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# Theoretical investigation about reactive properties of the Atrazine® herbicide

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**Abstract** – It is important understand the structure and reactivity chemical of the herbicides due to yours half-life in the environment. Atrazine herbicide degradation mechanism is dependent of several decomposition steps, which difficult your elimination of the ground. In this way, the present work shows a theoretical investigation based on computation chemistry about Atrazine herbicide identifying the HOMO and LUMO orbitals responsible by reactivity chemical of this herbicide.

6-clorine-N-etil-N'-(1-metiletil1)-1,3,5-triazine-2,4-diamine is known as Atrazine® and your structure chemical is shown in the Fig. 1b. This molecule can be degraded by chemical and microbiological process, where is yielding, mainly, the hidroxiatrazine and alquiles. Researchs report alterations in the development of frogs using low concentrations in relation to concentrations found in natural waters. Other investigations showed development of tumors in the pituritary and mammary glands of female rats[1,2]. Half-life of the Atrazine herbicide on ground is around 35 to 45 days depending of the factors: physical-chemistry, climatic conditions and existence of the microorganisms[3]. The aim of this work is present a theoretical investigation about structure molecular of the Atrazine molecule analyzing oxi-reductor properties, electronic density and wavelength excitation of the HOMO and LUMO orbitals.

Theoretical methodology employed in this work was choose to yield the equilibrium geometry and electronic properties of the Atazine® molecule. It is based on Density Functional Theory (DFT) with B3LYP functional and 6-31G(d,f) basis set for all atoms. It was analyzed the HOMO and LUMO orbitals density electronic and optical gap properties to investigate reactive properties of this system.

HOMO e LUMO orbitals were choose because represent the features of oxidation and reduction of a chemical system, respectively. In the Fig. 1a is shown the electronic density of the HOMO orbital. It is observed that the electronic density is localized, mainly, on nitrogen atoms of cycle and peripheral groups showing that the probability of any oxidation mechanism must occur on these atoms. In the Fig. 1c is shown the electronic density of the LUMO orbital which indicates that the probability of any reduction mechanism is associated to the atoms of the triazinic cycle. This simulation about HOMO and LUMO orbital of the Atrazine® herbicide demonstrated which regions with more probability of interaction in relation to oxi-reduction mechanisms.

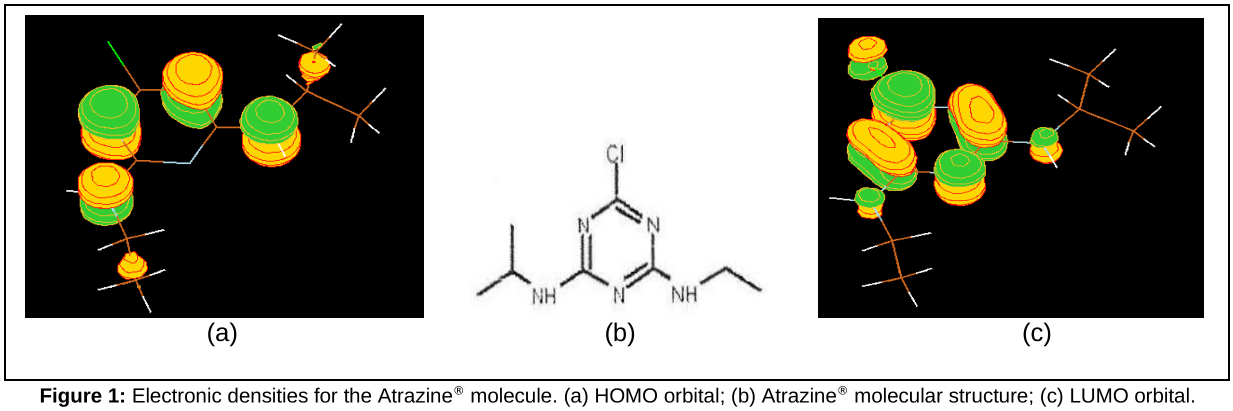


**Figure 1:** Electronic densities for the Atrazine® molecule. (a) HOMO orbital; (b) Atrazine® molecular structure; (c) LUMO orbital.

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