



The Possibility of Selective Sensing of the Straight-Chain Alcohols (Including Methanol to n-Pentanol) by Using the C₂₀ Fullerene and C₁₈NB Nano Cage

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ABSTRACT

Alcohol with its highly flammable nature to produce CO, and CO₂, and also its greenhouse gas emissions, has considerable effects in changing the ecosystem of earth. The high volumes of annual production of this species, as well as its powerful effects on tropospheric changes, have amplified its adverse impacts.

Due to these, in this project, by examining the possibility of C₂₀ fullerene (and its nitrogen-boron decorated form (C₁₈NB)) in selective sensing of the low weight straight-chain alcohols (including methanol to n-pentanol), we have attempted to find a new approach for detecting those species.

The results show that the C₁₈NB cage senses the existence of methanol ($\Delta E_g = 0.090$ eV) better than the C₂₀ fullerene ($\Delta E_g = -0.037$ eV). Also, the results indicate that both the C₂₀ fullerene and the C₁₈NB nanocage could sense methanol, clearer and more selective than other mentioned alcohols. Moreover, the results show, that adsorption of methanol by the two mentioned sorbents is thermodynamically more favorable compared to the other alcohols. Also, adsorption of this alcohol by C₁₈NB is significantly favorable than that of C₂₀ fullerene (in view of thermodynamics).

1. Introduction

In chemistry, an alcohol is an organic compound in which a hydroxyl functional group (-OH) is attached to a carbon atom [1]. There is a wide range of compounds with aliphatic or aromatic molecular segments which have a hydroxyl as the main functional groups; while, usually name of alcohol is referred to hydrocarbons with an aliphatic skeleton [2].

The straight-chain alcohols are known as the most famous ones. On the other hand, the low weight aliphatic straight-chain alcohols containing, methanol, ethanol, propanol, butanol, pentanol, and hexanol, are of the most produced, most used, and most famous alcohols [3].

Usually these compounds are produced by different types of industrial and mineral activities like

exploration, drilling, and extracting of oil, gas, and minerals and also petrochemical works [4,5], as well as production of those by natural ecosystems like metabolism of oceans [6].

Both these artificial and natural resources would annually produce hundreds tons of alcohols and release them to the atmosphere [7]. Since, alcohols intervene in a wide range of atmospheric changes especially in the greenhouse gas emission [8]; thus, considering, detecting and controlling these compounds is very important. In this regard, some precious researches were made [9,10]. Moreover, these toxic and flammable compounds [11] are being observed in some mineral activities and might jeopardize the health of miners. Thus, some of scientists have aided new technologies to control or detect the release of those compounds in especial places like mines; also, they used sensors for

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identifying these gases [12]. Due to the fact that the theoretical calculations have helped researchers in accurate design of some nano-sized actuators and molecular sensors, which are of the best and most advanced technologies [13,14].

Alcohol produces carbon oxide gases, and has also greenhouse gas emissions. Moreover, it has considerable effects in changing the ecosystem of our green planet. The high volume of annual production of this species, as well as its powerful effects on tropospheric changes, has amplified its adverse impacts. Beside the adverse effects of existence in troposphere, alcohols are extremely dangerous for miners, because these volatile compounds which may exist in mines; are toxic and highly flammable. Thus, fast and accurate detection of alcohols, especially by high-sensitive sensors, is very crucial.

Due to these, in this work, we have aided the theoretical calculations to find any possible state and energy minima for each of the mentioned aliphatic alcohols containing methanol, ethanol, n-propanol, n-butanol, n-pentanol, in presence of the C₂₀ fullerene, and C₁₈NB, in order to examine the suitability of these, for detection of the considered alcohols. The results showed that C₂₀ fullerene, and C₁₈NB are relatively able to sense these alcohols [15].

2. Computational

The isolated forms of the C₁₈NB, and C₂₀ fullerenes, and their associated systems with each of the alcohols mentioned above, were designed as input files and were then optimized to give the energy minima (Figure 1). The Gaussian 03 quantum chemical package was employed for performing the required calculations [16] and the related parameters were reached accordingly. Studies on all stationary points in addition to the other required calculation were performed by using B3LYP/6-31g(d) level of theory [17-18] which are shown to be suitable for these type of investigations [19,20].

Also, the frequency of each point was extracted to give the thermodynamic and kinetic parameters. The Global Electron Density Transfer (*GEDT*) was calculated by using the following formula [21];

$$GEDT = -\sum q_A \quad (1)$$

Where; q_A is the net Mulliken charge, and the sum of the entire atoms of the gases species.

The chemical potential of the system or the Fermi level (E_F), comes from the relation (2) [22]:

$$E_F = -(E_{HOMO} + E_{LUMO})/2 \quad (2)$$

Where; E_{HOMO} , and E_{LUMO} , are the energy surfaces of the HOMO, and the LUMO orbitals, respectively.

Also, the global hardness is calculated using the following relation [23,24]:

$$\eta = (E_{LUMO} - E_{HOMO}) / 2 \quad (3)$$

3. Results

For the first step, each isolated species containing C₁₈NB cage, C₂₀ fullerene, methanol, ethanol, n-propanol, n-butanol, and n-pentanol species was designed as input files and was then optimized, subsequently. Then, each of alcohols was placed near to C₁₈NB cage, and C₂₀ fullerene, in different orientations as input files. During the optimizations, some of the different proposed states turned into same orientations. Thus, among the input files, some orientations were come out after further optimizations (Figure1). An interesting point that was reached during the calculations was that adsorption of each alcohol was proceeded in one acceptable step.

One of the other points was that in the adsorption form of methanol by the C₁₈NB cage, a strong interaction occurred between the oxygen of methanol and boron of the fullerene which closed their interatomic distance (Figure 1).

The data presented in Table 1, showed that the adsorption of the smallest alcohol of the group (methanol) by C₂₀ fullerene or C₁₈NB cage, was favorable compared to all of the other considered alcohols. Somehow, the E_{ads} for the adsorption of methanol by C₂₀ fullerene was -3.328 kcal mol⁻¹; while, the values for the adsorption process of the other alcohols by this fullerene were -2.806 kcal mol⁻¹, -2.901 kcal mol⁻¹, -2.905 kcal mol⁻¹, and -2.944 kcal mol⁻¹ for methanol, ethanol, n-propanol, n-butanol, and n-pentanol, respectively. Also, the E_{ads} for adsorption of methanol by C₁₈NB cage was -26.29 kcal mol⁻¹ which was considerably higher compared the same values for adsorption processes of the other alcohols by this nano sized cage (-4.300 kcal mol⁻¹ (ethanol), -4.631 kcal mol⁻¹ (n-propanol), -4.739 kcal mol⁻¹ (n-butanol), and -4.723 kcal mol⁻¹ (n-pentanol)). Moreover, the *GEDT* values are 0.044, 0.054, 0.052, 0.021, and 0.022 for the adsorption states between C₂₀ fullerene and alcohols containing methanol, ethanol, n-propanol, n-butanol, and n-pentanol, respectively.

Also, the values of this parameter for the adsorption of alcohols containing methanol, ethanol, n-propanol, n-butanol, and n-pentanol by C₁₈NB fullerene are 0.284, 0.184, 0.064, 0.078, 0.182, respectively. It approximately shows that by increasing the molecular weight of the alcohols, the global charge transfer and also the electrical interactions between alcohols and fullerenes increase, while this order does not true for all cases. Since, the hydrocarbon parts of alcohols are nearly nonpolar, by increasing the number of CH₂ units (and therefore, increasing the nonpolar part), the total polarity of the alcohol would decrease. Thus, there is a possibility that (facing a certain sorbent) the total charge transfer decreases in parallel to increase of the CH₂ parts of alcohol.

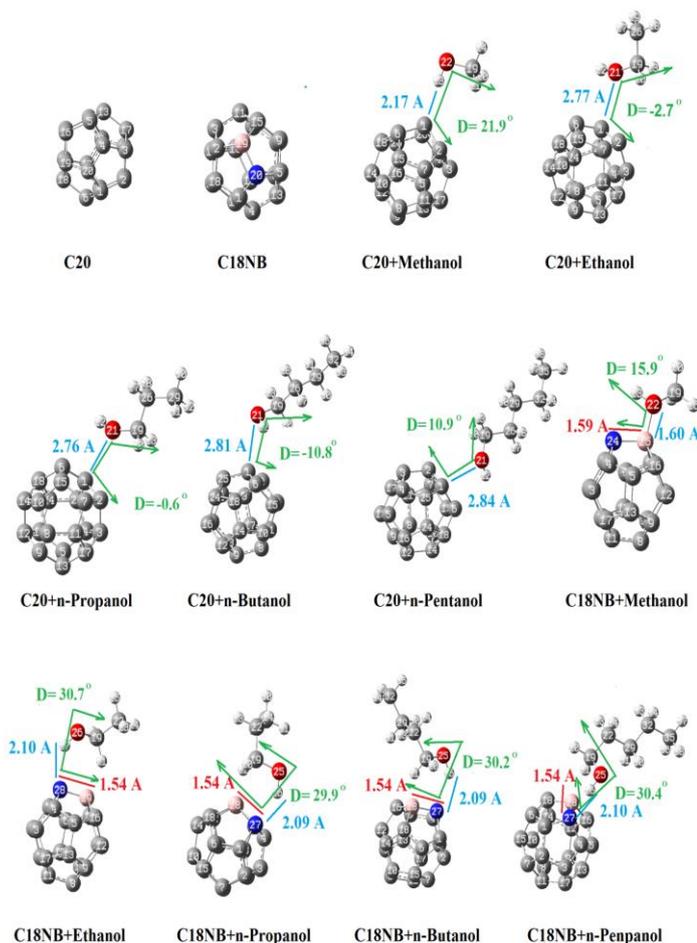


Figure 1. The geometrical situations for the adsorption systems optimized at B3LYP/6-31G(d) level of theory.

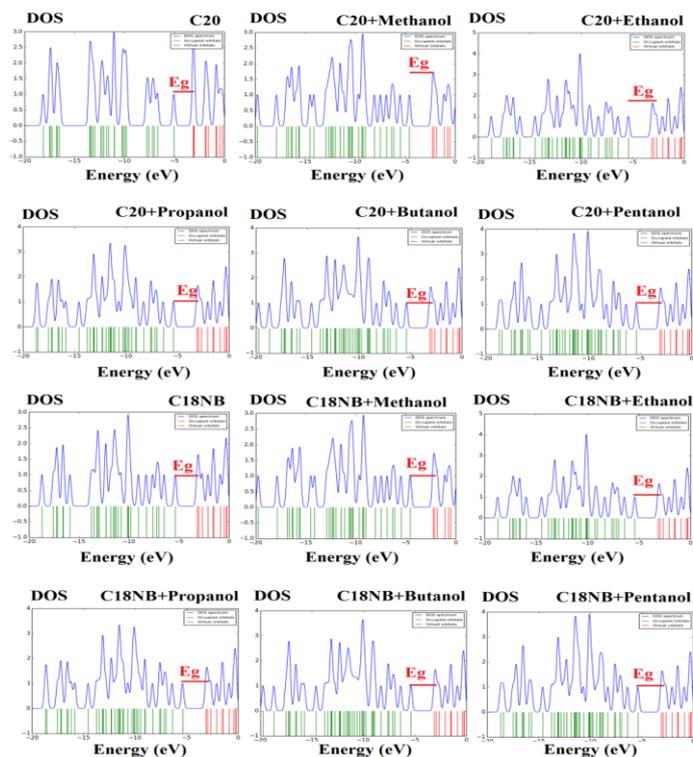


Figure 2. The DOS plots for the adsorption systems of the fullerene-alcohol at B3LYP/6-31G(d) level of theory.

Table 1. The key adsorption and frontier molecular orbital FMO parameters of the adsorption systems at B3LYP/6-31G(d) level of theory.

| System | E_{ads} (kcal mol ⁻¹) | $GEDT$ | E_{HOMO} (a. u.) | E_{LUMO} (a. u.) | E_g (eV) |
|-------------------------------|--|--------|---------------------------|---------------------------|------------|
| C ₂₀ fullerene | - | - | -0.1858 | -0.1145 | 1.925 |
| C ₂₀ +methanol | -3.328 | 0.044 | -0.1959 | -0.1260 | 1.888 |
| C ₂₀ +ethanol | -2.806 | 0.054 | -0.1823 | -0.1105 | 1.940 |
| C ₂₀ +n-propanol | -2.901 | 0.052 | -0.1817 | -0.1098 | 1.940 |
| C ₂₀ +n-butanol | -2.905 | 0.021 | -0.1839 | -0.1124 | 1.931 |
| C ₂₀ +n-pentanol | -2.944 | 0.022 | -0.1849 | -0.1128 | 1.947 |
| C ₁₈ NB fullerene | - | - | -0.1976 | -0.1163 | 2.195 |
| C ₁₈ NB+methanol | -26.29 | 0.284 | -0.1674 | -0.0828 | 2.285 |
| C ₁₈ NB+ethanol | -4.300 | 0.184 | -0.1987 | -0.1151 | 2.257 |
| C ₁₈ NB+n-propanol | -4.631 | 0.064 | -0.1980 | -0.1144 | 2.257 |
| C ₁₈ NB+n-butanol | -4.739 | 0.078 | -0.1975 | -0.1138 | 2.260 |
| C ₁₈ NB+n-pentanol | -4.723 | 0.182 | -0.1972 | -0.11347 | 2.260 |

In the issue of sensing this group of alcohols by the fullerenes, it would be mentioned that the C₁₈NB cage could sense the existence of methanol by a change in HOMO-LUMO gap of 0.090 eV (referenced to the isolated C₁₈NB cage), which is significantly higher than the HOMO-LUMO change for the presence of this alcohol by C₂₀ fullerene ($\Delta E_g = -0.037$ eV). Also, the existence of ethanol and n-propanol near to the C₂₀ fullerene leads to emergence of gaps with same values (0.015 eV). The presence of n-butanol creates a relatively weaker gap of 0.006 eV; while, the gap for n-pentanol was relatively clearer ($\Delta E_g = 0.022$ eV). As mentioned before, the gap for sensing methanol by C₁₈NB fullerene is about 0.090 eV; while, the existence of ethanol, and n-propanol change the HOMO-LUMO gap of the system in a same value ($\Delta E_g = 0.062$ eV). Moreover, the presence of n-butanol, and n-propanol molecules near to C₁₈NB fullerene, create a same HOMO-LUMO change gap of 0.065 eV. It seems that the gaps emerged by the presence of alcohols near to the C₁₈NB fullerene are much higher and clearer than that of C₂₀ fullerene; while, the C₂₀ fullerene could sense the existence of alcohols more selective than the C₁₈NB fullerene.

Figure 2 shows that, in contrary to the other studied alcohols, the DOS plot of methanol-sorbent system is relatively different compared to the DOS plot of the isolated C₁₈NB fullerene, and it may be due to the strong interaction between Oxygen atom of methanol and Boron atom of the nanocage. For example, in the DOS plot of the methanol-C₁₈NB system, in the area of unoccupied orbitals (red lines), there are only two peaks (opposite to the DOS plots of the other alcohol-C₁₈NBs); while in the same area for the DOS plot of the isolated

$C_{18}NB$, there are about five peaks. Moreover, in the case of C_{20} fullerene, the DOS plots indicate that in all adsorption systems, the peaks of the occupied molecular orbitals have increased compared to the isolated C_{20} fullerene, and it reveals that hybridizing has a key role in adsorption procedure. This event is also observed for $C_{18}NB$ case.

By a glance on Figure 3, it is observed that in all cases, LUMO is mainly localized on alcohol and it may show that under light irradiation (the excited state), the molecular orbitals are placed on the adsorption area. Also, it is clearly observed that in the case of the methanol- $C_{18}NB$ system, both HOMO and LUMO are continuously localized on alcohol and the cluster. It may reveal about the significant role of hybridization of orbitals along the adsorption process.

The values of the HOMO and LUMO surfaces of each considered alcohols (except methanol) are very near to each other, and thus, the total polarity (dipole moment), and also the volume of the molecules play the key roles in adsorption processes. It is observed for C_{20} fullerene as well as $C_{18}NB$ cage.

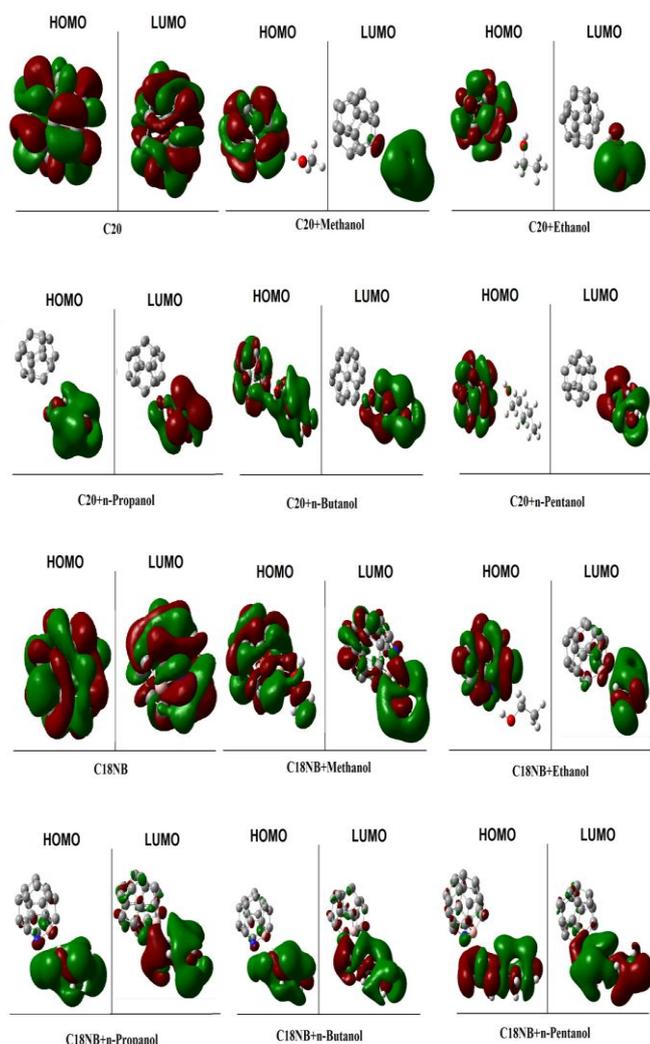


Figure 3. HOMO-LUMO distributions for each detected system, containing pedestrian fullerenes, and the adsorption states

Table 2 reveals that the binding distance for methanol- C_{20} fullerene is about 2.17 Å which is significantly lower than those for ethanol (2.77 Å), n-propanol (2.76 Å), n-butanol (2.81 Å), n-pentanol (2.84 Å). This difference is also observed for alcohol- $C_{18}NB$ systems. Somehow, the binding distance for methanol- $C_{18}NB$ fullerene is about 1.60 Å which is considerably lower than those for ethanol (2.10 Å), n-propanol (2.09 Å), n-butanol (2.09 Å), n-pentanol (2.10 Å). Thus, the results of the binding distances indicate that for each sorbent, methanol has the less binding distances compared to the other alcohols. It seems that the lowest molecular weight, lowest volume, and highest polarity of methanol, compared to others, lead to these priorities in adsorption and detection processes. In addition, the directions of the -OH group of alcohol and the heteroatoms of the fullerene, in methanol- $C_{18}NB$ case, may show that this system is stabilized by an O...B interaction (1.60 Å); while, for other studied alcohols, an hydrogen bonding (between Hydrogen of alcohol and Nitrogen of the $C_{18}NB$ cluster) stabilize the system.

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Moreover, the values of electrochemical potential or Fermi level (E_F) parameter for methanol, ethanol, n-propanol, n-butanol, and n-pentanol, are -2.585 eV, -2.503 eV, -2.503 eV, -2.503 eV, and -2.476 eV which show the E_F of the mentioned alcohols are much closed to each other. On the other hand E_F of $C_{18}NB$ is -4.082 eV which is relatively higher than that of C_{20} fullerene (-4.272 eV). Also, the Fermi level of the considered alcohols are much upper than E_F of the sorbents.

Table 2. The HOMO-LUMO energy surfaces (a. u.) for each isolated species, HOMO-LUMO gaps (a. u.), and Binding Distances (D_b ; Å)

| Species | E_{HOMO} | E_{LUMO} | $/E_{HOMO}(\text{sorbent}) - E_{LUMO}(\text{alcohol})/$ | $/E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})/$ | electron density transfer direction | D_b |
|----------------------|------------|------------|---|---|---|-------|
| C_{20} fullerene | -0.1858 | -0.1145 | - | - | - | - |
| methanol | -0.2645 | 0.0752 | 0.2610 | 0.1500 | $E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})$ | 2.17 |
| ethanol | -0.2616 | 0.0766 | 0.2624 | 0.1471 | $E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})$ | 2.77 |
| n-propanol | -0.2615 | 0.0777 | 0.2635 | 0.1470 | $E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})$ | 2.76 |
| n-butanol | -0.2611 | 0.0780 | 0.2638 | 0.1466 | $E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})$ | 2.81 |
| n-pentanol | -0.2609 | 0.0780 | 0.2638 | 0.1464 | $E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})$ | 2.84 |
| C_{18NB} fullerene | -0.1976 | -0.1163 | - | - | - | - |
| methanol | -0.2645 | 0.0752 | 0.2728 | 0.1482 | $E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})$ | 1.60 |
| ethanol | -0.2616 | 0.0766 | 0.2742 | 0.1453 | $E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})$ | 2.10 |
| n-propanol | -0.2615 | 0.0777 | 0.2753 | 0.1452 | $E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})$ | 2.09 |
| n-butanol | -0.2611 | 0.0780 | 0.2756 | 0.1448 | $E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})$ | 2.09 |
| n-pentanol | -0.2609 | 0.0780 | 0.2756 | 0.1446 | $E_{HOMO}(\text{alcohol}) - E_{LUMO}(\text{sorbent})$ | 2.10 |

Table 3. The thermodynamic parameters ΔG_{ads} , and ΔH_{ads} of adsorption (Kcal mol⁻¹); the electrochemical potential or Fermi level (E_F ; eV); and the global hardness (η ; eV).

| Species | ΔG_{ads} | ΔH_{ads} | η | E_F |
|----------------------|------------------|------------------|--------|-------|
| C_{20} fullerene | - | - | 0.979 | 4.082 |
| methanol | 5.36 | -2.18 | 4.626 | 2.585 |
| ethanol | 6.40 | -1.51 | 4.599 | 2.503 |
| n-propanol | 6.76 | -1.57 | 4.626 | 2.503 |
| n-butanol | 5.32 | -1.61 | 4.626 | 2.503 |
| n-pentanol | -18.88 | 24.39 | 4.599 | 2.476 |
| C_{18NB} fullerene | - | - | 1.116 | 4.272 |
| methanol | -12.88 | -24.49 | - | - |
| ethanol | 6.60 | -3.48 | - | - |
| n-propanol | 6.60 | -3.84 | - | - |
| n-butanol | 6.58 | -4.00 | - | - |
| n-pentanol | -19.30 | 21.99 | - | - |

As shown in Table 3, the enthalpies of adsorption ΔH_{ads} for adsorption processes of methanol on C_{20} fullerene, and C_{18NB} are -2.18 Kcal mol⁻¹, and -24.49 Kcal mol⁻¹, respectively; which are considerably lower compared to the adsorptions processes of the other alcohols on the fullerene or the C_{18NB} . It shows that the adsorption of methanol by the mentioned sorbents is thermodynamically more favorable compared to the other alcohols. Also, adsorption of this alcohol by C_{18NB} is significantly favorable than that of C_{20} fullerene (in view of thermodynamics).

Moreover, ΔH_{ads} of ethanol, n-propanol, and n-butanol by C_{20} fullerene are -1.51 Kcal mol⁻¹, -1.57 Kcal mol⁻¹, and -1.61 Kcal mol⁻¹ (respectively) that have same values (resulting in same favorability in adsorption processes). Also, ΔH_{ads} of adsorption of those three alcohols by C_{18NB} are the same (-3.48 kcal mol⁻¹, -3.84 kcal mol⁻¹, and -4.00 kcal mol⁻¹ for ethanol, n-propanol, and n-butanol, respectively). But, the average of the ΔH_{ads} of adsorption of those three alcohols by the C_{18NB} is relatively lower compared to those for C_{20} fullerene. The ΔH_{ads} for adsorption of n-pentanol both by C_{20} fullerene (24.39 Kcal mol⁻¹) and by C_{18NB} (21.99 Kcal mol⁻¹) are very unfavorable compared to the other mentioned alcohols. The same pattern is observed for the Gibbs free energies of adsorptions in most cases.

Due to Table 3, the global hardness (η) of C_{18NB} is 1.116 eV which is higher than that of C_{20} fullerene

(0.979 eV). Also, the values of η parameter for methanol, ethanol, n-propanol, n-butanol, and n-pentanol are 4.626 eV, 4.599 eV, 4.626 eV, 4.626 eV, and 4.599 eV, which show the total hardness of all mentioned alcohols are much closed to each other. Thus, the total reactivity of those alcohols is closed to each other. The average values for the total hardness of those alcohols are much higher than that of the C₁₈NB and the C₂₀ fullerene. It might show that the chemical of both two mentioned sorbents is much higher than the alcohols.

4. Conclusion

The results of the work showed that the adsorption of methanol by C₂₀ fullerene or its N-B decorated form (C₁₈NB), was considerably favorable than all of the other studied alcohols. Somehow, the E_{ads} for the adsorption of methanol by C₂₀ fullerene was -3.328 kcal mol⁻¹; while, the values for the adsorption of the other alcohols by this fullerene were -2.806 kcal mol⁻¹ (ethanol), -2.901 kcal mol⁻¹ (n-propanol), -2.905 kcal mol⁻¹ (n-butanol), and -2.944 kcal mol⁻¹ (n-pentanol). Also, the E_{ads} for adsorption of methanol by C₁₈NB fullerene was -26.29 kcal mol⁻¹ which was relatively higher than the same values for adsorption of the other alcohols by this form of fullerene (about -4 kcal mol⁻¹). In the case of sensing of the considered alcohols by those fullerenes, it could be mentioned that C₁₈NB cage senses the existence of methanol ($\Delta E_{\text{g}} = 0.090$ eV) better than the C₂₀ fullerene ($\Delta E_{\text{g}} = -0.037$ eV). The existence of ethanol and n-propanol near to C₂₀ fullerene create gaps with equal values ($\Delta E_{\text{g}} = 0.015$ eV). Moreover, the existence of n-butanol leads to emergence a relatively weaker gap ($\Delta E_{\text{g}} = 0.006$ eV); while, the same gap for n-pentanol was clearer ($\Delta E_{\text{g}} = 0.022$ eV). As said above, the gap for sensing methanol by C₁₈NB fullerene is about 0.090 eV; while, the existence of ethanol, and n-propanol change the HOMO-LUMO gap of the system in a same value ($\Delta E_{\text{g}} = 0.062$ eV). Also, the presence of n-butanol, and n-propanol near to C₁₈NB fullerene, lead to emergence of a same gap ($\Delta E_{\text{g}} = 0.065$ eV). It seems that the gaps created by the existence of alcohols near to C₁₈NB fullerene are relatively stronger compared to the C₂₀ fullerene. Thus, the results showed that both the C₂₀ fullerene and the C₁₈NB nanocage could sense methanol, clearer and more selective than other mentioned alcohols.

Also, the results of the binding distances indicate that for each sorbent, methanol has the lowest binding distances compared to the other alcohols. It seems that the lowest molecular weight, lowest volume, and highest polarity compared to others, lead to these priorities in adsorption and detection processes.

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