Commun. Comput. Chem
doi: 10.4208/cicc.2018.v6.n1.1

Vol.6, No.1, pp.1-12
Apr. 2018

REGULAR ARTICLE

Semi-Empirical and HOMO, LUMO Studies of Some Chlorinated Pesticides Compounds

Mamoun S.M. Abd El-Kareem*, M.A. Rabbih, E.T.M.Selim

Molcular and atomic physics unit., Experimental Nuclear Physics Dept., Nuclear Research Centre, Egyptian Atomic Energy Authority, Inshas, Cairo, Egypt

Received 7 Feb. 2018; Accepted (in revised version) 10 Apr. 2018

Abstract: Theoretical studies on some chlorinated pesticides compounds namely: Heptachlor, Heptachlorepoxide and Chlordane as a first group, Aldrin and Endrin as a second group, and DDT, Methoxychlor as a third group, were performed using semi-empirical quantum chemical calculation. Modified Neglect of Diatomic Overlap MNDO method was used to investigate the effect of positional variation of chlorine and oxygen atoms on the electronic and structure properties of the studied chlorinated pesticides. The structure optimization of some electronic parameters such as heats of formation, total energies, electronic energy, binding energy, nuclear energy, ionization energies, electron affinities and dipole moment were calculated and discussed. The energy of the Highest Occupied Molecular Orbital (HOMO) and the energy of the Lowest Unoccupied Molecular Orbital (LUMO) are also calculated. The LUMO - HOMO energy gap have been calculated and discussed. The stability and activity of the studied compounds based on the obtained values have been investigated.

Keyword: Semi-empirical calculations, HOMO & LUMO calculations and chlorinated pesticides.

1. INTRODUCTION

Pesticides found their way into wide applications and have played a significant part in constantly boosting agricultural and animal production. The hazards have brought along

* Corresponding author:mamoun_sarhan@yahoo.com

with them to food safety and human health has increasingly become the focus of world attention.[1-3]

Organochlorine pesticides are of great concern due to their occurrence at high concentrations in aquatic ecosystems; despite bans on production and usage.4 Many of the organochlorine compounds are substances that have high toxicity. They accumulated in organisms and biomagnified through the food chain, so consumption of fish from contaminated areas may be a real health risk for the consumers.[5]Most of these compounds are considered to act as environmental hormones, which disrupt reproductive cycles of wildlife and believed to be possible carcinogens or mutagens.[6]

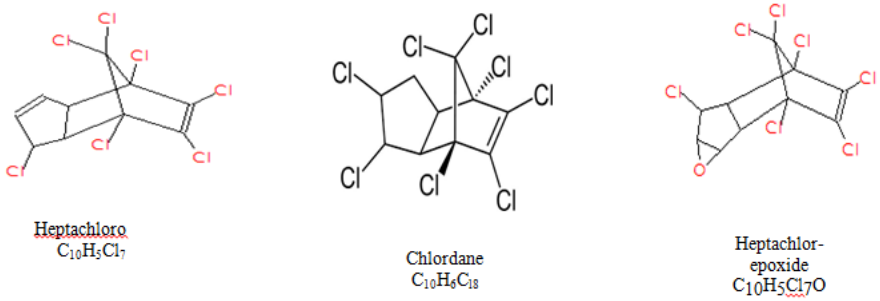

Figure 1: The chemical structures of Group (I).

Semi-empirical, Density Functional Theory, Molecular Mechanics and Ab-initio methods are often employed to investigate fundamental problems and to calculate geometrical and substantial parameters of theses chlorinated pesticides. These methods give information on the total energy, electron affinity, proton affinity, molecular geometry, heats of formation, charge densities, dipole moments, population analysis, chemical reaction pathways and thermodynamic properties. Semi-empirical methods provide the information of Primary calculations of different chemical properties using several methods viz. MNDO (Modified Neglect of Diatomic Overlap), AM1, PM3 and ZINDO9. [7-8]

Since the other quantum chemical calculation methods are time consuming, so, semi-empirical MNDO use with reasonably good results.[9] Also, authors have been used MNDO method in the investigation of the volatile components in basil oil and ginger extract.[10-11]

The frontier molecular orbital such as highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of the chemical species are serious in defining organic compounds reactivity. [12-13]

Few papers are dealing with pesticides structural elucidation, understanding its structure- activity relationship using quantum chemical calculations (semi-empirical methods) to predict their physical or thermochemical properties. The work of ZHU XiuHua