International Journal
of Discoveries and Innovations in Applied Sciences
Vol. 5 Issue 1 | **pp.** 18-22 | **e-ISSN:** 2792-3983
Available online @ https://oajournals.net/index.php/ijdias

OPEN ACCESS JOURNALS

Recognizing Some of the Structural Properties of a Group of Aromatic Compounds

Hakima Salman Jabr[1], Hanan dakhil idan alsaeedi[1]

1. Babylon university, College of Science, Physics Department, Babylon, Iraq
* Correspondence: autor@gmail.com

Abstract: Two components form organic compounds , Because of their association with fats, the former are referred to as aliphatic products. The second category of compounds is known as aromatic compounds, and is characterized by the presence of dimerization bonds resulting in a special ring system. In this paper, a group of aromatic compounds were studied using the hybrid function with three coefficients B3LYP with the base function 6-31G as one of the levels of the density functional theory. The calculated electronic properties included total energy, energies of the occupied upper molecular orbital and the lower unoccupied molecular orbital, energy gap, ionization energy, electronic affinity, electronegativity, electronic elasticity, chemical hardness, modulus of formation with medium, electronic density, and electrostatic potential. Calculations of the density function theorem were made using the Gaussian 09.

Keywords: Organic compounds ,(DFT), Graphene sheets, Gauss program.

Citation: Hakima Salman Jabr, Hanan dakhil idan alsaeedi. Recognizing Some of the Structural Properties of a Group of Aromatic Compounds Journal of Discoveries and Innovations in Applied Sciences 2025, 5(1), 18-22.

Received: 20th Apr 2025
Revised: 28th Apr 2025
Accepted: 7th May 2025
Published: 17th May 2025

1. Introduction

Homogeneous petroleum blocks are widely used in the production of plastics, fuels, perfumes and pesticides. In addition to the production of coatings and electrical insulators, the company operates in the pharmaceutical sector [1-2]. Many homogeneous and heterogeneous organic groups can be understood using benzoin as a basis. Brazens are the additional components in the components of the components that represent guest accounts and sensory groups, which affects its properties and industrial uses[3]. The presence of conjugated bonds, flatness, resistance to addition reactions, fulfillment of Huckel's rule, and electrophilic substitution are some of the requirements that must be met for a compound to be classified as aromatic[4]. Although aromatic compounds usually have a lower density than water, they can dissolve in nonpolar organic solvents because they are nonpolar [5]. Its properties can be enhanced by adding terminal groups, and it increases with increasing molecular weight, and it is stable, indicating that the electron distribution is even, and it has a unique odor[6-8]. As a result of these distinctive properties, they are used in many industries, but at the same time they have disadvantages. This study has dealt with homogeneous benzene complexes, represented by (Phenanthrene, Biphenyl, Pyrine, Coronene, Anthracene and Naphthalene) and we used in the calculations the density functional, which is a method for obtaining the electronic structure of the molecule, which shows that the density of the electron determines the wave function and the total energy of the system. Medium range for other electrons .Phenanthrene (C14H10) is a polycyclic aromatic hydrocarbon, a colorless solid that resembles a crystal, but can also appear yellow[9]. It is used in the manufacture of dyes, plastics, pesticides,

explosives and medicines, and was also used to make bile acids, cholesterol and steroids. **Biphenyl** ($C_{12}H_{10}$)A compound of two benzene rings bonded by a single bond whose density is evenly distributed over the two rings and is less effective compared to larger compounds. Pyrene ($C_{16}H_{10}$) consists of four aromatic rings and the electronic density is evenly distributed. **Coronene** ($C_{24}H_{12}$) It consists of six continuous gasoline rings, the rings are homogeneous in density due to resonance. Anthracene ($C_{14}H_{10}$) is also called paranaphthalene or green oil, a solid polycyclic aromatic hydrocarbon consisting of three benzene rings derived from coal-tar, is the simplest tricyclic aromatic hydrocarbon. **Naphthalene** ($C_{10}H_8$) **It consists of two benzene rings, and because of resonance the density is evenly distributed over the double bonds within the rings. [10-12].**

Theoretical Parts

Density functional is crucial in determining the electron density and determining the ground state properties of the system. A large variety of molecular properties can be accurately described by hybrid function. The calculations in this study are performed using Koopman's theory. The electron affinity of a molecule or atom is defined as the amount of energy change when an electron is added to a neutral atom to form a negative ion[13-14]. In this research, the electronic affinity, ionization energy, hardness, and the electrophilicity index with the medium were calculated. The energy gap and Fermi energy were also calculated, as shown in the equations below.

$IE = -E_{HOMO}$ …….. (1)

$EA = -E_{LUMO}$ …… (2)

$W = K^2 / 2H$ …..….. (3)

$H = (IE-EA) / 2$ …….. (4)

$$S = \frac{1}{2\eta} = (\frac{\partial^2 N}{\partial E^2})_{V(r)} = (\frac{\partial N}{\partial \mu})_{V(r)} \quad \text{……..(5)}$$

RESULTS AND DISCUSSION

The results obtained indicate that when the size of the compound increases or the number of aromatic rings in the compound increases, the Fermi energy becomes less negative, which indicates an increase in the stability of the electrons and a decrease in the energy gap as shown in Table (1). The Fermi energy is used to explain the electronic transition in organic materials, such as organic semiconductors, which means that it affects the optical and electronic properties, such as the property of light absorption. As for the electronic affinity, which represents the amount of energy absorbed when the atom gains an additional electron, one of the factors that affects it is that the smaller the size of the atom, the greater the electronic affinity, and its value also becomes high in the case of aromatic compounds, where the electronic distribution is stable, and it increases with the increase in the number of rings as in accordance with figures (1-4) , as it is more stable due to resonance. As for the hardness values of the studied compounds, hardness refers to the ability of the molecule to resist deformations, such as bending or twisting due to chemical reactions or physical effects. The more number of rings, the more the electronic interference and hardness as shown with figures (5-7) . We notice that in the coronine compound the hardness value is high compared to other compounds as shown in Table (2). As for the solubility factor or electrophilicity with the matter, which represents the ability of the molecule to interact or dissolve in a certain medium such as water or some other organic solvents, we conclude that the naphthalene compound is characterized by its weak solubility in water, but it is a good solvent in ethanol, while anthracene is less soluble in water, and the reason is the large molecular size of the compound. The experimental results agree well with these findings [15-16].

Structure	EHOMO (eV)	ELUMO (eV)	Eg (eV)	EF (eV)	ET (eV)
Phenanthrene	-5.82152134	-0.93687473	4.8846466	-6.2899587	-14678.12759
Biphenyl	-6.0816585	-0.66612528	5.4155332	-6.4147211	-12604.2585
Pyrene	-5.38641745	-1.44871364	3.9377038	-6.1107743	-16752.03861
Coronene	-8.31785848	-1.0585079	7.2593506	-8.8471124	-25080.06921
Anthracene	-5.51675	-1.93198	3.5847	-6.48274	-14682.1
Naphthalene	-5.82097712	-0.9605483	4.8604288	-6.3012513	-63199.72

Table No. (1) Shows the electronic characteristics of the facilities under investigation .

Structure	IE (eV)	EA (eV)	H (eV)	S (eV)-1	W (eV)
Phenanthrene	5.822	0.937	5.353084	2.67654	105.894
Biphenyl	6.082	0.666	5.748596	2.8743	118.273
Pyrene	5.386	1.449	4.662061	2.33103	87.0443
Coronene	8.318	1.059	7.788605	3.8943	304.812
Anthracene	5.517	1.932	4.55076	2.27538	95.6249
Naphthalene	5.821	0.961	5.340703	2.67035	106.028

Table No. (2): Presents additional calculated structure characteristics

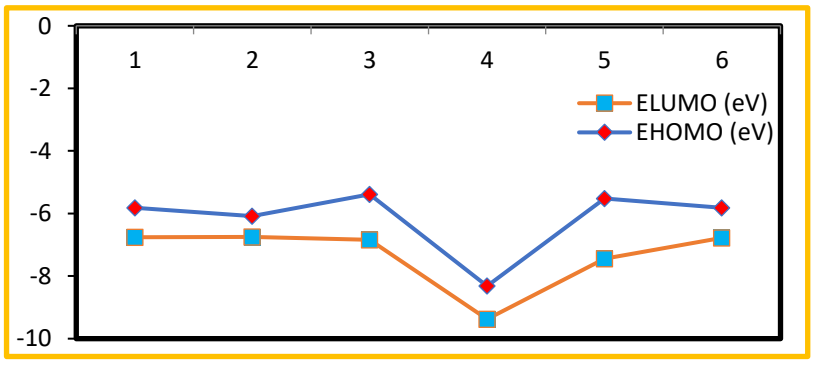

Figure (1) : Electronic states for HOMO and LUMO.

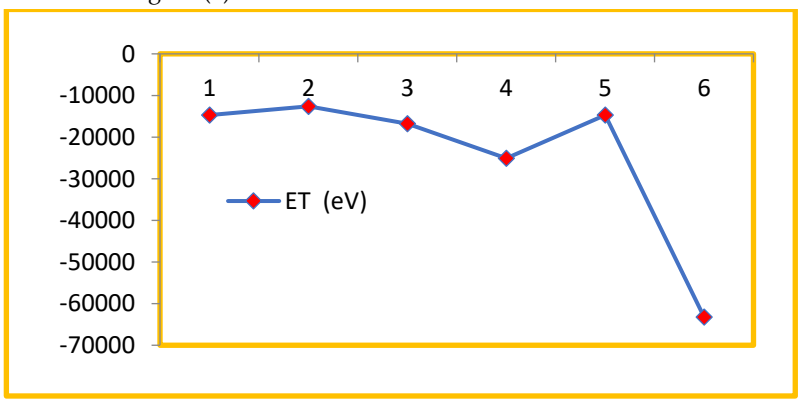

Figure (2) : Total amount of energy examined.

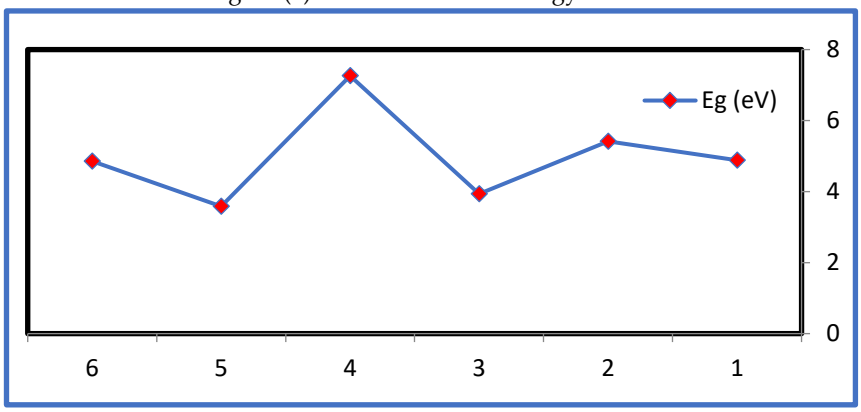

Figure (3) : The energy gap being investigated.

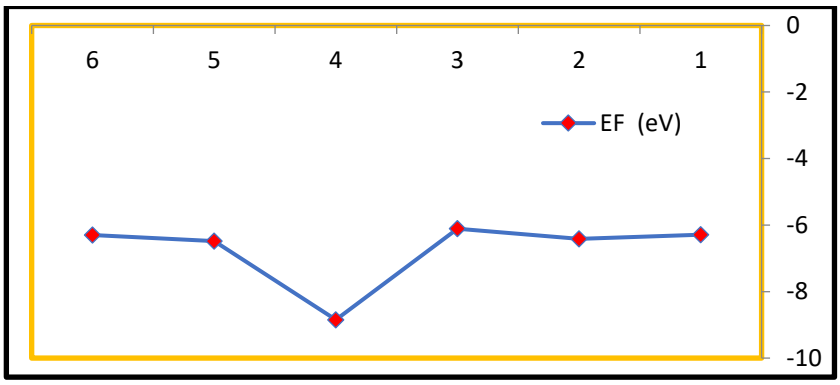

Figure (4): Fermi energy under investigation

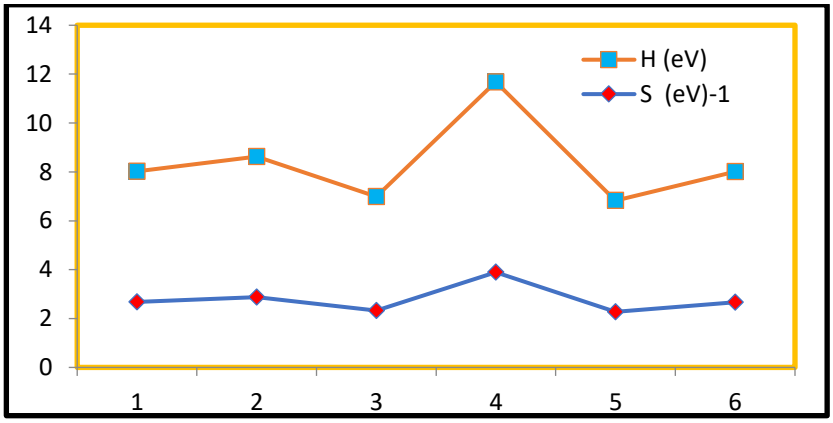

Figure (5) : Study of softness(S) and chemical hardness (H) conditions.

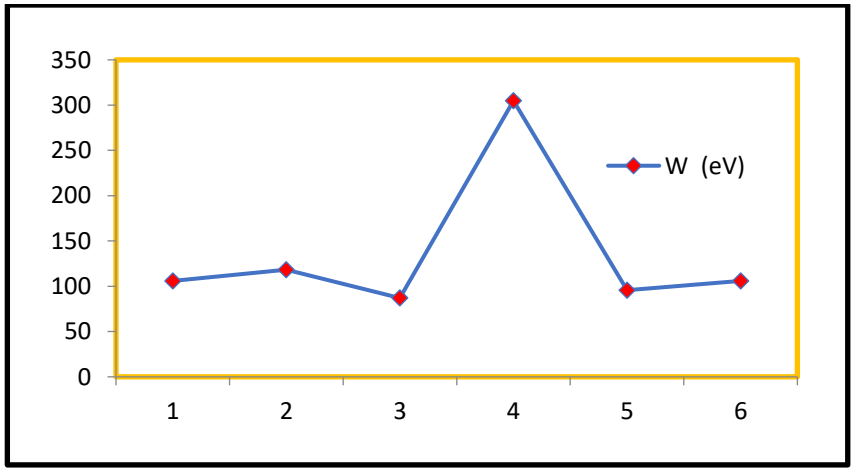

Figure (6) : Calculation of the electronegativity index of the medium

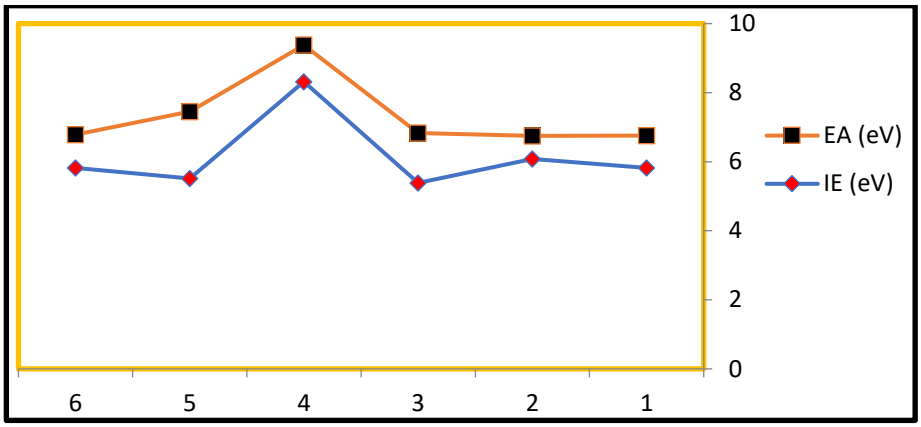

Figure (7): Shown curves for The ionization energy (IE) and electron affinity (EA) .

Conclusion

The main electronic properties of each of the following compounds were determined in this study (Pyrene, Phenanthrene, Biphenyl , Coronene, Anthracene and Naphthalene) were found, such as the energy gap and Fermi energy, Which depends on the number of rings; as it increases, the energy difference between HOMO and LUMO decreases. Consequently this causes a decrease in Fermi's energy and thus the total energy decreases. Regarding the remaining attributes, like ionization energy, we observe that it decreases when the number of rings increases, and the more stable the compound becomes, the less the electronic affinity, Additionally, the energy gap determines the hardness; a large gap indicates high hardness. These characteristics were examined using the density function theorem, which was created using the Gaussian 09

References

(1) Balakshin, M. Y., Capanema, E. A. ,"Comprehensive Structural Analysis of Biorefinery Lignins with a Quantitative 13C NMR",Approach. RSC Adv., 5 (106), 87187−87199, 1, 200-212, 2015.
(2) Franco, I., Solomon, G. C., Schatz, G. C., Ratner, M. A., J. Am. Chem. Soc., 133, 15714, 2011.
(3) Vazquez, H., Skouta, R., Schneebeli, S., Kamenetska, M., Breslow, R.; Venkataraman, L.; Hybertsen, M. S., Nature Nanotech., 7, 663, 2012.
(4) Fernández, I.; Wu, J. I.; Schleyer, P. v. R., Org. Lett., 15, 2990, 2013.
(5) Daryna Diment, Oleg Tkachenko, Philipp Schlee, Nadine Kohlhuber, Antje Potthast, Tetyana M. Budnyak, Davide Rigo, and Mikhail Balakshin ,"Study toward a More Reliable Approach to Elucidate the Lignin Structure−Property−Performance Correlation", 2024.
(6) Hakima Salman Jabr," THE INFLUENCE OF ADDING ALUMINUM ATOMS ON PROPERTIES OF GRAPHENE SHEETS USING DFT", Synergy: Cross-Disciplinary Journal of Digital Investigation, (ISSN 2995-4827), VOLUME 02ISSUE 9,2024.
(7) Limacher, P. A.; Lüthi, H. P., WIREs Comput. Mol. Sci., 1, 477, 2011.
(8) Miessler, Gary L., Fischer, Paul J., Tarr, Donald A." Inorganic Chemistry", Pearson Education. ISBN 978-0-321-91779-9,2013.
(9) *Chachiyo, Teepanis* , "Communication: Simple and accurate uniform electron gas correlation energy for the full range of densities", *Journal of Chemical Physics, 2016.*
(10) Muellller, R. Aromatic Compounds and Their Reactions. Wiley-VCH, (2011).
(11) March, J. Advanced Organic Chemistry: Reactions, Mechanisms, and Structure. 4th Edition. Wiley, (1985).
(12) Clayden, J., Greeves, N., Warren, S., & Wothers, P. Organic Chemistry. 2nd Edition. Oxford University Press, (2012).
(13) Robinson, B. Heterocyclic Chemistry. 3rd Edition. Wiley, (2007).
(14) Alejandro C. Olivieri and Graciela M. Escandar, "Practical Three-Way Calibration", Elsevier, (2014).
(15) Hakima Salman Jabr1, Rajaa Hussein Abd Ali," The Effect of Nitrogen on the Structural and Electronic Properties of Graphene Sheet using Density Functional Theory", Acta Scientifica Naturalis, ASN, Vol. 9, No 2, Pages 1–9, 2022.
(16) C. J. Cramer , "Essentials of Computational Chemistry: Theories and Models" ,2nd Edition , Wiley.com. Retrieved, 2021.