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Evaluating Adsorption of Proline Amino Acid on the Surface of Fullerene (C_{60}) and Carbon Nanocone by Density Functional Theory

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ABSTRACT

Determination of proline is of great importance and investigating the interaction of this amino acid with nanostructures play a key role in the construction of novel appropriate sensors for proline measurement. In this regard, proline adsorption on the surface of fullerene and carbon nanocone was studied by density functional theory. For this purpose, the structures of fullerene, nanocone, proline and proline-adsorbent complexes at two different configurations were optimized geometrically. Then, IR and Frontier molecular orbital calculations were done in the temperature range of 298.15-398.15 K at 10° intervals. The obtained adsorption energies, adsorption enthalpy changes, Gibbs free energy variations and thermodynamic equilibrium constants showed that the adsorption of proline on the surface of nanocone is exothermic, spontaneous, one sided and experimentally feasible. In this sense, proline adsorption on the fullerene is endothermic, non-spontaneous, balanced and experimentally impossible. The achieved specific heat capacity values reveal that carbon nanocone can be used in the development of thermal sensors for the determination of proline. The effect of temperature on the adsorption process was also checked out and the results indicate that 298.15 is the optimum temperature for the studied procedure. Some HOMO-LUMO parameters such as energy gap, electrophilicity, maximum charge capacity, chemical hardness and chemical potential were also evaluated. Accordingly, the findings demonstrate that carbon nanocone can be utilized in the electrochemical determination of proline.

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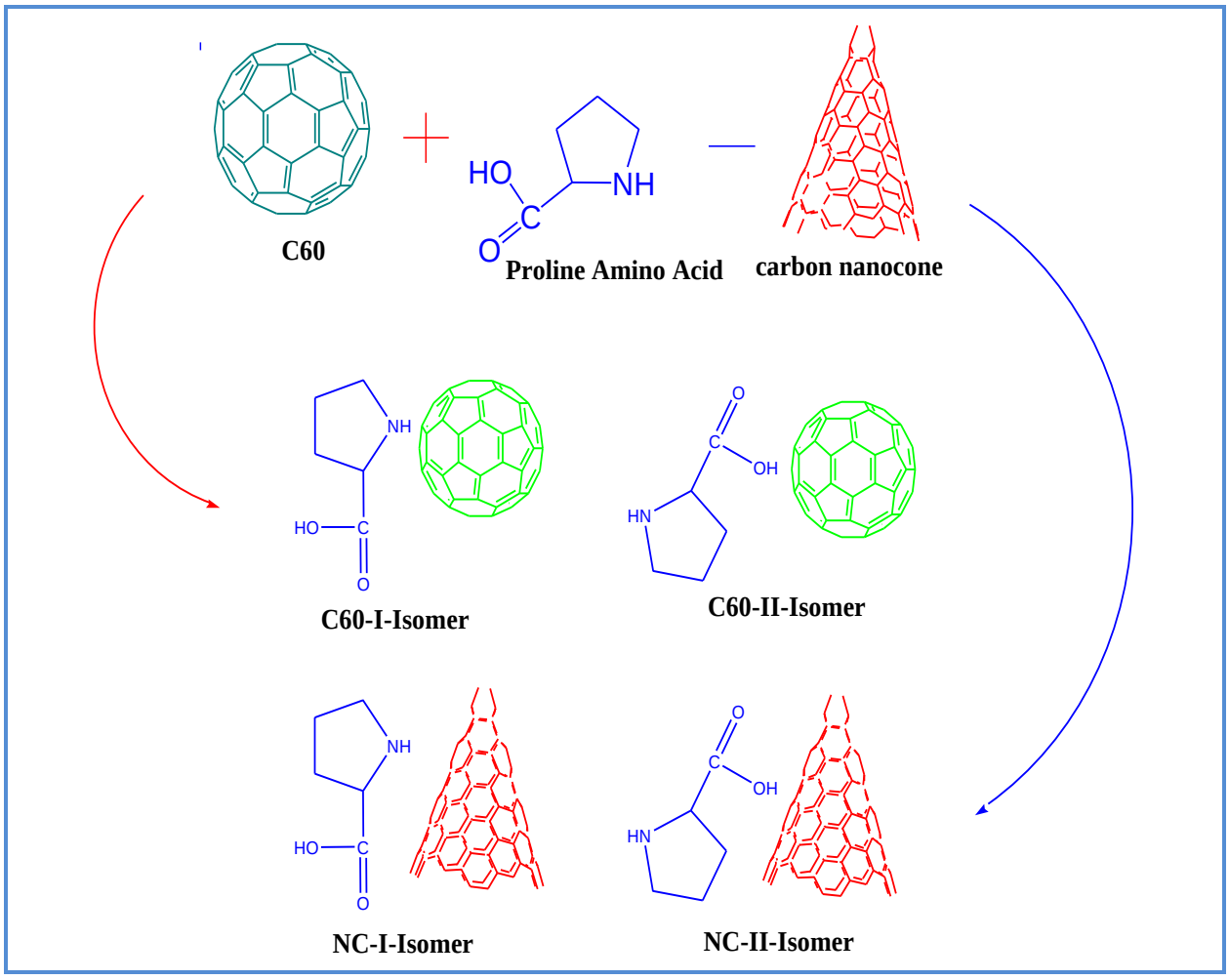
Graphical Abstract



Introduction

Proline with $C_5H_9NO_2$ chemical formula (Figure 1) is one of the main 20 amino acids that is used in the construction of proteins. Proline is an osmotic regulator in plants and can alleviate the salt and drought stress effects, significantly [1]. Moreover, this vital nutrition is a strong antioxidant that acts as an energy reservoir in the cells which adjust the cellular reduction potential. Protection of super molecules like proteins and decreasing the internal acidity of the cells are other functions of proline [2-4]. This amino acid which is the precursor of hydroxyl proline in our body is one of the principal constituents of collagen. Collagen is a protein that acts as a natural glue and is the major component of skin, tendons, bones, cartilages and teeth [5]. Hence, proline is important for the proper function of our body and also the health of other living organisms. In this regards, its determination is very significant. Various analytical techniques such as high performance liquid chromatography (HPLC), fluorescence,

electrochemiluminescence and UV-visible spectrophotometry have been reported for the determination of this biological molecule. However, the mentioned techniques have remarkable downsides like requiring expensive and intricate instruments, needing experienced operators, having sample pre-treatment steps, being time-consuming and lack of selectivity. The referred disadvantages motivate chemists to concentrate on new analytical methods like biosensors because this type of sensors are economical, time saving, selective, straightforward, portable, sensitive and applicable in turbid and colored specimens without any sample pre-treatment procedures [6-8]. But, the main step in the development of a biosensor is to find an appropriate sensing material which has a good interaction with the desired analyte.

Moreover, carbon nanostructures such as C_{60} fullerene and carbon nanocone have attracted the scientific community because of their ideal physical and chemical properties [9-11]. C_{60} which is called bucky ball, due to its similarity to the utilized balls in football (Figure 2), was synthesized for the first time at 1985 [12]. This zero dimensional nanostructure have prominent features like broad absorption in UV-visible area, structural angel strain, photo-thermal effect, long living triplet state and having dual nature of electrophilic and nucleophilic traits [13]. These eminent characteristics show that fullerene can be an excellent sensing material in designing various kinds of sensors for the determination of different biological compounds so that it has been used successfully for the detection of some important analytes; including, glucose, urea, proteins, dexamethasone and prednisolone [14]. Besides, carbon nanocone is an intermediate conical nanostructure between a graphene sheet and a carbon nanotube (Figure 1) [15]. This nanostructure can be produced by cutting 1-5 sectors of angle 60° from a graphene sheet connecting the originated edges by the cut, with 1-5 pentagons at the aspects [16]. The mechanical stability and also the electrochemical features of carbon nanocone make it a unique choice for developing novel biosensors. The adsorption of NO, H_2, HCl and NH_3 on the surface of carbon nanocone has also been evaluated. In this regard, herein, the adsorption of proline amino acid on the fullerene and carbonanocone was investigated by density functional theory for the first time [17-18].

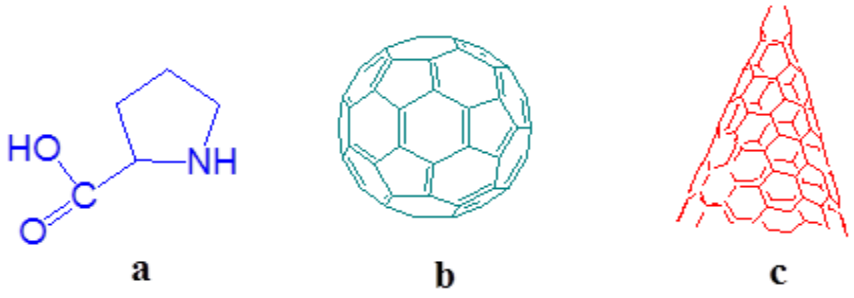


Figure 1. The structure of proline amino acid (a), the structure of C_{60} (b), and the structure of carbon nanocone (c)

Experimental

Computational methods

The structures of C_{60}, carbon nanocone, proline and the produced derivatives from the interaction of proline with the evaluated nano adsorbents were designed by Gauss view software. Then, the designed structures were geometrically optimized and in the next step, IR and Frontier molecular orbital calculations were implemented on them in the temperature range of 298.15-398.15 K at 10° intervals. All of the computations were done in the aqueous phase and atmospheric pressure using density functional theory method in the B3LYP/6-31G (d) level of theory. This basis set was selected because in our prior research, it has produced results which were in a good agreement with the experimental findings [19-30]. Spartan software was selected for performing the calculations. The evaluated process in this study was as follows:

Proline + adsorbent→ proline-adsorbent (1)

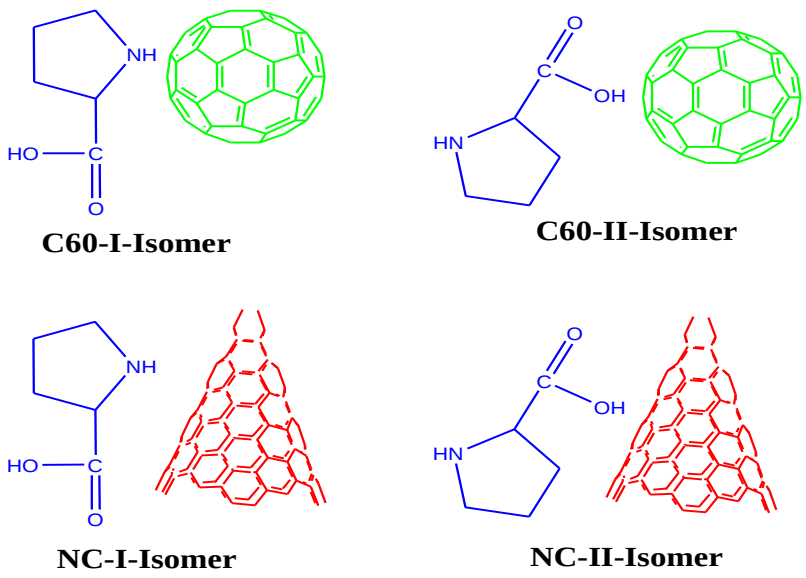


Figure 2. The optimized structures of proline complexes with fullerene and carbon nanocone at two different configurations

Results and discussion

Adsorption energy values

As it can be seen from Figure 2, the proline amino acid was inserted near the surface of fullerene and carbon nanocone at two different configurations. In one configuration, proline is adsorbed on the adsorbent from the carbonyl functional group and in the other; the proline is oriented towards

the surface of nanostructure from the nitrogen atom. The derivatives that are produced from the interaction of carbon atom of carbonyl group with the fullerene and carbon nanocone are demonstrated by C_{60}-I-Isomer and NC-I-Isomer abbreviated names, respectively. C_{60}-II-Isomer and NC-II-Isomer stand for the two other complexes which are originated from the interaction of the nitrogen atom with the surface of fullerene and nanocone, respectively. The adsorption energy (E_{ads}) for the desired process was calculated by equation 2. In this formula, E is the symbol of total energy for the products and reactants of the studied procedure. The provided data in (Table 1) reveals that the adsorption of proline on the nanocone structure is experimentally feasible at both configurations because of the negative obtained adsorption energies. On the other hand, proline adsorption is experimentally impossible on the surface of fullerene due to the positive values of adsorption energy. The bond lengths between the nearest carbon atom of the adsorbents and the nitrogen and carbon atoms of proline are also reported in the table. As it is obvious, the interaction of nanocone and proline is stronger than fullerene because the bond lengths between nanocone and proline are shorter than the bond lengths between proline and fullerene. The mentioned finding is also in a good agreement with the calculated adsorption energy values. It should be noted that no negative frequency in the studied structures was observed as the reported values in the table confirm this.

$$E_{ads}=E_{\text{proline-adsorbent}} - (E_{\text{proline}} + E_{\text{adsorbent}}) \quad (2)$$

Table 1. The values of adsorption energy, lowest frequency and bond lengths for the proline adsorption process

Derived complexes	The total electronic energy of proline (KJ/mol)	The total electronic energy of adsorbents (KJ/mol)	The total electronic energy of the derived products (KJ/mol)	E_{ads} (KJ/mol)	Lowest frequency (cm^{-1})	CO-C (Å)	N-C (Å)
NC-I-Isomer	-839736.488	-1963404.140	-2801384.745	-859.217	74.614	1.457	-
NC-II-Isomer	-839736.488	-1963404.140	-2801590.559	-1065.031	78.523	-	1.408
C_{60}-I-Isomer	-839736.488	-5892188.564	-6731279.629	645.424	304.202	1.532	-
C_{60}-II-Isomer	-839736.488	-5892188.564	-6731247.253	677.800	311.089	-	1.460

Thermodynamic survey

Some important thermodynamic parameters of the adsorption process were also investigated. The

Gibbs free energy changes (ΔG_{ad}), adsorption enthalpy Changes (ΔH_{ad}) and thermodynamic equilibrium constants (K_{th}) were calculated via equations 3-5 respectively.

$$\Delta H_{ad} = \Delta E^{\circ} + (H_{th\ proline\text{-}adsorbent} - (H_{th\ proline} - H_{th\ adsorbent})) \quad (3)$$

$$\Delta G_{ad} = \Delta E^{\circ} + (G_{th\ proline\text{-}adsorbent} - (G_{th\ proline} - G_{th\ adsorbent})) \quad (4)$$

$$K_{th} = \exp(-\Delta G_{ad} / RT) \quad (5)$$

In the equations 3 and 4, ΔE° refers to the total energy variations of the system which can be calculated by subtracting the total energy of the products from the total energy of reactants. H_{th} and G_{th} stand for the thermal enthalpy and thermal Gibbs free energy that were computed by the software for each structure. In equation 5, R and T are ideal gas constants and the temperature respectively. All of the thermodynamic parameters were calculated in the temperature range of 298.15-398.15 K at 10° intervals in order to inspect the effect of the temperature on the adsorption procedure. The achieved adsorption enthalpy alterations are given in Table 2. As it is clear, adsorption of proline on the carbon nanocone is exothermic owing to the calculated negative values of ΔH_{ad}. In this sense, proline adsorption is endothermic on the surface of fullerene. By a closer look, it will be perceived that the adsorption of proline is more exothermic from its nitrogen atom in comparison to the carbonyl functional group. Because, the ΔH_{ad} values of NC-II-Isomer is more negative than the enthalpy changes of NC-I-Isomer. Moreover, by enhancing temperature this parameter has become more negative. Therefore, the adsorption process has become more exothermic by increasing of temperature.

Table 2. The values of adsorption enthalpy changes in the temperature range of 298.15-398.15 K

ΔH_{ad} (KJ/mol)				
Temperature (K)	**NC-I-Isomer**	**NC-II-Isomer**	**C_{60}-I-Isomer**	**C_{60}-II-Isomer**
298.15	-1629.202	-1981.716	470.435	499.587
308.15	-1631.778	-1984.292	471.349	500.476
318.15	-1634.397	-1986.911	472.250	501.380
328.15	-1637.062	-1989.576	473.175	502.285
338.15	-1639.782	-1992.296	474.092	503.185
348.15	-1642.518	-1995.032	475.114	504.196
358.15	-1645.218	-1997.732	476.180	505.246
368.15	-1647.932	-2000.446	477.241	506.325
378.15	-1650.661	-2003.175	478.307	507.416
388.15	-1653.431	-2005.945	479.402	508.514
398.15	-1656.242	-2008.756	480.524	509.612

The calculated Gibbs free energy changes are tabulated in Table 3. As it can be witnessed, the proline adsorption on the nanocone surface is spontaneous whereas the adsorption of proline on the fullerene is non-spontaneous. Because the obtained ΔG_{ad} values for NC-I-Isomer and NC-II-Isomer are considerably negative, this parameter is positive for C_{60}-I-Isomer and C_{60}-II-Isomer derivatives. The impression of temperature on this variable was also checked out. As it is obvious from the table, by incrementing the temperature, ΔG_{ad} has become more positive. Hence, rising the temperature makes the adsorption process less spontaneous. The next point that can be understood from the table is that proline adsorption from its nitrogen atom on the nanocone is more spontaneous because NC proline N derivative has lower ΔG_{ad} than NC proline CO derivative.

Table 3. The values of adsorption Gibbs free energy changes in the temperature range of 298.15-398.15 K

ΔG_{ad} (KJ/mol)				
Temperature (K)	**NC-I-Isomer**	**NC-II-Isomer**	**C_{60}-I-Isomer**	**C_{60}-II-Isomer**
298.15	-1398.611	-1751.125	519.477	547.431
308.15	-1394.402	-1746.916	518.119	546.067
318.15	-1390.099	-1742.613	516.700	544.673
328.15	-1385.706	-1738.220	515.255	543.233
338.15	-1381.283	-1733.797	513.752	541.742
348.15	-1376.855	-1729.369	512.305	540.315
358.15	-1372.271	-1724.785	510.852	538.949
368.15	-1367.584	-1720.098	509.389	537.574
378.15	-1362.814	-1715.328	507.971	536.164
388.15	-1358.031	-1710.546	506.552	534.791
398.15	-1353.181	-1705.695	505.151	533.411

The thermodynamic equilibrium constants are presented in Table 4. One of the advantages of this parameter is that it can show the influence of temperature more sharply in comparison to other variables. The results indicate that proline interaction with carbon nanocone is one-sided and non-equilibrium, whereas, its interaction with C_{60} is weak, two-sided and reversible. In addition, by increasing of temperature, K_{th} has been significantly reduced in the proline-nanocone derivatives. Thus, it can be deduced that the adsorption procedure has become weaker. On the other hand, this variable has increased by incrementing of temperature in the case of fullerene-proline derivatives. It seems that proline adsorption on the fullerene gets stronger by increasing of temperature. But, it is worth mentioning that at the highest temperature, the thermodynamic constants of C_{60}-I-Isomer and C_{60}-II-Isomer are 5.311×10^{-67} and 1.041×10^{-70}, respectively, which shows that giving energy and heat to the system cannot make the proline adsorption process experimentally possible. As it was expected from the previous results, NC-II-Isomer derived product has greater thermodynamic constant in comparison to NC-I-Isomer. Thus, proline has the best interaction with nanocone from its nitrogen atom.

Table 4. The thermodynamic equilibrium constants for the proline adsorption process in the temperature range of 298.15-398.15 K

K_{th}				
Temperature (K)	**NC-I-Isomer**	**NC-II-Isomer**	**C_{60}-I-Isomer**	**C_{60}-II-Isomer**
298.15	$1.096\times10^{+245}$	$6.322\times10^{+306}$	9.694×10^{-92}	1.227×10^{-96}
308.15	$2.367\times10^{+236}$	$1.353\times10^{+296}$	1.480×10^{-88}	2.707×10^{-93}
318.15	$1.730\times10^{+228}$	$1.308\times10^{+286}$	1.458×10^{-85}	3.725×10^{-90}
328.15	$3.833\times10^{+220}$	$4.994\times10^{+276}$	9.533×10^{-83}	3.353×10^{-87}
338.15	$2.382\times10^{+213}$	$6.798\times10^{+267}$	4.334×10^{-80}	2.057×10^{-84}
348.15	$3.834\times10^{+206}$	$2.985\times10^{+259}$	1.360×10^{-77}	8.532×10^{-82}
358.15	$1.403\times10^{+200}$	$3.644\times10^{+251}$	3.103×10^{-75}	2.476×10^{-79}
368.15	$1.110\times10^{+194}$	$1.157\times10^{+244}$	5.286×10^{-73}	5.298×10^{-77}
378.15	$1.799\times10^{+188}$	$8.921\times10^{+236}$	6.767×10^{-71}	8.626×10^{-75}
388.15	$5.773\times10^{+182}$	$1.593\times10^{+230}$	6.747×10^{-69}	1.069×10^{-72}
398.15	$3.426\times10^{+177}$	$6.082\times10^{+223}$	5.311×10^{-67}	1.041×10^{-70}

The computed specific heat capacity values (C_V) of proline and its derived products with fullerene and carbon nanocone are given in Table 5. As it is obvious from the table, there is a tangible gap between the specific heat capacity values of proline and the investigated nano-adsorbents. Moreover, after the adsorption of proline, a significant surge has brought about in the C_V values of the evaluated nanostructures. According to equation 6, C_V has a direct relationship with thermal conductivity [25]. In this formula, n, $<v>$, λ, C_V and N are particles per unit, mean particle speed, mean free path, molecular specific heat capacity and Avogadro's number, respectively. Therefore, the thermal conductance of the fullerene and nanocone has been improved after the adsorption of proline amino acid. In this sense, in the development of thermal biosensors, a meaningful variation in the thermal conductivity of the sensing material plays a key role in the sensitivity of the designed analytical method. It can be concluded that nanocone is a promising sensing material in the construction of thermal biosensor for the detection of proline. The prior results proved that the interaction of proline and nanocone is exothermic and heat is transmitted from the system to the environment. So, the heat production which is necessary for appropriate function of this type of sensors is spontaneously implemented in the adsorption of proline on the nanocone.

$$K = \frac{n < v > \lambda\, Cv}{3N} \tag{6}$$

The impact of changing temperature on the specific heat capacity was also inspected. As it can be seen, the C_V value of each material has increased by incrementing of temperature. Thus, the thermal conductivity has ameliorated by rising of the temperature.

Table 5. The values of specific heat capacity for the proline adsorption in the temperature range of 298.15-398.15 K

C_V (J/mol.K)							
Temperature (K)	**proline**	**Nanocone**	**NC-I-Isomer**	**NC-II-Isomer**	**C_{60}**	**C_{60}-I-Isomer**	**C_{60}-II-Isomer**
298.15	88.159	300.432	328.693	322.339	403.7009	509.388	511.425
308.15	90.767	306.842	337.546	331.517	424.0389	532.518	534.446
318.15	93.431	312.982	346.289	340.578	444.2032	555.506	557.330
328.15	96.144	318.860	354.919	349.516	464.1699	578.322	580.048
338.15	98.901	324.485	363.433	358.329	483.9179	600.942	602.573
348.15	101.696	329.867	371.827	367.014	503.4289	623.342	624.882
358.15	104.524	335.014	380.098	375.567	522.6869	645.500	646.954
368.15	107.379	339.936	388.245	383.985	541.678	667.398	668.770
378.15	110.254	344.642	396.264	392.267	560.3903	689.019	690.314
388.15	113.146	349.142	404.152	400.409	578.8135	710.349	711.570
398.15	116.048	353.444	411.909	408.409	596.9387	731.375	732.526

Frontier molecular orbital analysis

In chemistry, HOMO is the highest occupied molecular orbital (E_H) and LUMO (E_L) is the lowest unoccupied molecular orbital, and the energy discrepancy between them is known as energy gap (HLG). This variable which was calculated by equation 7 is an admissible standard for measuring the electrical conductivity of a compound. Due to the fact that the conductometric analytical methods are designed on the basis of remarkable alterations in the conductivity of a special reaction, estimating HLG can be so helpful. As the provided data in (Table 6) illustrates, the HLG values of fullerene and carbon nanocone are 8.66 and 9.16 (eV), respectively, which have a considerable discrepancy with proline HLG (15.97). And after the adsorption of proline on the surface of nano-adsorbents, HLG has abated, dramatically. The conductivity and energy gap have a vice versa relationship with each other. Hence, the conductivity of the system has defused after the interaction of proline with the nanostructures. In this regard, owing to former results which indicated proline does not have a good interaction with fullerene it seems carbon nanocone can be utilized in the conductometric determination of proline.

$$HLG=E_{LUMO} - E_{HOMO} \quad (7)$$

$$\eta = (E_{LUMO} - E_{HOMO})/2 \quad (8)$$

$$\mu = (E_{LUMO} + E_{HOMO})/2 \quad (9)$$

$$\omega = \mu^2/2\eta \quad (10)$$

$$\Delta N_{max}=- \mu/\eta \quad (11)$$

Chemical hardness (η) was also calculated for each structure using equation 8. Chemical hardness is an acceptable criterion for estimating the softness and reactivity of a substance. In fact, a material with a negligible HOMO-LUMO gap is chemically smoother than a compound with a high value of HOMO-LUMO gap. With a more precise glance at Table 6, it can be realized that the chemical hardness of proline has declined drastically after its adsorption on the evaluated adsorbents. Given the fact that soft substances can change their electron density more easily in comparison to hard compounds, they will be more reactive because the electron transmission that is essential for the implementation of a reaction can be done in soft compounds more comfortably. So, proline derived products with fullerene and nanocone are more reactive than pure amino acid and nano-adsorbents. The chemical potential (μ) was also obtained *via* equation 9. This parameter is important for calculating electrophilicity (ω) and maximum amount of electronic charge index (ΔN_{max}). When two molecules react with each other, one of them acts as an electrophile whereas the other behaves as a nucleophile. Both ω and ΔN_{max} which were calculated by equations 10 and 11 respectively, exhibit the tendency of a molecule towards electron so that the compounds with higher electrophilicity and maximum charge capacity values are more eager to absorb electron from the environment. The obtained results in the table indicate that proline cannot participate in the complexation reactions with nanocone and C_{60} because their propensity to the electron is similar to each other.

Table 6. Calculated E_H and E_L, HLG, chemical hardness (η), electrophilicity index (ω), and the maximum amount of electronic charge index (ΔN_{max}) for the proline adsorption process

	E_H (eV)	**E_L (eV)**	**HLG (eV)**	**η (eV)**	**μ (eV)**	**ω (eV)**	**ΔN_{max} (eV)**
Proline	-8.12	-7.85	15.97	7.98	-0.14	0	0.02
C_{60}	-5.62	3.04	8.66	4.33	-1.29	0.19	0.30
C_{60}-I-Isomer	-9.70	-2.31	7.39	3.70	-6.01	4.88	1.63
C_{60}-II-Isomer	-8.9	-2.3	6.6	3.30	-5.60	4.75	1.70
Nano cone	-6.29	2.87	9.16	4.58	-1.71	0.32	0.37
NC-I-Isomer	-10.51	-3.33	7.18	3.59	-6.92	6.67	1.93
NC-II-Isomer	-9.78	-3.07	6.71	3.36	-6.43	6.15	1.92

Conclusions

Various analytical methods have been developed for proline determination. However, most of them are expensive, time-consuming and sophisticated. Fortunately, biosensors can be a good alternative because of being economical, having simple instrumentation and eminent selectivity. In this regard, the performance of fullerene (C_{60}) and carbon nanocone as a sensing material for proline detection was evaluated by density functional theory. The results revealed that proline adsorption on fullerene is endothermic, non-spontaneous and experimentally impossible. On the other hand,

proline adsorption on the surface of carbon nanocone was exothermic, spontaneous and experimentally feasible. In addition, the findings proved that carbon nanocone can be used for designing a thermal sensor for proline measurement. The orbital molecular analysis exhibited that carbon nanocone is also a prominent sensing material for conduct metric determination of proline. Owing to the fact that the obtained theoretical results substantiate the capability of carbon nanocone as an eminent sensing material for proline detection, an experimental investigation on the usage of this nanostructure for the construction of new proline biosensors is recommended to the experts of this field.

Conflict of Interest

We have no conflicts of interest to disclose.

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