



Modeling the Effect of Functional Groups on the Electronic Properties of Benzene, Pyridine and Pyrimidine



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MOLECULAR modeling at B3LYP/6-31G (d, p) level is utilized to study the effect of some functional groups on the electronic properties of aromatic compounds such as benzene and heterocyclic aromatic compounds as pyridine and pyrimidine. Proposed compounds are supposed to study the effect of some functional groups such as CHO, OH, Br, CH₃ and NH₂. Total dipole moment (TDM) and band gap energy (ΔE) are calculated for all supposed structures. Also, electrostatic potentials (ESP) are calculated for all model molecules as contour. From all results, there is a change in the negativity and hence in the reactivity of studied models. Furthermore, bond length and bond angle are also calculated. Functional groups showed their ability to make a change in electronic properties of the studied structures.

Keywords: Benzene; Pyridine; Pyrimidine; B3LYP/6-31G (d, p) and ESP.

Introduction

Heterocyclic compounds are of the most important organic compounds which represent the center of most scientific chemical articles. [1, 2]. They represent a very distinguished category of chemical structures [3]. Benzene is one of the most popular heterocyclic organic compounds at all. It is always obtained from the processes of oil-refining. Physically, it is a volatile, clear, flammable and colorless liquid. Chemically, it is the magic solvent of various organic hydrophobic

substances that do not solubilize in aqueous media. It is also used in synthesizing various structures. Therefore, it has a great concern from the industrial point of view. However biologically, benzene is considered as one of the toxic hazardous materials. It causes several lethal effects on the biological tissues [4]. Various chemical modifications were carried out on the benzene ring in order to create new structures with novel characteristics. One of the most commonly synthesized benzene derivatives is the nitrogen-

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containing six-membered derivatives [5]. They are widely involved in various applications related with medicine, agriculture and industry [6]. Pyridine is one of the popular nitrogen-based six-membered derivatives of benzene. Its name can be divided into two parts; 'Pyr' which means fire in the Greek words and 'idine' is the suffix used for all aromatic hydrocarbons [7]. It is obtained by replacing one of the CH Groups from benzene structure a nitrogen atom [8]. Bone pyrolysis process was the first sort to obtain pyridine bases [9]. Anderson was the first to extract pyridine in 1846 using bone oil. Korner in 1869 reached its correct chemical structure and then verified by Dewar in 1871 which is a nitrogen-based benzene derivative [10-12]. During the late 19th century and early 20th century, Pyridines started to take attentions. However, at the second half of the 20th century pyridine and its derivatives had an important and effective participation for various medical and industrial applications [13]. Another biologically important compound is pyrimidine which is considered one of the most active chemical structures structured as Nitrogen-based six-membered derivative of benzene and pyridine. Pyrimidine consists of a benzene ring with two nitrogen atoms in the positions 1 and 3 replacing two CH groups of benzene. Chemically, pyrimidine has similar nature of pyridine. Furthermore, adding nitrogen atoms increases the electron density of the ring due to the lone pair electrons of N atom. Therefore, the electrophilic substitution reactions become less probable while the nucleophilic ones get easier. From another point of view, the nitrogen addition increases the total dipole moment and hence reactivity, and that is why pyrimidines are biologically active compounds [14]. Pyrimidine ring forms the core structure of nitrogen bases in nucleic acids; both DNA and RNA, named cytosine, uracil, thymine and also in uric acid and barbituric acid [15]. Pyrimidine and its derivatives are extensively investigated in biological applications and synthesis of many drugs due to their antibacterial, antifungal, antiallergic, antihypertensive, antiasthmatics, bronchodilator, cardiotoxic and antitumor activity [16-20].

Molecular modeling shows potential application which is used as a tool to clarify some properties such as electronic, geometrical, chemical and biological functions and properties for many systems and molecules [21-24]. It is stated that total dipole moment (TDM), electrostatic potential (ESP) and HOMO/LUMO band gap energy (ΔE) are considered as tools for estimating the reactivity of a given structure [25-27].

Based on these considerations, this work is conducted to study the effect of some functional groups on benzene, pyridine and pyrimidine.

The studied structures are subjected to Density Functional Theory (DFT) calculations to calculate their electronic properties.

Computational Details

All calculations were conducted using GAUSSIAN 09 soft code which is implemented at Spectroscopy Department, National Research Centre (NRC) [28]. Structures of both pyridine and pyrimidine were optimized using DFT level at Becke-style 3-Parameter DFT (using the Lee-Yang-Parr correlation functional) (B3LYP) [29-31] and 6-31G(d,p) as a basis set. Physical and electronic properties of both structures were calculated such as total energy (E), TDM and HOMO/LUMO band gap energies (ΔE) at the same theoretical level.

Results and Discussion

Model molecules for benzene, pyridine and pyrimidine were supposed as in Fig. 1(a), 2(a) and 3(a) respectively, pyridine and pyrimidine are structurally related to benzene by replacing one methine group (=CH-) with Nitrogen atom (N) for pyridine and 1,3 two methine group (=CH-) with two Nitrogen atom (N) for pyrimidine. TDM and HOMO/LUMO band gap energy ΔE were calculated for the proposed structures. For benzene, pyridine and pyrimidine TDM were 0.0000, 2.1848 and 2.2869 Debye while HOMO/LUMO band energy ΔE are equal to 6.7926, 6.2415 and 5.7609 eV respectively. According to the presence of the two Nitrogen atom (N) in pyrimidine which make difference in electronegativity, TDM increased and band gap energy ΔE decreased. TDM and HOMO/LUMO band gap energy ΔE result indicated that pyrimidine is the most reactive compound compared with benzene and pyridine.

The proposed structures benzene, pyridine and pyrimidine are supposed to interact with the following functional groups: CHO, OH, Br, CH₃ and NH₂ to study the influence of the reactivity of each structure.

Firstly, benzene is supposed to interact with the functional groups: CHO, OH, Br, CH₃ and NH₂. As present in table 1, TDM for benzene with CHO increased from 0.0000 to 3.0282 Debye while HOMO/LUMO band gap energy ΔE changed from 6.7926 to 5.2186 eV. Also, for benzene with OH TDM increased to 1.3354 Debye and HOMO/LUMO band gap energy ΔE 5.9822 eV. For benzene with Br TDM increased

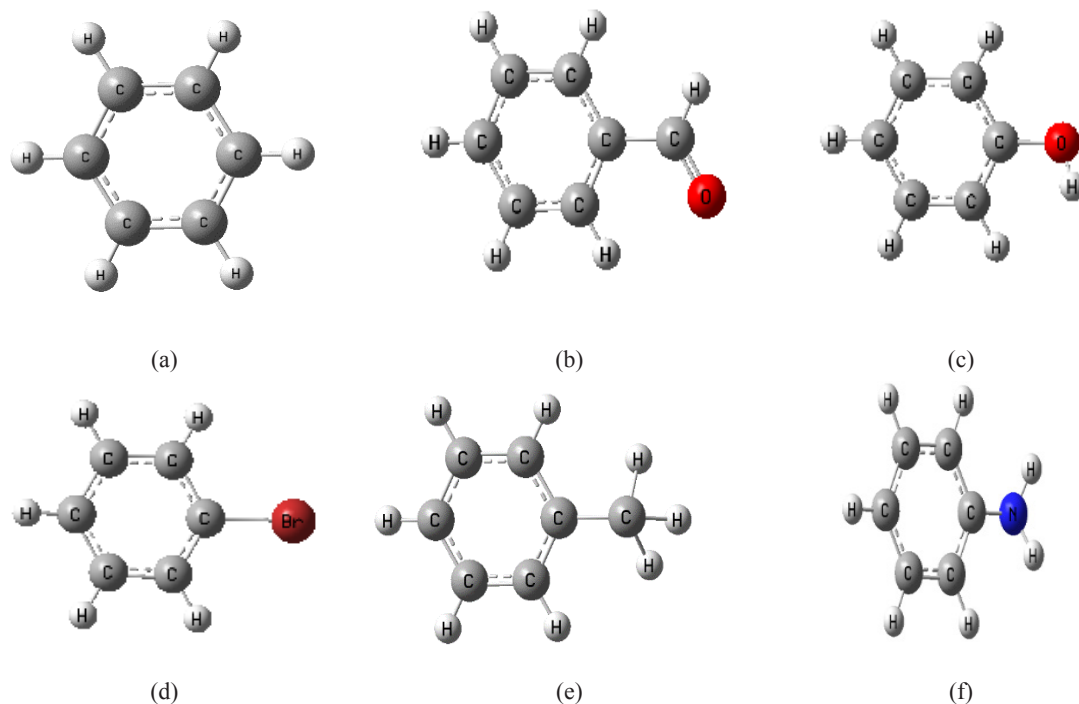


Fig.1. B3LYP/6-31G(d,p) optimized structures for (a) benzene and benzene functionalized with (b) CHO, (c) OH, (d) Br, (e) CH₃ and (f) NH₂.

to 1.8054 Debye while band gap energy ΔE decreased to 6.2274 eV. Furthermore, TDM increased to 0.3424 Debye for benzene with CH₃ and band gap energy ΔE decreased to 6.5340 eV. Similarly, for benzene with NH₂ TDM changed from 0.0000 to 1.7097 Debye and band gap energy ΔE changed from 6.7926 to 5.6263 eV. TDM and band gap energy ΔE results indicated that benzene with CHO is the most reactive structure related to benzene and benzene with the functional groups. Secondly pyridine interact with the functional groups: CHO, OH, Br, CH₃ and NH₂ according to table 2 TDM decreased to 1.6513 Debye for pyridine with CHO and HOMO/LUMO band gap energy ΔE decreased to 4.9482 eV.

While TDM of pyridine Br increased to 2.7464 Debye and HOMO/LUMO band gap energy ΔE decreased to 6.2306 eV. When adding CH₃ to pyridine TDM changed from 2.1848 to 2.6639 Debye. Furthermore, TDM of pyridine NH₂ increased to 3.9862 Debye and band gap energy ΔE decreased to 6.0864 eV.

Results of band gap energy (ΔE) and TDM of pyrimidine functionalized with CHO, OH, Br, CH₃ and NH₂ reactive groups are illustrated in table 3. TDM of pyrimidine-CHO decreased to 1.6473 Debye and band gap energy ΔE decreased to 4.9239 eV. While TDM of pyrimidine -OH increased to 2.7464 Debye and band gap energy

ΔE increased to 6.5526 eV. For pyrimidine -Br, TDM decreased to 0.8443 Debye and band gap energy ΔE 5.6763 eV. Furthermore, TDM of pyrimidine -CH₃ increased to 2.7755 Debye and band gap energy ΔE 5.7188 eV. TDM of pyrimidine -NH₂ changed to 2.8051 Debye and band gap energy ΔE changed to 5.6809 eV.

Studying the geometrical parameters such as bond distance and bond angles considered an indication for the stability/ reactivity of the studied models. As a result of substitution of benzene with CHO, OH, Br, CH₃ and NH₂ bond distance increased from 1.0864 Å to 1.4803, 1.3679, 1.9135, 1.0941 and 5.6263 Å but the bond angle changed from 120.014° to 124.711°, 117.324°, 119.302°, 120.089° and 120.695° respectively as presented in table 4. Also for pyridine according to table 5, the bond distance increased from 1.0799 Å to 1.4871, 1.4300, 1.9100, 1.5400 and 1.3826 Å but the angles increased ongoing from pyridine to pyridine substituted with CHO and then starts to decrease ongoing from pyridine substituted with OH, Br, CH₃ and NH₂ to 118.833°, 118.833°, 118.737° and 116.682° respectively. Similarly for pyrimidine, as represented in Table 6 bond distances increased from 1.3378 Å to 1.4804, 1.4300, 5.6763, 1.5056 and 1.4700 Å and the angles between the bonds decreased from 127.377° to 123.936°, 118.737°,

118.737°, 126.886° and 118.737° for substitution of pyrimidine with CHO, OH, Br, CH₃ and NH₂, respectively

Also, molecular electrostatic potentials ESP are calculated at the same level of theory as it considered one of the most important parameters that presents the more active sides of the studied model molecules. ESP can be described according to the distribution of charges around the model molecules by following a color map ranging from red to orange, yellow, green and finally blue where the red color indicates that this site is the most active site. Calculated ESPs for benzene, functionalized benzene, pyridine, functionalized pyridine, pyrimidine and functionalized pyrimidine are illustrated as contour actions in Fig. 7-9.

Fig.7 shows that benzene has no active site (that is neutral compound) but by adding functional groups on benzene such as CHO, OH, Br and NH₂ the red color and the electro-negativity of benzene increased and hence the reactivity increased. But by adding functional group on benzene such as CH₃ the ESP shows green contour which means that electro-negativity decreased and also the reactivity decreased.

Fig. 8 shows that pyridine has active site at place of hetero atom as red color appears at this place so it has more electro-negativity and becomes more reactive. But on the other hand, for pyridine substituted with CHO, OH, Br and NH₂ the studied models possess two active sites which considered an indication for increasing the reactivity of the models under investigation. But pyridine substituted with CH₃ has one active site Fig.9 illustrated that pyrimidine also has two active sites while pyrimidine substituted with CHO, OH and NH₂ have three active sites but pyrimidine substituted with CH₃ also has two active sites. This indicated that the reactivity of pyrimidine increases with the presence of functional groups like CHO, OH and NH₂.

Conclusion

The reactivity of benzene increased as HOMO/LUMO band gap energy decreased while TDM increased as a result of substitution. For substituted benzene, benzene substituted with CHO is the most reactive structure in comparison with the other studied models. For heterocyclic compounds such as pyridine and pyrimidine, the most reactive compounds are pyridine substituted with CHO and pyrimidine substituted with CHO

TABLE 1. B3LYP/6-31G(d,p) calculated total dipole moment TDM as Debye, HOMO /LUMO band gap energy ΔE as eV for benzene and benzene functionalized with CHO, OH, Br, CH₃ and NH₂.

| Structure | ΔE | TDM |
|--------------------------|------------|--------|
| Benzene | 6.7926 | 0.0000 |
| Benzene -CHO | 5.2186 | 3.0282 |
| Benzene -OH | 5.9822 | 1.3354 |
| Benzene -Br | 6.2274 | 1.8054 |
| Benzene -CH ₃ | 6.5340 | 0.3424 |
| Benzene -NH ₂ | 5.6263 | 1.7097 |

TABLE 2. B3LYP/6-31G(d,p) calculated total dipole moment TDM as Debye, HOMO /LUMO band gap energy ΔE as eV for pyridine and pyridine functionalized with CHO, OH, Br, CH₃ and NH₂.

| Structure | ΔE | TDM |
|---------------------------|------------|--------|
| Pyridine | 6.2415 | 2.1848 |
| pyridine -CHO | 4.9482 | 1.6513 |
| pyridine -OH | 6.5526 | 2.7464 |
| pyridine -Br | 6.2306 | 0.6570 |
| pyridine -CH ₃ | 6.2927 | 2.6639 |
| pyridine -NH ₂ | 6.0864 | 3.9862 |

TABLE 3. B3LYP/6-31G(d,p) calculated total dipole moment TDM as Debye, HOMO /LUMO band gap energy ΔE as eV for pyrimidine and pyrimidine functionalized with CHO, OH, Br, CH₃ and NH₂.

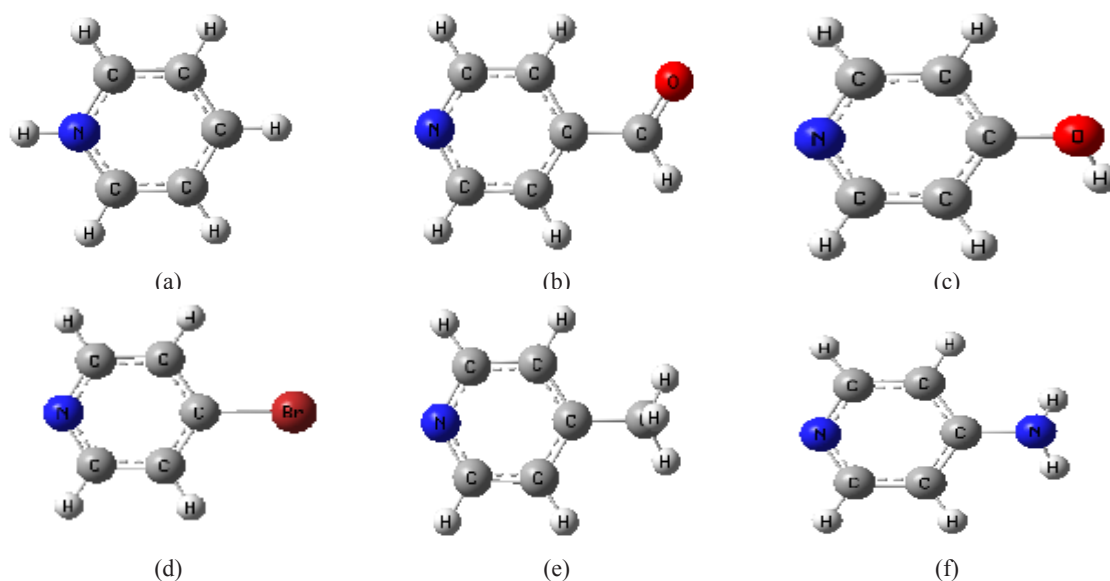
| Structure | ΔE | TDM |
|-----------------------------|------------|--------|
| Pyrimidine | 5.7609 | 2.2869 |
| pyrimidine -CHO | 4.9239 | 1.6473 |
| pyrimidine -OH | 6.5526 | 2.7464 |
| pyrimidine -Br | 5.6763 | 0.8443 |
| pyrimidine -CH ₃ | 5.7188 | 2.7755 |
| pyrimidine -NH ₂ | 5.6809 | 2.8051 |

TABLE 4. B3LYP/6-31G(d,p) calculated bond length as Å and bond angles as degree for benzene and benzene functionalized with CHO, OH, Br, CH₃ and NH₂.

| Structure | Bond distance | Bond angle |
|--------------------------|---------------|------------|
| Benzene | 1.0864 | 120.014 |
| Benzene -CHO | 1.4803 | 124.711 |
| Benzene -OH | 1.3679 | 117.324 |
| Benzene -Br | 1.9135 | 119.302 |
| Benzene -CH ₃ | 1.0941 | 120.089 |
| Benzene -NH ₂ | 5.6263 | 120.695 |

TABLE 5. B3LYP/6-31G(d,p) calculated bond length as Å and bond angles as degree for pyridine and pyridine functionalized with CHO, OH, Br, CH₃ and NH₂.

| Structure | Bond distance | Bond angle |
|---------------------------|---------------|------------|
| Pyridine | 1.0799 | 119.985 |
| pyridine -CHO | 1.4871 | 124.096 |
| pyridine -OH | 1.4300 | 118.833 |
| pyridine -Br | 1.9100 | 118.833 |
| pyridine -CH ₃ | 1.5400 | 118.737 |
| pyridine -NH ₂ | 1.3826 | 116.682 |

**Fig. 2.** B3LYP/6-31G(d,p) optimized structures for (a) pyridine and pyridine functionalized with (b) CHO, (c) OH, (d) Br, (e) CH₃ and (f) NH₂.

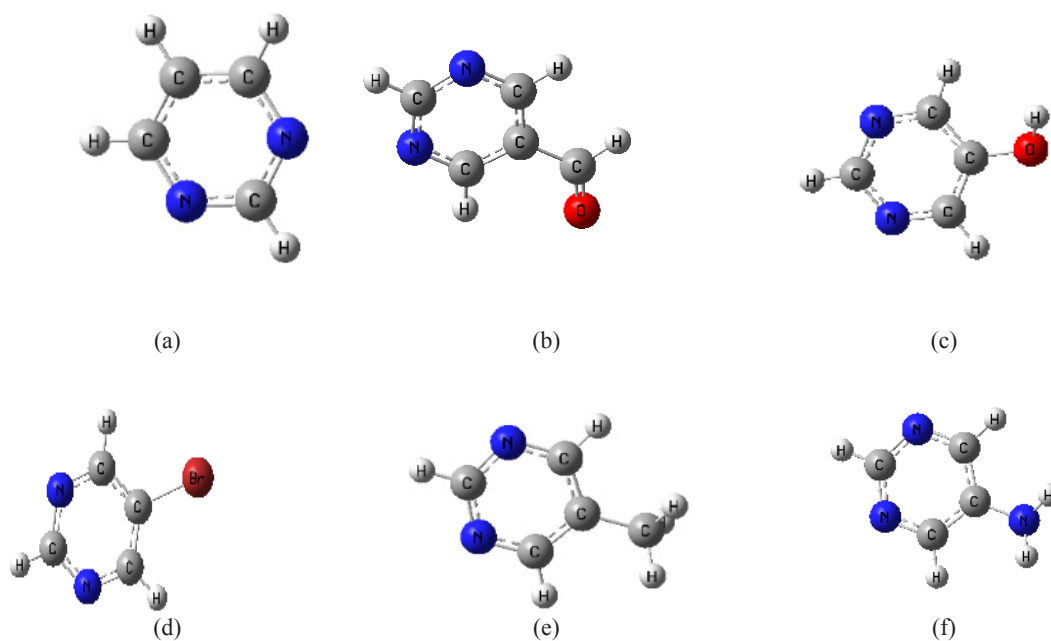


Fig. 3. B3LYP/6-31G(d,p) optimized structures for (a) pyrimidine and pyrimidine functionalized with (b) CHO, (c) OH, (d) Br, (e)CH₃ and (f) NH₂.

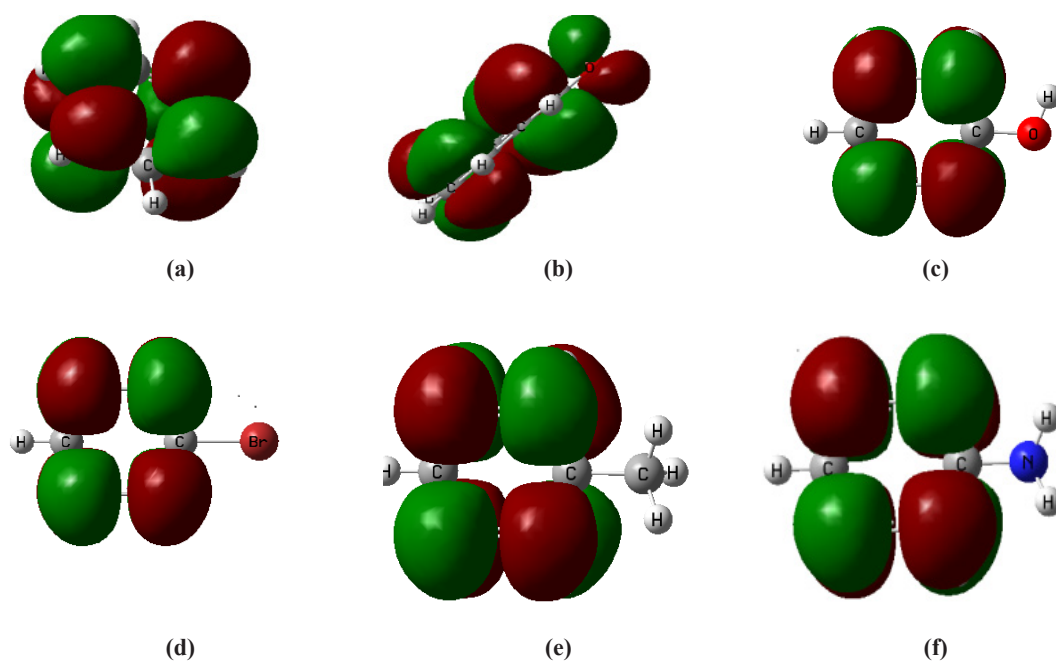


Fig. 4. B3LYP/6-31G(d,p) calculated HOMO/LUMO band gap energy for (a)benzene and benzene functionalized with (b)CHO, (c) OH, (d) Br, (e) CH₃ and (f) NH₂.

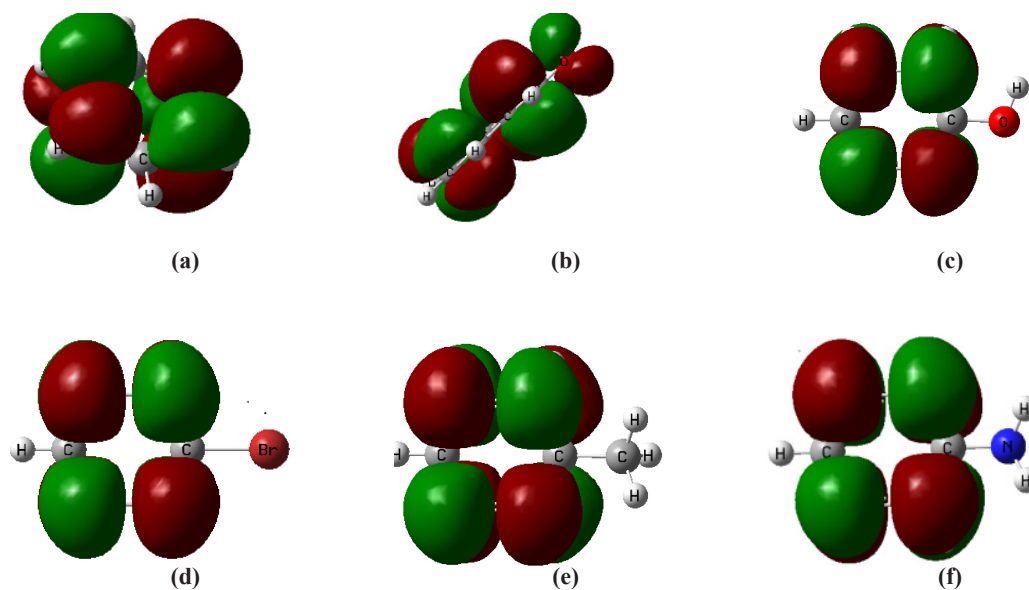


Fig. 5. B3LYP/6- 31G(d,p) calculated HOMO/LUMO band gap energy for (a)pyridine and pyridine functionalized with (b)CHO, (c) OH, (d) Br, (e) CH₃ and (f) NH₂.

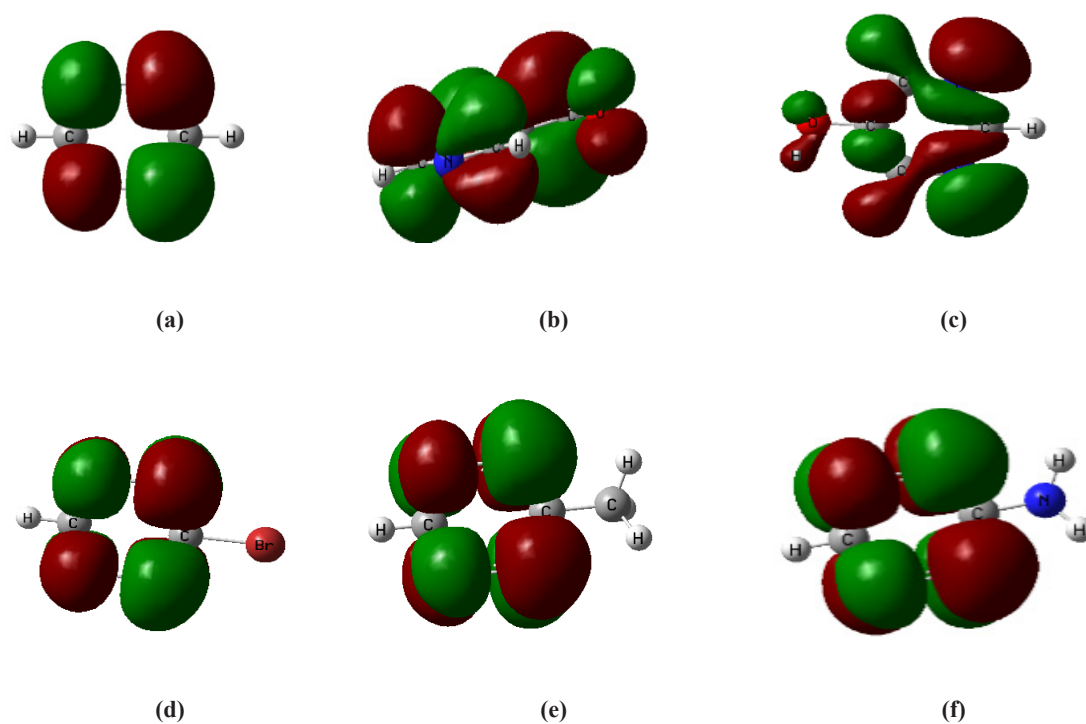


Fig. 6. B3LYP/6- 31G(d,p) calculated HOMO/LUMO band gap energy for (a)pyrimidine and pyrimidine functionalized with (b) CHO, (c) OH, (d) Br, (e) CH₃ and (f)NH₂.

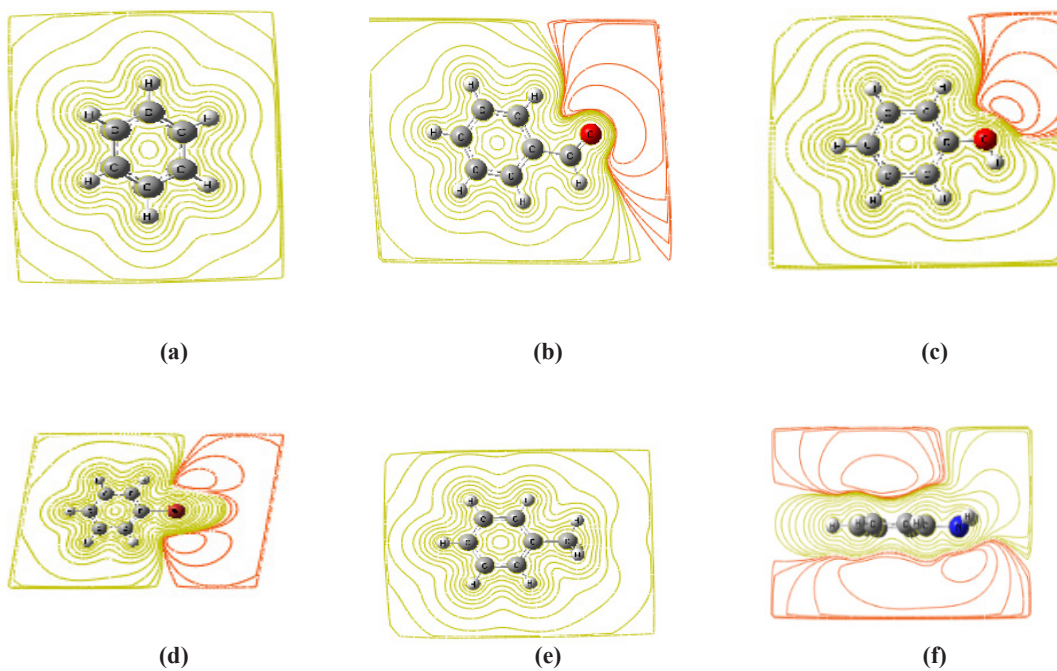


Fig.7. B3LYP/6-31G(d,p) calculated electrostatic potential ESP as contour for (a)benzene and benzene functionalized as (b)CHO,(c)OH, (d)Br, (e) CH₃ and (f) NH₂.

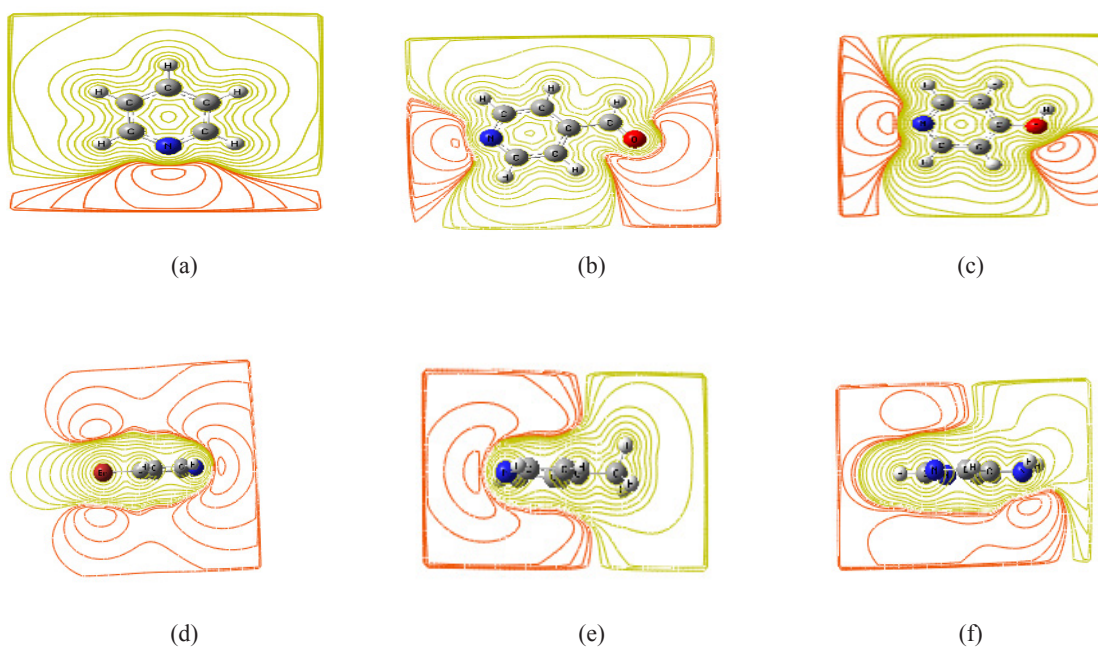


Fig. 8. B3LYP/6-31G(d,p) calculated electrostatic potential ESP as contour for (a)pyridine and pyridine functionalized with (b)CHO, (c)OH, (d)Br, (e)CH₃ and (f)NH₂.

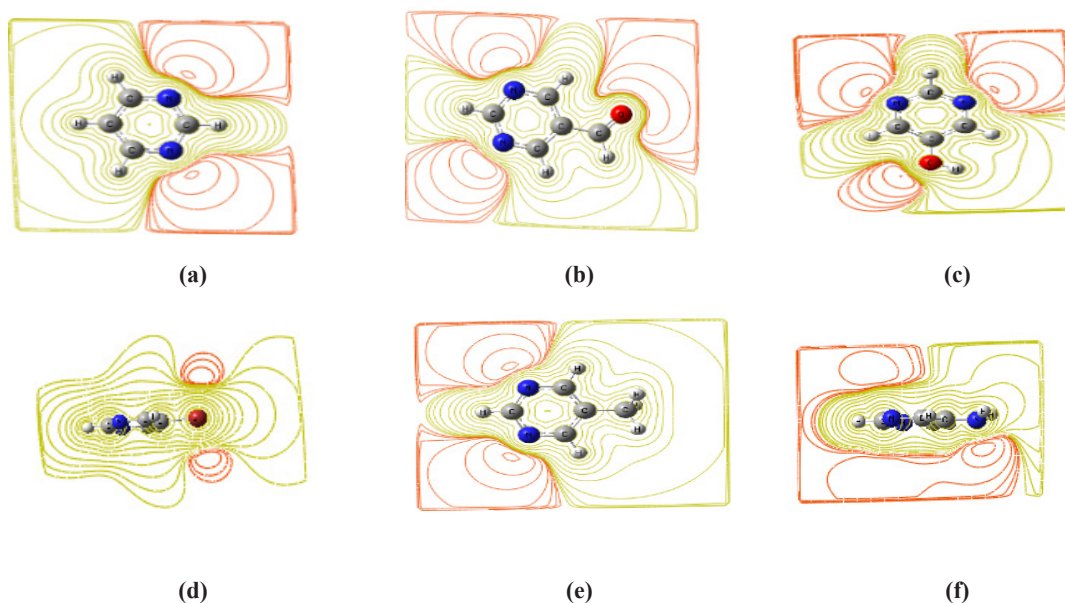


Fig. 9. B3LYP/6-31G(d,p) calculated electrostatic potential ESP as contour for (a)pyrimidine and pyrimidine functionalized with (b)CHO, (c)OH, (d)Br, (e)CH₃ and (f)NH₂.

in comparison with other studied functional groups. Based on the results one can state that, the Pyrimidine is the most reactive compound and CHO is the most reactive functional group compared to all the studied model molecules. It could be concluded also that the studied functional groups are changing the electronic properties of the studied organic structures. Furthermore, DFT is suitable technique for elucidating physical as well as chemical properties of functional organic structures. The present computational work confirms the previous findings that the calculated TDM, HOMO/LUMO and ESP are good indicators for reactivity of the given chemical structure.

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نمذجة تأثير المجموعات الفعالة علي الخواص الالكترونية للبنزين، البيريدين و البيريميدين

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⁴المعهد القومي للبحوث الفلكية والجيوفيزيقية، حلوان، القاهرة، مصر.
⁵قسم الطيف، المركز القومي للبحوث، 33 شارع البحوث، 12622 الدقى، الجيزة، مصر.

تستخدم النمذجة الجزيئية علي نطاق واسع لفهم الصفات التركيبية والكميائية والفيزيقية للعديد من المركبات. لذا يتم في هذا البحث استخدام نظرية الكثافة الفعالية (DFT) عند مستوى B3LYP/6-31G (d,p) لدراسة تأثير المجموعات الفعالة التالية CHO, OH, Br, CH₃, NH₂ علي الصفات الالكترونية للبنزين، البيريدين و البيريميدين وسيتم حساب التركيب شاملًا اطوال الروابط والزوايا بين الذرات وكذلك حساب عزم ثنائي القطب الكلي بالإضافة الي كل من طاقة الفجوة والجهد الكهربائي الاستاتيكي. وقد اظهرت النتائج قدرة كبيرة للمجموعات الفعالة علي احداث تغيير ملحوظ في الصفات الالكترونية للمركبات محل الدراسة.