ISBN 978-85-63274-02-4

# International Conference on Food and Agriculture Applications of Nanotechnologies

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São Pedro, SP
2010

1st Edition
1st print: 500 copies

Anais da 1. International Conference of Food and Agriculture Applications of Nanotechnologies – São Pedro: Aptor Software, 2010.
284 p.

ISBN 978-85-63273-02-4

1. Nanotechnologies – Events. 2. Ribeiro, Caue. 3. Assis, Odílio Benedito Garrido de. 4. Mattoso, Luiz Henrique Capparelli. 5. Mascarenhas, Sergio

International Conference on Food and Agriculture Applications of Nanotechnologies

NanoAgri 2010

# Simulation of the structure molecular and HOMO and LUMO orbitals of the Linuron herbicide

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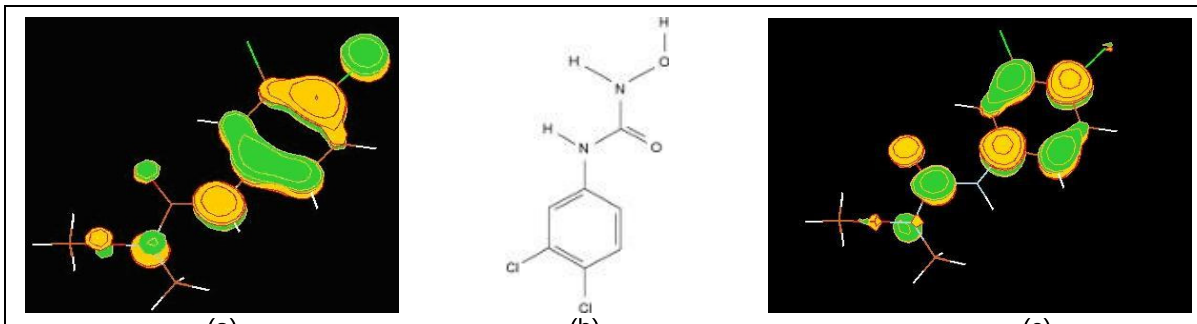
**Abstract** – It is important understand the structure and reactivity chemical of the herbicides due to yours half-life in the environment. Linuron herbicide degradation mechanism is dependent of several decomposition steps, which difficult your elimination of the ground. In this way, the present work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

Linuron herbicide has molecular formula $C_9H_{10}Cl_2N_2O_2$ with aqueous solubility of 81 mg.$L^{-1}$ at 25ºC. Its molecular geometry is shown in the Figure 1b. This herbicide is selective and it absorbed by root and, mainly, by leaves of plants. Linuron's herbicide action is based on interruption of the photosynthesis through Hill's process [1]. It is usual find Linuron in mixture with other herbicides such as Atrazine®, Metribuzin and Oxadiazon [2]. Aim of this work is present a theoretical investigation about structure molecular of the Linuron 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 Linuron 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 Linuron herbicide demonstrated which regions with more probability of interaction in relation to oxi-reduction mechanisms.




(a) (b) (c)

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

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