by symmetry of the frontier molecular orbitals [7]. These predications follow the *Woodward-Hoffmann* rules about the pericyclic reactions [8], and also the hypothesis of the *Mobius topology* [9].

A [1,5] shift involves the migration of apart of a molecule (especially hydride or alkyl group) from atom 1 to the atom 5, of a π system. Hydrogen has been shown to shift in both cyclic and open chain π network, while; it seems the [1,5] alkyl shifts in an open-chain system is not favorable [10]. However, many reports revealed about rate preferences for [1,5] alkyl shifts in cyclic systems [11].
The [1,5] alkyl shift in absence of the light irradiation must occur in an antarafacial migration (which are impossible for transformations) or the carbon center takes under inversion. But when the light is irradiated to the system and the π electrons of the system become excited, the pattern of the HOMO orbital transforms to LUMO and thus, the [1,5] alkyl shift would be possible [12].
In this work, we have investigated the possibility of [1,5] sigmatropic shift of C_{20} fullerene carbon atoms on the benzene ring, both, in absence and in presence of light irradiation (Scheme 1). The results showed that this sigmatropic process is favorable under light irradiation with triplet excited state. Moreover, the results of the FMO calculations and the DOS plots reveal about the

∗ Corresponding author. chemistry_2021@yahoo.com