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DFT study of azo linkage effect on homoaromatization of some 1,4-dihydropryridines

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ABSTRACT

1,4-dihydropryridine derivatives revealed various biological activities and pharmacological properties such as antiviral, antibacterial and anti-inflammatory activities. In this research, density functional theory (DFT) calculations at the B3LYP level are used to optimize the geometry of the compounds. In this study, we were interested in evaluation of homoaromaticity of the selected compounds using nucleus independent chemical shifts NICS(0), NICS(0.5), NICS(1), NICS(1.5) and NICS(2), bond lengths, bond angles and HOMO-LUMO gap.

1. Introduction

1,4-dihydropryridines (DHP's) and their derivatives, have shown several biological and pharmacological properties, such as anti-analgesic, anti-tubercular, anti-tumor, anti-inflammatory, hepatoprotective, cardiovascular disease, geroprotective and stress protective activities [1-4].

Computational chemistry is an important part of chemistry which studies the properties of compounds, their reactions and optimization of existing chemical methods by using advanced and specialized soft wares. One the important areas of study is to analyze that the compounds are aromatic or homoaromatic which this is done through theoretical methods. The index of nuclear independent chemical shift (NICS) is one the most famous criteria which for the first time was proposed by Schleyer et al. in 1996, and received attention from many chemists [5]. By this method we can measure magnetic flux in hypothetical points in the center of molecule and at different distances from it, in a way that at the distance $1\ ^{\circ}A$ upper than the middle of the ring, the effects of σ bond decreases in the molecule and by this method we can better analyze the effects of π ~~unstable~~ electrons under field effect. This criterion has been used for justifying aromatic property of many systems [6-13].

Homoaromatic compounds are named according to the number of saturated linkages they contain mono for one interruption etc. such as cycloheptatriene, [14] and dihydro-1,2,4,5 tetrazine, [15] Three types of homoaromatic interactions exist: through-bond, through-space, and transannular. The best established homoaromatic molecules are cationic in nature, and only recently have anionic counterparts been identified as homoaromatic. A truly neutral homoaromatic structure has eluded researchers thus far. The focus of this report will be to review recent efforts towards the synthesis and characterization of neutral and anionic homoaromatic compounds [13, 14].

2. Results and Discussion

The main purpose of this research is to calculate density functional theory (DFT) at level B3LYP of those 1,4-dihydropryridine compounds which have aryl azo bridge in order to study the effects of these bridges on the extent of homoaromatic property of these compounds. For this reason, first, all these structures (Figure 1) have been optimized by using Gaussian 2009