



Anti-corrosion studies of a tryptamine Schiff base ligand

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INTRODUCTION

Schiff bases are characterized by the -C=N- (imine functional group). They have found various applications in medicines as anti-inflammatory, antimicrobial and anti-tumor agents. Their other uses include catalysis, herbicidal, antiseptic, dyes and polymers [1]. Recent researches have reported their application as corrosion inhibitors because their electron rich imine centers adsorbed and form corrosion inhibiting surface films [2, 3].

Tryptamine is an alkaloid with an indole ring and a primary amine (Figure 1). It is an important precursor to serotonin (a neurotransmitter). Both **indole** and tryptamine have been reported to have been isolated from plants and animals [4, 5].

Tryptamine Schiff base Several Schiff bases have been studied for the prevention of corrosion, however the tryptamine Schiff base 2-((2-(1H-indol-3-yl)ethyl) methylene) - λ^4 -azanyl)- λ^3 -methyl)-6-methoxyphenol (**HL²**), with chemical formula C₁₈H₁₈N₂O₂ has not been investigated for its anti-corrosion characteristics. Hence this study was done using Density Functional Theory (DFT) to determine the behavior of a previously synthesized and characterised tryptamine Schiff base HL² [6], as an anti-corrosion compound.

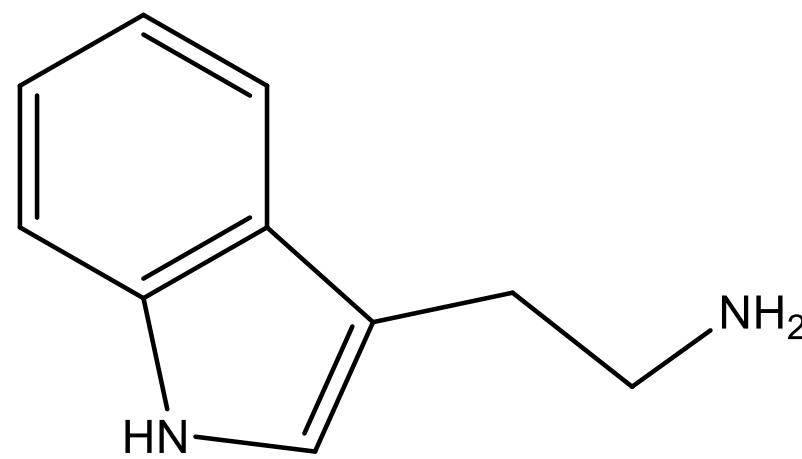


Figure 1: Tryptamine

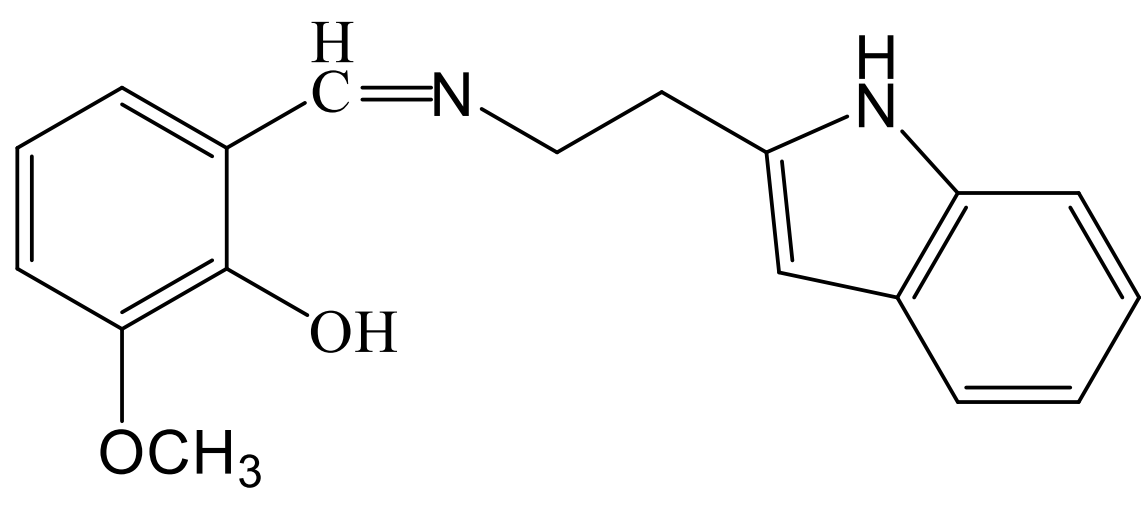


Figure 2: HL²

METHODOLOGY

To study the mechanism of inhibition of HL², the computational simulation of its molecular properties was carried out using Density Functional Theory (DFT) calculations, using the Becke-3-Lee-Yang-Parr exchange (B3LYP), together with the standard double-zeta plus polarization 6-311G (d, p) basis set [B3LYP/6-31G(d)] implemented in the GAUSSIAN 03 software. Chemical parameters obtained include:

- ✓ Energy gap (ΔE),
- ✓ absolute electro negativity (χ),
- ✓ global hardness (η)
- ✓ softness (σ)
- ✓ number of transferred electrons (N)
- ✓ back donation (ΔE_{d-b})

RESULTS AND DISCUSSION

The results obtained from the DFT calculations of the molecules of the HL² are presented in Table1. Frontier molecular orbital maps are also presented in Figures 3 and 4.

Table 1: Electronic properties of HL² calculated by DFT

Compounds	E _{HOMO}	E _{LUMO}	ΔE eV	IP eV	EA eV	χ eV	eV	σ Ev	ΔE_{b-d}
HL ²	-5.5725	-1.4895	4.0830	5.5725	1.4895	3.531	2.0415	0.4898	-0.5104

Frontier molecular orbital diagrams of HL²

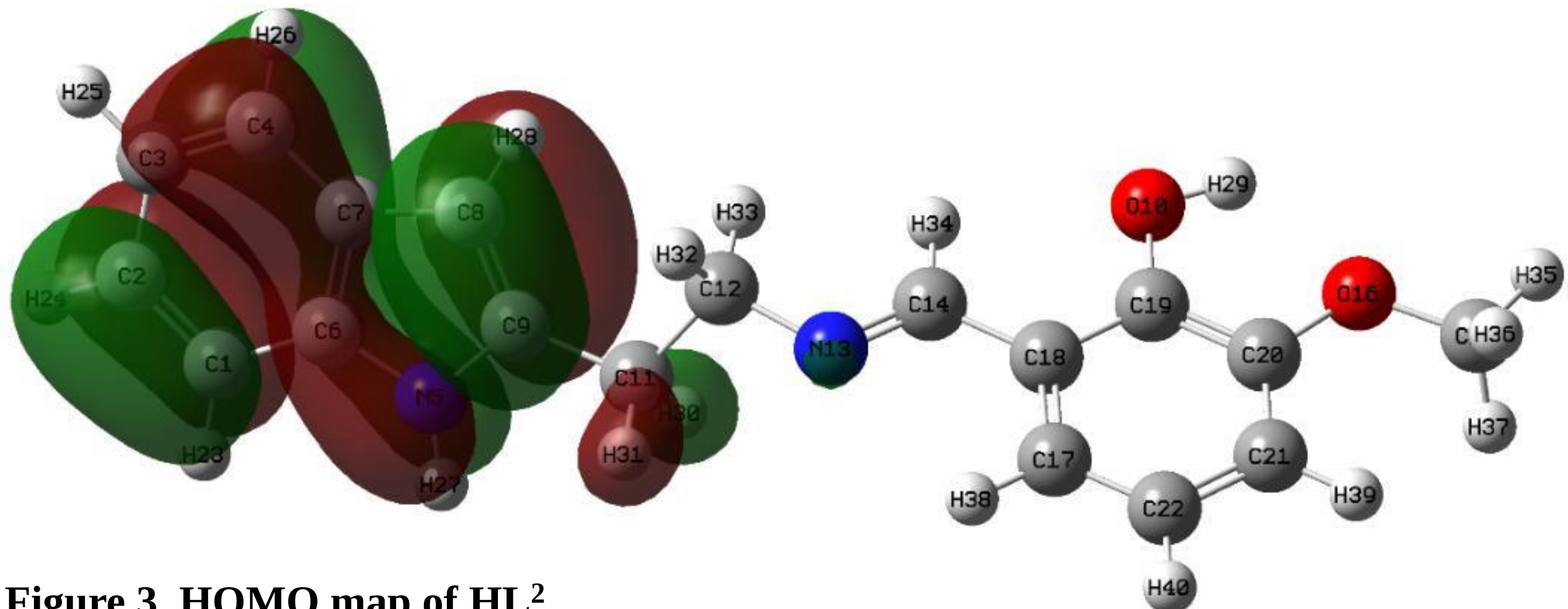


Figure 3. HOMO map of HL²

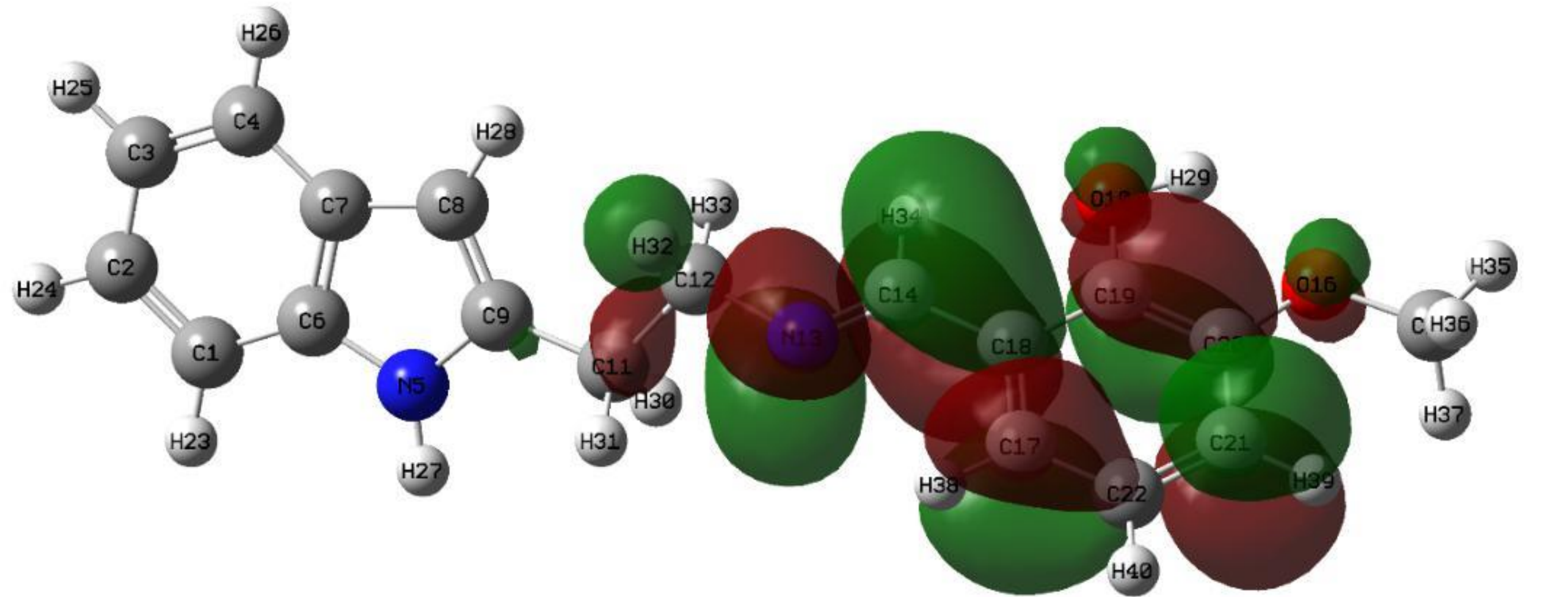


Figure 4. LUMO map of HL²

CONCLUSION

The energy of highest occupied molecular orbital (E_{HOMO}), energy of lowest unoccupied molecular orbital (E_{LUMO}), energy gap (ΔE), and electronegativity (χ) values obtained for HL² using the Density Functional Theory at B3LYP/6-311G are all in agreement with values reported for effective transfer of electrons between an inhibiting system and metal surface [7,8]. Hence, HL² has a good potential to act as a corrosion inhibitor

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