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# Absorption of tranylcypramine on C60 nanocage: Thermodynamic and electronic properties

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**Abstract**: Reactivity characteristics of Tranylcypramine and adopting on C60 (ih) in gas and water phases have been focused in the present work, using DFT B3LYP/6-311+G (d, p). Calculation of chemical structure (dipole momentum), thermodynamic features (gibbs free energy, enthalpy, entropy, as well as thermal capacity) and electronic parameters (σ, μ, ω, χ and η) were carried out. Based on the calculations of HOMO and LUMO energy, Tranylcypramine indicated the properties of stability and reactivity. There are two active sites for Tranylcypramine, which both show thermodynamic stability.

**Keywords**: DFT, Tranylcypramine, C60, bucky ball, reactivity, stability.

## INTRODUCTION

Tranylcypromine can be defined as a non-hydrazine monoamine oxidase (MAO) inhibitor which acts and it is used in a similar capacity as phenelzine; however, it has less prolonged inhibition. The half-life of Tranylcypromine has been reported between 90 to 190 minutes. It has structural relations with amfetamine and in case of overdose, its metabolism to amfetamine occurs (Cheeseman *et al*., 2000; Kuganathan *et al*., 2019). Catalysis of the oxidative deamination of the neurotransmitters (noradrenaline, dopamine, serotonin), a primary amino group to the relative aldehydes, takes place by Monoamine oxidase (MAO) as a flavoprotein that exists in mitochondria1 membranes. The aldehyde is then converted into relative alcohol or carboxylic acid by other enzymes. The additional neurotransmitters are catabolized by MA0 after inducing their action. The transmitter action is prolonged due to interferences in the activity of MA0, which are reported as useful therapeutic factors in depression treatment (Cheeseman *et al*., 2000; Ghasemi *et al*., 2018). Trans (+)-2-Phenylcyclopropanamine (Tranylcypromine) (I) is a monoamine oxidase (MAO) inhibitor which is mainly applied in psychiatric depression treatment. It inhibits MAO and other enzymes through blockage of oxidative deamination of different naturally-occurring monoamines (sympathomimetic, 5-hydroxytryptamine) I. It also shows some impacts which are not associated with enzyme inhibition. "I" has applications in conditions of close medical control due to acute and chronic toxicities, which are dependent on their dose. The approach of brain-specific chemical delivery system (CDS) has the potential of enhancing utilization of I in therapeutic applications through dosage reduction. It consequently extends drug presence at the site of receptor and reduces toxicity. Successful application of the dihydropyridine-quaternary pyridinium s~lt- type redox carrier-based CDSs has been reported in different drugs, while the functional principles are clearly defined (Petrovic *et al*., 2012, Ralser *et al*., 2016).

Backy ball (C60) has applications as an absorbing agent (Kang *et al*., 2011; Saraswati *et al*., 2019) in several toxic, as well as nontoxic chemical ingredients (Mallawaarachchi *et al*., 2018), dyes (Kalaugher, 2005), and wastewater (Wang *et al*., 2002; Adolfsson-Erici *et al*., 2002; Zhao *et al*., 2020; Lopez-Fernandez *et al*., 2012). Theoretical calculations in all disciplines (Shirai *et al*., 2005) including nanocage (Kang *et al*., 2011) have been performed using density functional theory (Yavuz *et al*., 2009; Garelli *et al*., 2005; Takzare *et al*., 2019; Ceulemans *et al*., 2008; Muya *et al*., 2009) and molecular dynamic calculations (Jo *et al*., 2018; Wang *et al*., 2020; Xu *et al*., 2013).

The present work has applied backyball (C60) as an absorbent for Tranylcypramine in gas and water phases by density functional theory with 6-311+G(d, p) basis set.

## MATERIALS AND METHODS

### *Method of Computation*

Application of the chemical quantum estimations has been used because of the Gaussian 03 (GESMJ *et al*., 2009) package that runs on the supercomputer. The three parameter hybrid functional of Becke B3LYP and the 6-311+g(d, p) basis set were used for full geometry optimizations, electric field gradient, thermodynamic features, and electronic parameters. The current work has been used Backyball C-C (C60 ih) as an absorbent. The following formula was used to calculate the energy of absorption:

$E_{ads}=E_{(B\text{-}T)}-(E_{\text{ Tranylcypramine}}+E_{backyball})$

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## RESULTS

According to the calculation results of prior studies, nanocage adoption with metallic atoms is accompanied with efficient modifications of electrical features, chemical activities, and the potential to react in them (Lee *et al*., 2008). Thus, B3LYP/6-311+G(d, p) has been used used in the present work to optimize all the structures, including Tranylcypramine and buckyball (C60, fullerene), as well as adopted Tranylcypramine on buckyball. Tranylcypramine optimized structure is shown in fig. 1. Tranylcypramine has two active sites, namely N and phenyl rings. Each site has its own chemical and electrochemical position in Tranylcypramine, as shown in fig. 2. Various effects for reaction on chemical reactions have been reported for TDensity electrons in each positions. It is possible to obtain more desirable chemical behaviors in gas phase by the presence of phenyl ring.

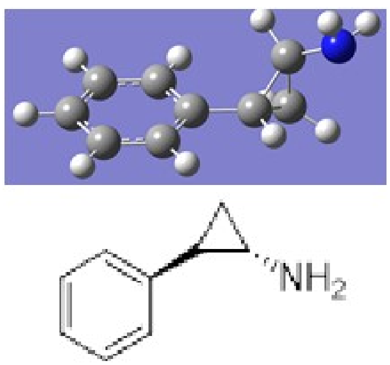


**Fig. 1**: Optimized structure of Tranylcypramine by B3LYP/6-311+G(d, p)

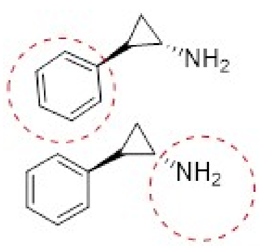


**Fig. 2**: Different Active Place in Tranylcypramine

## DISCUSSIONS

HOMO and LUMO energies can be considered as significant features of chemical reactivity. Larger amounts of LUMO are related to the higher electron acceptance capacity in molecules. HOMO and LUMO energies are responsible for recognition and prediction of how strong or stable chemical compound are. Given the energies of these frontier orbitals near orbitals with different energy levels, the highest electron excitations take place at HOMO-LUMO band gap energy. Particularly, in the case of large chemical aromatic systems, small HOMO-LUMO band gaps result in $\pi$ electrons which are mobile. Thus, the electron can easily jump to higher energy levels close in energy. Higher energy distribution across the molecule takes place due to greater $\pi$ electrons mobility, leading to more stable conditions. Therefore, higher stability will result from smaller gaps of HOMO-LUMO. The $\pi$ electrons mobility indicates good conductivity of large aromatic systems (such as graphene nanoribbons), which makes them excellent semiconductors because of small conduction band gap, which leads to electrical current of the electrons movement. The HOMO and LUMO can be regarded interesting issues because of providing valuable insights into the reaction conditions according to the interaction of orbitals to control the reaction outcomes. Weak electrons are provided by HOMO energies for reaction in chemical conditions. Tranylcypramine shows high participation in chemical reactions because of HOMO energy. It also donates electrons in all chemical reactions due to electro negativity of atoms (O, Cl) in Tranylcypramine chemical structure. The Details of Tranylcypramine frontier (HOMO and LUMO) orbitals are shown in table 1.

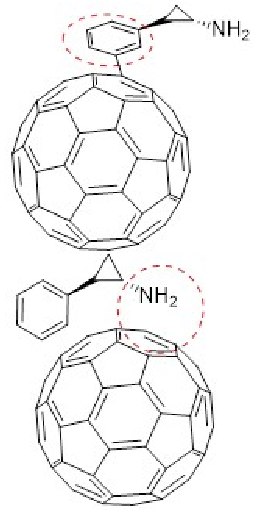


**Fig. 3**: Tranylcypramine -C60 Complexes in Different Active Side (three different position)

Compounds polarity in reaction media is introduced by dipole momentum of chemical compounds. As shown in table 1, Tranylcypramine dipole momentum equals 1.2936 D in gas, indicating Tranylcypramine polarity due to electronegative atoms in Tranylcypramine (N atom) chemical structure.

**Table 1**: Energy Data and Dipole Momentum of Tranylcypramine by B3LYP/6-311+G(d, p)

| Tranylcypramine | Gas |
|---|---|
| Energy | -1061.93kJ |
| Dipole moment | 1.2936 |
| HOMO | $-380.49\times10^{19}$eV |
| LUMO | $-26.24\times10^{19}$eV |

**Table 2**: Electronic Parameters of Tranylcypramine in Gas and Water Phase by B3LYP/6-311+G(d, p)

| Tranylcypramine | IP (eV) | EA (eV) | μ (eV) | η (eV) | χ (eV) | σ (eV) | ω (eV) |
|---|---|---|---|---|---|---|---|
| gas | 380.49E19 | 26.24E19 | -203.36E19 | 177.12E19 | 203.36E19 | 5.64E-22 | 1.16E21 |

There are three active sites of Tranylcypramine for adopting C60, as shown in fig. 3. C60 has (ih) symmetry which means that all sites have similar conditions for participation in chemical reactions. In other words, it does not matter which position is considered in reactions. The principal and optimized buckyball structure can be observed in fig. 4.

**Table 3**: Energy and Dipole Momentum in Tranylcypramine-C60 Complexes

| | 1 | 2 |
|---|---|---|
| E(kcal/mol) | -2050.214 | -2045.206 |
| μ(D) | 1.6817 | 1.8541 |
| ΔE(ads/kJ) | -6810.639 | -6789.605 |

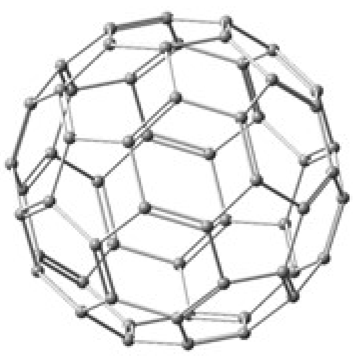

**Fig. 4**: Optimized Structure of C60(ih) by B3LYP/6-311+G(d, p) E(-738.33kJ)

The capacity of performing works and supplying heat is called energy. The energy saved in chemical bonds is called chemical potential, which can be regarded as a significant thermodynamic property. Chemical potential can be applied in different sciences related to materials, including chemistry, physics, biology, as well as chemical engineering. It makes calculation of all chemical materials' thermodynamic parameters possible at different spatial pressures and temperatures.

Assuming that the pressure and temperature are constant, it is possible to determine how stable the substances, chemical compounds and solutions are through chemical potential. Given the value of chemical potential μ for Tranylcypramine which is -203.36 in gas phase, Tranylcypramine shows stability in gas phase. Energy negativity indicates hidden energy in Tranylcypramine chemical bonds and its activity. The definition of the atom's energy is based on the loss or gain of energy by the atom, due to chemical reactions, which results in a loss or gain of electrons. A chemical reaction, in which energy is released, is known as an exothermic reaction. On the other hand, a chemical reaction, in which energy is absorbed, is known as an endothermic reaction. The former leads to negative energy, which is indicated by a negative sign; however, the latter leads to positive energy, which is indicated by a positive sign. In the case of adding an electron to a neutral atom ($1^{st}$ electron affinity), the release of energy will takes place, which means that the first electron affinity is negative.

Nevertheless, adding an electron to the negative ions ($2^{nd}$ electron affinity) requires higher amounts of energy. Accordingly, there is an energy release from the process of electron attachment, which leads to positivity of electron affinities. Tranylcypramine shows positivity in electron affinity energy (EA), indicating its reluctance to donate electrons. Reactivity parameters of a molecule, such as electro negativity (χ), softness (σ), hardness (η), as well as electrophilicity index (ω), were obtained based on the theory of Koopman using the DFT technique. Electro negativity (χ) can be defined as value of power attraction of atoms or molecules, which is obtained from HOMO and LUMO. η leads to stable and reactive chemical molecules. σ parameter indicates the potential to accept electrons of chemical molecules. Tranylcypramine reactivity parameters in gas and water phases are shown in table 2. As it is found in the study, Tranylcypramine is significantly stable and reactive in chemical reactions. In fact, adopting Tranylcypramine on C60 took place. The energy of every complex in fig. 3 is shown in table 3. According to the dipole momentum of every complex, all active sites have the ability of acting in polar media. Based on the relative adopting energy, among all active sites led to structural stability in chemical media, structure 1 had the highest stability.

## CONCLUSION

Tranylcypramine chemical reactivity and its adopting on bulky ball (C60) was studied in this research with the application of DFT B3LYP/6-311+G(d, p) in gas phase. It was found from the chemical structure and electronic parameters that Tranylcypramine was active and capable of adopting on C60 while keeping its stability. There are three active sides for Tranylcypramine, which all of them show thermodynamic stability, while structure 1 shows the highest stability of all.

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