



## A theoretical study about Substituted effect in current ring and aromaticity with NICS index in nano carrier Xylometazoline drug

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### Abstract

Xylometazoline is a drug which is used as a topical nasal decongestant. It is applied directly into the nose, either as a spray or as drops. Xylometazoline is an imidazole derivative which is designed to mimic the molecular shape of adrenaline. It binds to alpha-adrenergic receptors in the nasal mucosa. Due to its sympathomimetic effects, it should not be used by people with high blood pressure, or other heart problems. In this report, At the first compounds [C60- Xylometazoline -C65-X] (X=F, Cl, Br) were optimized, then NMR calculations have been done. The results indicate In all noticed carbons atoms Chemical shielding tensor ( $\sigma$ ) is lowest and chemical shift tensor( $\delta$ ) is highest in R-F. On the other hand with increasing electroneativity in substituted atom, NICS Index shows this trend: R-F>R-Cl>R-Br. nucleic independent chemical shift (NICS) is considered for Aromaticity. If aromaticity is increased, so , stability is increased and reactivity is increased. All calculations is performed in 6-31g\* basis set in HF method and in gas phase.

**Keywords:** Xylometazoline, Fullerenes, Chemical potential, Nano drug carriers.

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### 1. Introduction

Nanostructures can be categorized into following forms according to their structures: diamonds with  $sp^3$  hybridization, Graphite with  $sp^2$  hybridization, Hexagonal diamonds with  $sp^3$  hybridization, fullerenes with  $SP^2$  hybridization, Nanoparticles, Graphene, single-layer and multi-layer nanotubes, Crystal Nanostructures. All these forms of nanostructures produce unique Pharmaceutical and