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# Initial study of the effect of substrates on Tetrahydrozoline and its nano-constituent drugs

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## Abstract

In this paper, the effect of halogen compounds on tetrahedrozoline with nanosized fullerene was investigated. First, the structures of Tetrahydrozoline on a fully vectorized nanoclay were optimized with halogen compounds on carbon 69 (R-X: X = F, Cl, Br; R = C60-Tetrahydrozoline-C69-). Then orbital calculations were performed using NBO technique, and structural parameters and bipolar moments of compounds were also analyzed. The results showed that the energy levels of the molecular orbitals (LUMO and HOMO) in the R-F have the lowest values, and C69-F are the shortest bond and the strongest among the C69-X bonds. Comparison of bipolar moments of compounds shows that the more the halogen is heavier, the lower the dipole moment of the compound. All computations were performed using the Hartree-Fake method and the base series 6-31G * in the Gaussian 2003 software and in the gas phase.

**Keywords:** Tetrahydrosulin, Fullerene, Dipole Moment, LUMO and HOM.

## 1. Introduction

Tetrahydrozoline is a drug that causes vascular contraction and is produced from imidazoline. Figure 1-1 shows the structure of this drug.