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Original Research Article

Adsorption of Procarbazine Anti-cancer Drug on the Surface of Graphene: A DFT Study

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ABSTRACT

The present study aimed to assess the adsorption of graphene with anticancer drug procarbazine in a gas and solvent phase (water) at the B3LYP/6-31G (d) theoretical level. Initially, the structures of procarbazine and graphene complexes were optimized in three configurations. Afterwards, IR calculations and molecular orbital analysis were performed. In addition, some important parameters were assessed, including the adsorption energy, Gibbs free energy changes (ΔGad), enthalpy (ΔHad) variations, thermodynamic equilibrium constant, specific heat capacity, chemical hardness, energy gap, and electrophilicity. According to the results, Gibbs free energy changes (ΔGad), enthalpy (ΔHad) variations, I-Isomer and II-Isomer and III-Isomer were negatives at various temperatures, throughout the temperature range of 298.15-310.15 K. Since according to the obtained results for adsorption of procarbazine on the graphene in I-Isomer and II-Isomer and III-Isomer were spontaneous at various temperatures, throughout the temperature range of 298.15-310.15 K. Structural properties calculated, including the density and length of C-N bonds, and the findings of the analysis of molecular orbitals indicated that the reactivity, electrophilicity, and conductivity of procarbazine are reduced after this reaction. Also the calculated specific heat capacity values indicated that graphene could be utilized as a sensing material in the construction of thermal biosensors for procarbazine determination.

Keywords: Procarbazine, Anticancer drugs, Functional density theory, Graphene

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Introduction

The Rapid advance in drug discovery methods has led to an exponential increase in new drugs. Due to the diverse physicochemical properties of various drugs, we need smarter drug delivery systems. The use of nano compounds is increasingly growing, so that it has penetrated all aspects of life. In the meantime, the use of nano compounds in medical processes has also become more and more used. One of the important aspects of nanotechnology that has been considered today is the use of nanoscience as a drug carrier in the treatment of cancer, in some cases the use of these compounds as therapeutic targets. Due to the rapid advances in the discovery of drugs and their different physical and chemical properties, it is necessary to have intelligent drug delivery systems. [1] Delivery systems have many limitations on the use of materials and production processes [2]. The materials of these systems should have a biocompatibility with the body so that they can be easily attached to the drug, can be removed from the body, and the production process is carefully controlled so that the product containing the drug does not reduce the biological activity of the drug [3-4]. The chemical structure of procarbazine is shown in figure (1). In this study, the effect of graphene's compromise on the energetic properties of procarbazine was first considered computatively [5-9].

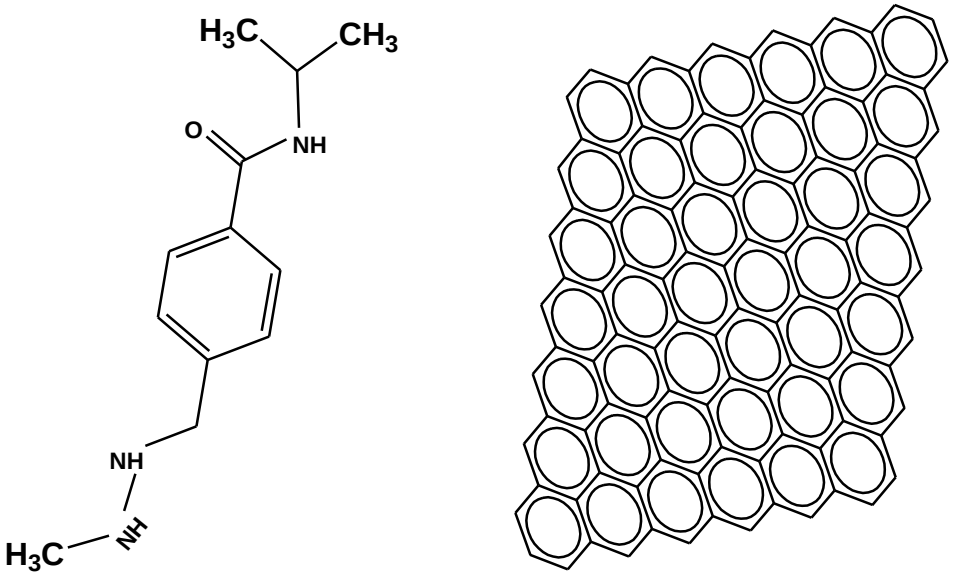

Figure 1: Chemical structure of procarbazine and graphene structure

Computational methods

Initially, the structure of the procarbazine, graphene and the derivatives of the cited nanostructure reaction with the procarbazine were computed in three different modes using Gauss View 6.1 software, and in the next step, geometric optimization calculations, IR, and molecular orbitals on them The use of the theory of density function and base series 6-31 g * was performed with the B3LYP hybrid functions. And done with the Gaussian calculation software. This basic series was selected as in previous reports, the results of that match were in good experimental data. All calculations performed using Spartan software in the temperature range from 278.15 to 314.15 K over the temperatures range from 3˚ -3˚. The responses are examined in general using Equation

Procarbazine + graphene→ procarbazine-graphene (1)

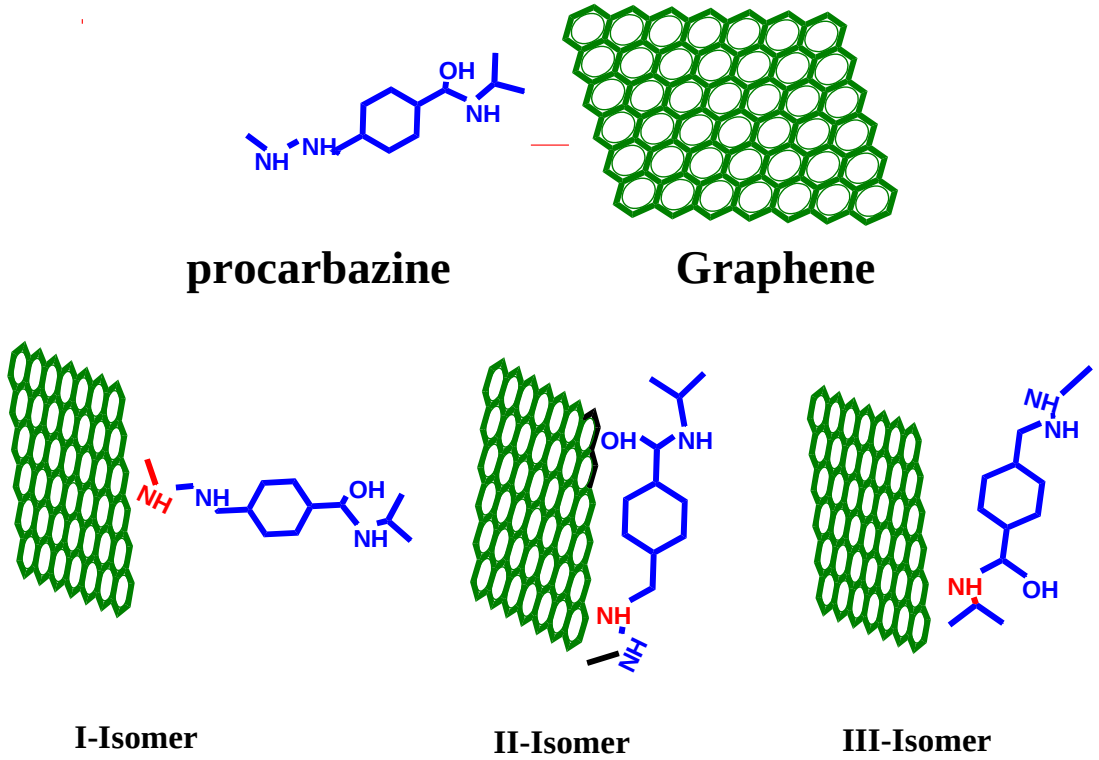

Figure 2: Optimized structure of procarbazine and its derivatives with graphene

Study of structural properties

As is seen in Figure 2, Graphene adsorption has been obtained from three positions. To understand more easily, each complex of the procarbazine derivate with graphene is named with an abbreviation, which will be explained. The links formed between the nitrogen groups in the structure of procarbazine can play a key role in the effectiveness of synthesized

procarbazine. In other words, as these links are looser and easier to disassociate, procarbazine can react more easily. Thus, after geometric optimization was performed on all compounds, the length of C-N bonds, in the procarbazine complexes, as well as their derivatives with graphene was measured and the values obtained in Table 1. As the data in Tables 1 indicate, after C-N attachment has increased, meaning that these bonds become looser and these derivatives can more easily enter the process of effectiveness. Density is another parameter that has direct and special relationship with effective power. As is seen in the data in the tables, the procarbazine density has decreased after the connection to the pure Graphene. Other structural features, such as surface and zero point energy have also increased dramatically after fullerene substituent.

Table 1: Total energy values, the lowest observed frequency, bond distances, bond type, zero point energy, surface, mass, volume and density for procarbazine and its derivatives with graphene in the gas phase(a) and the water solvent phase(b)

		Procarbazine	I-Isomer	II-Isomer	III-Isomer
ΔE_{ad}	a	-	-848.5074481	-868.4953811	-884.0627594
	b		-836.8840963	-859.2289409	-877.4517501
Lowest frequency (cm^{-1})	a	20.5806	8.0393	8.3767	7.0302
	b	16.7771	7.5658	8.0428	5.4443
$N13-C35$ (Å)	a	-	1.49029	-	-
	b		1.48997		
$N28-C35$ (Å)	a	-	-	1.50704	-
	b			1.50389	
$N30-C35$ (Å)	a	-	-	-	1.50126
	b				1.50311
$\sigma_{N13-C35}$ (Å)	a	-	3.057888	-	-
	b		3.052399		
$\sigma_{N28-C35}$ (Å)	a	-	-	3.36945	-
	b			4.573155	
$\sigma_{N30-C35}$ (Å)	a	-	-	-	3.633627
	b				3.638822
Area ($Å^2$)	a	284.39	575.02	583.64	591.86
	b	284.39	575.02	583.64	591.86

Calculating and analyzing the value of enthalpy changes, the formation of the graphene reaction

To obtain the values of the enthalpy formation for adsorption of graphene and procarbazine from the Equation (2). In this equation, ΔH0 is the total energy variation in the process obtained by reduction in the total energy of the products of a reaction from the sum of the total energy of the raw material. ΔH0 also represents the enthalpy sign for each of the reaction components.

$$\Delta H_{ad} = H_{\text{graphene- Procarbazine}} - (H_{\text{graphene}} + H_{\text{Procarbazine}}) \qquad (2)$$

As the results in Table (2) show, graphene reaction is done by exothermic procarbazine, and energy is transferred from the system to the environment, as the values of ΔHad are obtained for all the derivatives are negative. However, this phenomenon cannot have an effect on the reaction run, because despite this increase, the enthalpy changes remains negative. Moreover, to examine the effect of temperature on graphene substituent process, all thermodynamic parameters were calculated at the temperature range from 278.15 to 314.15 Kelvin in the 3˚-3˚ range and the values were reported. As is seen in Table (2), the temperature of the enthalpy changes gradually increases with increasing temperature. Thus, the process of forming the desired compounds becomes warmer with increasing temperature, and the optimum temperature for the synthesis of all derivatives is 298 Kelvin

Table 2: The values of enthalpy variations in the formation of substituent reaction of graphene and procarbazine in the gas phase (a) and the water solvent phase (b) at the temperature range from 278.15 to 314.15 Kelvin

Temperature(K)		I-Isomer	II-Isomer	III-Isomer
278.15	a	-778.82	-814.08	-847.08
	b	-671.27	-706.52	-739.52
281.15	a	-778.83	-814.08	-847.07
	b	-671.27	-706.53	-739.52
284.15	a	-778.83	-814.08	-847.08
	b	-671.28	-706.53	-739.52
287.15	a	-778.83	-814.08	-847.08
	b	-671.28	-706.52	-739.52
290.15	a	-778.83	-814.08	-847.08
	b	-671.28	-706.52	-739.52
293.15	a	-778.84	-814.08	-847.08
	b	-671.28	-706.52	-739.52
296.15	a	-778.84	-814.08	-847.08
	b	-671.29	-706.52	-739.53
299.15	a	-778.84	-814.07	-847.08
	b	-671.29	-706.52	-739.53
302.15	a	-778.84	-814.07	-847.08
	b	-671.29	-706.52	-739.53
305.15	a	-778.85	-814.07	-847.08
	b	-671.3	-706.52	-739.54
308.15	a	-778.85	-814.06	-847.08
	b	-671.3	-706.51	-739.54
311.15	a	-778.85	-814.06	-847.08
	b	-671.3	-706.51	-739.54
314.15	a	-778.85	-814.06	-847.08
	b	-671.31	-706.51	-739.54

Calculation and Investigation of Gibbs free energy changes and procarbazine derivatives with graphene

Equation (3) was used to calculate the Gibbs free energy variation (ΔGad). Regarding this, ΔGad is the thermal energy released by the Gibbs calculated by the software for each component of the reaction. The results, all of which are presented in Table (3), show that substituent of carbon nanotubes on procarbazine are spontaneous. This is because its ΔGad is much less than the Gibbs III-Isomer free energy variation. It is noteworthy that the process of

forming both derivatives is significantly more volatile by replacing the procarbazine at the fullerene bonding site. Since ΔGad value has experienced a sharp decrease after the process. However, in general, as the value of this parameter is significantly negative in all cases, it can be expected that the reaction of forming all compounds is empirically possible. The effect of temperature on this quantity was also evaluated as is evident the temperature rises, the amount of Gibbs free energy changes gradually increases as well. Thus, the highest synthesis efficiency appears at room temperature or 298 Kelvin.

$$\Delta G_{ad} = E_{graphene\text{-}\ Procarbazine} - (E_{graphene} + E_{Procarbazine}) \qquad (3)$$

Table 3: Gibbs free energy change of graphene and procarbazine in the gas phase(a) and the water solvent phase(b) at the temperature range from 278.15 to 314.15 Kelvin

	ΔGad(KJ/mol)			
Temperature(K)		I-Isomer	II-Isomer	III-Isomer
278.15	a	-710.11	-745.53	-778.92
	b	-602.69	-638.12	-671.51
281.15	a	-709.86	-745.3	-778.67
	b	-602.45	-637.89	-671.27
284.15	a	-709.61	-745.06	-778.43
	b	-602.2	-637.65	-671.02
287.15	a	-709.37	-744.82	-778.18
	b	-601.96	-637.41	-670.77
290.15	a	-709.12	-744.58	-777.94
	b	-601.71	-637.17	-670.53
293.15	a	-708.87	-744.34	-777.69
	b	-601.46	-636.94	-670.28
296.15	a	-708.62	-744.1	-777.44
	b	-601.22	-636.7	-670.04
299.15	a	-708.38	-743.86	-777.2
	b	-600.97	-636.46	-669.8
302.15	a	-708.13	-743.62	-776.95
	b	-600.73	-636.22	-669.56
305.15	a	-707.88	-743.37	-776.71
	b	-600.48	-635.98	-669.31
308.15	a	-707.63	-743.12	-776.46
	b	-600.24	-635.73	-669.07
311.15	a	-707.38	-742.87	-776.22
	b	-599.99	-635.48	-668.82
314.15	a	-707.13	-742.63	-775.97
	b	-599.73	-635.23	-668.57

Calculation and evaluation of the thermodynamic properties of procarbazine and their derivatives with graphene

The constant thermodynamic formation of the synthesis of procarbazine derivatives with graphene was also calculated using Equation (4). In this equation, ΔGad is the same as the Gibbs free energy variation obtained at the previous stage, R is the ideal gas constant, and T is the temperature in Kelvin as the results presented in Table (6) clearly show.

$$K_{th} = \exp(-\Delta G_{ad} / RT) \quad (4)$$

The thermodynamic parameters showed that the procarbazine drug reaction with graphene is exothermic, spontaneous, one-way and non-equilibrium and this reaction has the highest efficiency at room temperature. Molecular orbit analysis also proved that graphene derivatives have less conductivity, electrophilicity, and reactivity compared to pure procarbazine. As theoretical studies have shown that the graphene reaction with procarbazine is empirically possible, so the empirical investigation of the synthesis of these derivatives is highly recommended by experts in this field.

Analysis of the results of calculations of molecular orbitals

The most important frontier molecule orbital cell (FMOS), such as the highest occupied molecule orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) have a decisive role in the chemical stability of the molecule [10]. The energy gap between HOMO and LUMO determines the reactivity, polarization, and hardness-softness of a molecule, which is represented by the Gap mark and used to calculate it using Equation (5). The energy gap is directly related to the molecular electrical conductivity. In fact, compounds that have small energy gaps can easily pass electrons from the barrier to the conductive strip, which means that materials that have less energy bands have more electrical conductivity than molecules with higher energy chats. The results presented in Table (5) clearly show that the energy gap after adsorption of graphene has increased significantly. Indeed, the rate of conductivity of procarbazine has significantly decreased after fullerene substituent. The next parameter examined is the chemical hardness (η), whose value can be obtained using Equation (6). Chemical hardness is a good measure to estimate the reactivity of a new compound. This is because molecules that are structurally softer and have low chemical

hardness can easily change their electron density. Thus, electronic transmissions essential for chemical reactions are better and easier to use in soft compounds [11-15].

Table 4: The values of thermodynamic equilibrium constants for the procarbazine adsorption process with graphene in the gas phase (a) and the water solvent phase (b) at the temperature range from 278.15 to 314.15 Kelvin

	K_{th}			
Temperature(K)	I-Isomer		II-Isomer	III-Isomer
278.15	a	$1.1629\times10^{+35}$	$6.914\times10^{+38}$	$5.9431\times10^{+41}$
	b	$3.9204\times10^{+15}$	$6.3\times10^{+11}$	$4.4673\times10^{+17}$
281.15	a	$3.7462\times10^{+34}$	$2.1749\times10^{+38}$	$1.8219\times10^{+41}$
	b	$1.5776\times10^{+15}$	$2.4305\times10^{+11}$	$1.637\times10^{+17}$
284.15	a	$1.217\times10^{+34}$	$6.8946\times10^{+37}$	$5.6294\times10^{+40}$
	b	$6.3716\times10^{+14}$	$9.4065\times10^{+11}$	$6.0318\times10^{+16}$
287.15	a	$3.9703\times10^{+33}$	2.20E+37	$1.753\times10^{+40}$
	b	$2.592\times10^{+14}$	$3.6621\times10^{+11}$	$2.2409\times10^{+16}$
290.15	a	$1.306\times10^{+33}$	7.091410^{+36}	$5.5013\times10^{+39}$
	b	$1.0604\times10^{+14}$	$1.4341\times10^{+11}$	$8.3733\times10^{+15}$
293.15	a	$4.3277\times10^{+32}$	$2.2969\times10^{+36}$	$1.739\times10^{+39}$
	b	$4.3617\times10^{+13}$	$5.6484\times10^{+19}$	$3.1504\times10^{+15}$
296.15	a	$1.4445\times10^{+32}$	$7.48\times10^{+35}$	$5.5412\times10^{+38}$
	b	$1.8047\times10^{+13}$	$2.2393\times10^{+19}$	$1.1925\times10^{+15}$
299.15	a	$4.8508\times10^{+31}$	$2.452\times10^{+35}$	$1.7762\times10^{+38}$
	b	$7.5192\times10^{+12}$	$8.932\times10^{+18}$	$4.5501\times10^{+14}$
302.15	a	$1.6386\times10^{+31}$	$8.0906\times10^{+34}$	$5.7178\times10^{+37}$
	b	$3.1521\times10^{+12}$	$3.5842\times10^{+18}$	$1.7464\times10^{+14}$
305.15	a	$5.566\times10^{+13}$	$2.692\times10^{+34}$	$1.855\times10^{+37}$
	b	$1.3274\times10^{+12}$	$1.4446\times10^{+18}$	$6.7396\times10^{+13}$
308.15	a	$1.9025\times10^{+13}$	$9.0251\times10^{+133}$	$6.0625\times10^{+36}$
	b	$5.621\times10^{+11}$	$5.8407\times10^{+17}$	$2.617\times10^{+13}$
311.15	a	$6.5506\times10^{+29}$	$3.0484\times10^{+33}$	$1.9949\times10^{+36}$
	b	$2.3927\times10^{+11}$	$2.3764\times10^{+17}$	$1.0221\times10^{+13}$
314.15	a	$2.2746\times10^{+29}$	$1.0377\times10^{+33}$	$6.6221\times10^{+35}$
	b	$1.021\times10^{+11}$	$9.7323\times10^{+16}$	$4.0144\times10^{+12}$

The data in the table shows that the reaction of procarbazine is reduced after the reaction with graphene since all the derivatives obtained from the carbon nanotubes subtraction

reaction have a higher chemical hardness than the pure drug. The chemical potential (μ) used to obtain the rest of the parameters was calculated using equation (7). Electrophilicity (ω) and the maximum load transmitted to the system (ΔNmax) are both suitable quantities, showing the tendency of a compound to absorb electrons [16-24]. These two parameters were calculated using Equations (8) and (9), respectively. When two molecules react with each another, one acts as an electrophile while another plays the role of a nucleophile and the compound whose electrophilicity and charge capacity are higher will tend to behave as an electron receptor. On the other hand, a molecule with low electrophilicity and capacity tends to accept the electron system. As shown in the table, electrophilicity of procarbazine has been greatly reduced after graphene binding. Hence, one can be conclude that the desire of procarbazine to absorb electrons has decreased. The bipolar state of the studied structures has also been studied. This parameter is a good criterion for evaluating the solubility of molecules in polar solvents. Molecules with higher dipole moments have better solubility in water and compounds with less bipolar moments will be weaker in polar solvents. As can be seen, the dipole moment of procarbazine decreases after graphene connection. Thus, graphene derivatives with procarbazine have less solubility in water compared to pure procarbazine [25-32].

$$\mathbf{Gap = E_L - E_H} \quad \mathbf{(5)}$$

$$\mathbf{\eta = (E_L - E_H)/2} \quad \mathbf{(6)}$$

$$\mathbf{\mu = (E_L + E_H)/2} \quad \mathbf{(7)}$$

$$\mathbf{\omega = \mu^2/2\eta} \quad \mathbf{(8)}$$

$$\mathbf{\Delta N_{max} = -\mu/\eta} \quad \mathbf{(9)}$$

Table 5: calculated HOMO and LUMO, band gap, chemical hardness(η), chemical potential, electrophilicity(ω),the maximum amount of electronic charge index(ΔNmax) and dipole moment for the procarbazine adsorption process in the gas(a) and water solvent(b)phase.

	E_{HOMO} (eV)	E_{Lumo} (eV)	Gap (eV)	η(eV)	μ(eV)	ω (eV)	ΔN_{max} (eV)	Dipole Moment(Deby)
procarbazine	-7.42[a]	6.10	617.42	308.71	301.29	158.16	-0.98	3.34
	-7.29[b]	6.21	13.50	0.75	-0.54	-42.19	0.08	3.59
I-Isomer	-6.87[a]	0.85	7.72	3.86	-3.01	-2.48	0.78	2.39
	-6.81[b]	0.93	7.74	3.87	-2.94	-2.55	0.76	2.84
II-Isomer	-6.96[a]	0.77	7.73	3.87	-3.10	-2.41	0.80	2.62
	-6.89[b]	0.84	7.73	3.87	-3.03	-2.47	0.78	2.52
III-Isomer	-6.86[a]	0.89	7.75	3.88	-2.99	-2.52	0.77	1.89
	-6.83[b]	0.93	7.76	3.88	-2.95	-2.55	0.76	2.23

Conclusion

According to the evaluation of the thermodynamic parameters. Procarbazine drug reaction with graphene was exothermic, spontaneous, one-way, and non-equilibrium. In addition, the reaction had the highest efficacy at room temperature. Molecular orbit analysis also confirmed that fullerene derivatives had higher conductivity, electrophilicity, and reactivity compared to pure Procarbazine. As proposed in theoretical studies, the reaction of fullerene with Procarbazine is empirically possible. Therefore, the empirical investigation of the synthesis of these derivatives by the experts in this field is strongly recommended.

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