



4TH National Conference of Iran Chemistry, Chemical Engineering And Nano

PHOTOISOMERIZATION STUDIES OF NEW AZO TWEezer: THE REPORT ON INTERACTION WITH C₆₀

B. Ghanbari¹, M. Mahdavian²

**¹Department of Chemistry, Sharif University of Technology, Tehran, Iran,
GHANBARI@SHARIF.EDU, ²Department of Chemistry, Sharif University of
Technology, Tehran, Iran, MAHSA.MAHDAVIAN@YAHOO.COM**

Abstract: In the present communication, a novel bimacrocylic tweezer linked through diazobenzene moiety was synthesized and characterized by ESI MS, IR, ¹H and ¹³C NMR, UV-vis spectroscopy as well as CHN microanalysis. UV light was irradiated the tweezer to promote the cis-trans isomerization. The molecular structure of the tweezer was calculated by using DFT method. A significant interaction between the cis isomer of the tweezer with C₆₀ was also found in terms of the association constant calculated by ¹H NMR spectroscopy. More importantly, these calculations suggested a novel unprecedented interaction between the HOMO's of diazobenzene moiety on the tweezer instead of the aromatic groups with C₆₀.

Keywords: azo tweezer, C₆₀, diazobenzene, cis-trans

1. INTRODUCTION

Adjusting three-dimensional arrangement of chemical structures in a reversible ways on the molecular level unlocks enormous possibilities in chemistry, as well as in material and biological sciences [1]. In this background, light suggests superior prospects, as it has typically nondestructive nature and can be applied to several photoactive functional groups to meet the mentioned requirement. Among the photoactive functional groups, azobenzenes have been explored for decades as influential molecular switches and employed in numerous different areas stretching from liquid crystals to biomolecules and switchable catalysts [2]. On the other hand, C₆₀ displays several specific photophysical and electronic properties as electronic, magnetic properties and conducting which present C₆₀ as a potential electron acceptor candidate, frequently applied in electron-transfer components of molecular electronic devices. Basically, the exceptional size and symmetry of the delocalized π -electron on C₆₀ provides it a noble electron acceptor [3].

In continuation of our systematic studies on complex formation of aza-crown host molecules with C₆₀ [4], we found that these molecules were efficient for supramolecular interaction with C₆₀ guest, although they suffered from capability to rapid uncomplexation of the fullerenes. In the present research, we report the synthesis of a new tweezer-like molecule containing azobenzene group in a multistep route. It was expected that the supramolecular interaction of the aza-crown moiety on **L** with C₆₀ could be triggered by photochemical *cis-trans* isomerization process preferentially centered on the aza-conjugated units. Although, a diversity of C₆₀-based high order photo- and/or electro-active systems and donor-acceptor dyads [5], have also been considered and reported, but to the best of our knowledge, this is the first independent example of photochemical-triggered interaction of a host molecule with C₆₀.

2. EXPERIMENTAL

2.1. Materials and general considerations

C₆₀ (98%) was obtained from BuckyUSA and the other reagents were purchased in analytical and/or chemical grade from commercial sources without further purification. ¹H and ¹³C NMR spectra were recorded in CDCl₃ on a Bruker-ARX500