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DFT/QTAIM analysis of favipiravir adsorption on pristine and silicon doped C₂₀ fullerenes

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Abstract: Fullerenes have received attentions due to their versatile properties. Molecular structures and electronic properties namely binding energy, band gap, electrophilicity index and molecular topological analysis were studied for undoped and silicon doped C₂₀ fullerenes and favipiravir in order to search for possible application of the systems as drug delivery vehicles. Density functional theory (DFT) and quantum theory of atoms in molecules (QTAIM) were used for the research. Molecular structures having the interaction edges of SiC₁₉...OH in water and SiC₁₉...C=O in gas phase were found as those most stable with binding energies of -57.28 kcal/mol and -43.46 kcal/mol correspondingly. The results and parameters found in this research may provide additional insights into drug delivery systems.

Keywords: C₂₀; favipiravir; DFT; QTAIM

1 Introduction

Molecular modelling, designing of new nanostructural devices and studies revealing the interaction mechanisms between various types of molecular systems have been reported (Cheng and Zhao, 2012; Zhang and Zhao, 2012; Zhao and Han, 2008; Zhao and Han, 2012; Zhao et al.,

2007). Due to their functional properties, fullerenes have attracted a wide range of interest, especially in the field of nanomaterials and biomedical sciences (Guo et al., 1992; Koshio et al., 2000; Kroto et al., 1985). Fullerene incorporated drug systems have been examined because of their low toxicity and minimal side effects (Bakry et al., 2007; Shi et al., 2013; Singh and Lillard, 2009). In addition to these, by doping fullerenes with heteroatoms, it is possible to change their properties such as hydrogen adsorption capacities, molecular stabilities and conductivities (Baei, 2012; Cruz-Silva et al., 2008; Ganji et al., 2011; Wang et al., 2012). It has been also reported that boron doped carbon nanostructures have the potential to act as p-type conductors which include electronic holes and silicon doped carbon nanotubes showed metal conductivity (Hassani and Tavakol, 2016; Wang et al., 2012). By doping fullerene structures with different heteroatoms, it is also possible to change the charge distributions of the fullerene systems which is an important parameter determining the systems adsorption behaviour and possible usage as sensors by leading alterations in the band gap energy (Amiraslanzadeh, 2016).

As a pyrazinecarboxamide derivative, favipiravir (6-fluoro-3-hydroxy-2-pyrazinecarboxamide; C₅H₄FN₃O₂), known also as T-705, is an antiviral compound used against for many RNA and Ebola type viruses. It is active against influenza, West Nile, yellow fever, foot-and-mouth disease viruses as well as other flaviviruses, arenaviruses, bunyaviruses and alphaviruses (Furuta et al., 2002; Furuta et al., 2013; Sissoko et al., 2015).

Recently, we have carried out a study to investigate the adsorption between favipiravir and undoped or silicon doped C₆₀ fullerenes and to make an assessment about their possible usage as drug delivery vehicles (Parlak et al., 2017). In the search of the stable structures, nine different possible structures using various interaction edges of the molecule were optimized using M062X/6-31G(d) method. It was observed that the binding energy (E_b) is dependent on the solvent and interaction edge. The C=O and OH edges were effective in the gas phase and water correspondingly. In view of the above and in continuation with our interests in the investigation of doped fullerenes

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(Parlak et al., 2016; Parlak et al., 2017), the primary scope of this study was to use DFT and QTAIM in conjunction with the M062X/6-31G(d) method to understand the possible interaction mechanism of C₂₀ and Si-doped C₂₀ fullerenes with favipiravir molecule. Within this scope, we were interested in understanding the usage of the C₂₀ cage as a potential candidate to carry this important drug.

2 Results and discussion

2.1 Interaction of favipiravir and C₂₀

Several possible interaction edges may be proposed upon examining electrostatic potential (ESP) map of the drug molecule and fullerene systems (Figure 1). Colour ranges (in a.u.) of the drug and SiC₁₉ in gas and water are

Figure 1: ESP maps of the structures.

more positive than 0.025 for blue and more negative than -0.025. Areas of low and high potentials, red and blue, are characterized by an abundance of electrons and a relative absence of electrons respectively. Therefore, the lowest electrostatic potential area corresponds to the greatest electron concentration area. Taking into account these possible interaction sites and by considering our previous study (Parlak et al., 2017), three possible structures were built and optimized (Figure 2). The optimized structure for C₂₀...Drug system shows that the plane indicated by pentagon of C₂₀ is almost parallel to the plane constructed by the ring atoms of the drug molecule and this leads to a parallel displaced π - π interactions (Hunter and Sanders, 1990). Equilibrium distance from the center of the pentagon of C₂₀ to the hexagon of the drug molecule and binding energy of the system were found to be 3.43 Å and -3.96 kcal/mol in the gas phase (Table 1). The binding energy obtained indicates a physisorption occurring between C₂₀ nanocage and the drug like C₆₀ fullerene (Bhushan, 1999; Parlak et al., 2017). In water, the binding energy of C₂₀...Drug system is reduced by 39% in magnitude and the distance increases from 3.43 Å to 3.45 Å. Density of states (DOS) spectra of the related system are shown in Figures 3 and 4 together with plots of frontier orbitals. Introduction of drug molecule to C₂₀ fullerene leads to a slight change (0.006 and 0.008 eV) in the energy

Table 1: BSSE corrected binding and solvent energies (kcal/mol) of the structures.

Structure	M062X/6-31G(d)		
	E _b (gas)	E _b (water)	E _s
C ₂₀	-	-	-0.50
Drug	-	-	-6.84
C ₂₀ ...Ring	-3.96	-2.42	-6.86
SiC ₁₉	-	-	-3.88
SiC ₁₉ ...C=O	-43.46	-51.24	-18.52
SiC ₁₉ ...OH	-39.75	-57.28	-28.38
SiC ₁₉ ...N&O	-39.58	-57.19	-28.09

Figure 2: Interatomic distances (a-c) and optimized structures for the investigated systems.

Figure 3: DOS spectra of C₂₀ and C₂₀...Drug in gas phase.

gaps of frontier orbitals (E_g) for both the gas phase and in water. The interaction between C₂₀ and the drug molecule leads to a slight decrease in the electrophilicity index (ω) for gas phase and an increase for water (Table 2).

2.2 Interaction of favipiravir and SiC₁₉

In order to determine the possible interaction sites for a given molecular system, the determination of partial charges or charge distribution along the surfaces of the investigated systems is important for effective interaction (Armaković et al., 2014; Ashrafian, 2015; Shariatinia and Shahidi, 2014). Therefore, charge distribution analysis is important in the examination of adsorption processes. Accurate determination of charge distribution of molecular systems depends on various factors such as the types of the atoms included in the system, computational methods and the basis sets employed in the calculations (Brom et al., 2003; Easton et al., 1996; Kelly et al., 2005;

Figure 4: DOS spectra of C₂₀ and C₂₀...Drug in water.

Table 2: Energetic parameters (eV) of doped and undoped C ₂₀ fullerenes.					
Structure	E _{HOMO}	E _{LUMO}	E _g	η	ω
M062X/6-31G(d) Gas					
C ₂₀	-6.314	-2.429	3.885	1.943	4.919
SiC ₁₉	-6.222	-3.212	3.010	1.505	7.392
C ₂₀ ...Drug	-6.301	-2.422	3.879	1.940	4.904
SiC ₁₉ ...Drug					
C=O	-5.198	-3.074	2.124	1.062	8.054
N&O	-4.602	-3.224	1.378	0.689	11.111
OH	-4.596	-3.241	1.355	0.678	11.332
Water					
C ₂₀	-6.264	-2.368	3.896	1.948	4.781
SiC ₁₉	-6.167	-2.747	3.420	1.710	5.808
C ₂₀ ...Drug	-6.289	-2.401	3.888	1.944	4.856
SiC ₁₉ ...Drug					
C=O	-5.505	-2.265	3.240	1.620	4.658
N&O	-5.271	-2.361	2.910	1.455	5.004
OH	-5.271	-2.360	2.911	1.456	5.001

Thompson et al., 2002). Interaction between molecular systems is governed by the electrostatic potentials due to the nuclei and electron distribution (Stone, 2002). ESP maps indicate the charge distributions of molecular systems in three dimension which makes it possible to visualize the charge distribution of a molecule. This information of the charge distributions allows the determination of how and which site the molecules interact with each another (Hunter, 2004; Kenny, 2009; Weiner et al., 1982).

It can be observed from the ESP map of the Si-doped C₂₀ fullerene that the silicon atom can be considered as the active sites for the ligand interaction (Figure 1). The favipiravir molecule may prefer to interact via its oxygen atom of carbonyl group (C=O), oxygen atom of hydroxyl group (OH) and nitrogen of ring and oxygen of hydroxyl group at the same time (N&OH) based on the ESP analyses. It is observed that E_b energies show dependence on the molecular environment. The strongest binding interaction including correction for basis set superposition error (BSSE) within the investigated sites occurs with oxygen atom of the carbonyl group for SiC₁₉...Drug system with -43.46 kcal/mol in the gas phase. In water, the strongest connection occurs from the OH edges with -57.28 kcal/mol (Table 1). A similar trend was observed for Si-doped C₆₀ fullerenes with favipiravir drug molecule (Parlak et al., 2017). The binding energies of the interactions of doped C₂₀ fullerene with drug molecule are given in Table 1 and these suggest that chemisorption occurs between silicon doped C₂₀ and the drug molecule (Bhushan, 1999) like Si-doped C₆₀ (Parlak et al., 2017). In chemisorption, new chemical bonds are formed between interacting molecules and therefore, the interatomic distances where the bonding occurs must be at a feasible length (Oura et al., 2003). As seen in Figure 2, calculated interatomic bond distances make it possible for chemisorption (De Silva et al., 2014; El Mahdy, 2016).

Chemical hardness (η) and electrophilicity character can be used to evaluate the chemical stability and reactivity of chemical species (Suliman et al., 2014). For the SiC₁₉...Drug system, the calculated values for chemical hardness increases from gas phase to water and electrophilicity indices decrease (Table 2). Further, electrical band gaps follow same trend with chemical hardness. In general, it is seen that the band gap values are sufficient for the systems to be biologically active. It is also important to note that all the complexes of SiC₁₉...Drug system shows larger (more negative) binding energies or stronger interaction in water compared to the gaseous phase (Table 1). The values of solvent energy (E_s) for both silicon doped C₂₀ and C₆₀ (Parlak et al., 2017)

Table 3: Carbonyl stretching vibration (cm⁻¹) for the structures.

Structure	M062X/6-31G(d)	
	Gas	Water
	Carbonyl stretching	
Drug	1818	1779
SiC ₁₉ ...C=O	1752	1737
SiC ₁₉ ...(N&O)	1756	1788
SiC ₁₉ ...(OH)	1755	1788

complexes indicate that the complexes by OH edge have higher solubilities.

The carbonyl stretching vibrations show characteristic band properties and thus these are convenient to follow the effect of adsorption on the fullerene complexes undertaken in this work. In the gas phase and water, the C=O stretching vibrations were calculated as 1818 and 1779 cm⁻¹ for the free drug molecule. The effect of adsorption of the favipiravir on the Si-doped fullerenes lead to alterations on the vibrational wavenumbers of C=O band confirming the existence of interaction between the drug and the doped fullerene system (Table 3).

2.3 Topological analysis

The QTAIM method was used to analyse the electron density and bonding characteristics of the systems (Bader, 1990). In order to gain further insights into the bonding, the topological analysis has been performed and the corresponding wave functions were generated at the same level of theory. The characteristics of the bond critical point (BCP) were obtained in terms of the electron density (ρ) and it's Laplacian ($\nabla^2\rho$), the total electron energy density (H), the potential electron energy density (V) and the Lagrangian kinetic energy (G). The computed summation of QTAIM parameters at the intramolecular BCP's is provided in Table 4. The observed molecular topological map of SiC₁₉...C=O is provided in Figure 5 as an example.

C₂₀...Drug configurations in both gas phase and water have positive values of $\nabla^2\rho$ (0.022 and 0.021 a.u.) and H (0.001 a.u.), indicating their electrostatic character. Further, for this interaction, the electron density value is 0.007 a.u. These results indicate that the bonds possess the typical characteristic of closed-shell interactions. It is claimed that the nature of interaction in the case of positive Laplacian of charge density and H is electrostatic while the nature of interaction in case of positive $\nabla^2\rho$ and negative of H is partly covalent (Ravaei et al., 2019).

Table 4: Properties (a.u.) of QTAIM analysis for the structures.

Structure	ρ	$\nabla^2\rho$	G	V	H
Gas					
C ₂₀ ...Drug	0.007	0.022	0.005	-0.004	0.001
SiC ₁₉ ...Drug					
C=O	0.085	0.500	0.139	-0.152	-0.013
*N&O	0.098	0.623	0.171	-0.186	-0.015
OH	0.097	0.618	0.170	-0.185	-0.015
Water					
C ₂₀ ...Drug	0.007	0.021	0.004	-0.003	0.001
SiC ₁₉ ...Drug					
C=O	0.096	0.618	0.169	-0.183	-0.014
*N&O	0.103	0.686	0.188	-0.204	-0.016
OH	0.103	0.688	0.188	-0.204	-0.016

*No any BCP for N atom.

Figure 5: Molecular topography map for SiC₁₉...C=O. Nuclear and bond critical points are represented by purple and orange spheres correspondingly. Green and yellow circles are cage and ring critical points, respectively. The lines are bond paths.

Hence, the silicon doped configurations have positive $\nabla^2\rho$ and negative of H values and the Si-O bonds are polar covalent bonds for both medium.

3 Computational details

In the search of stable configurations, input geometrical structures of the C₂₀, SiC₁₉ and favipiravir drug molecule were built and then they were optimized with applying no geometrical restrictions using the M062X functional with the 6-31G(d) basis set. In order to check, if the final structures belong to a transition state or not, frequency calculations were carried out with the same level of theory. No imaginary frequencies were encountered. Therefore, none of the investigated geometries are in the transition state. In order to make an assessment about

the relative stabilities and adsorption mechanisms of the present systems, electrostatic potential, binding energies, energy gaps of frontier orbitals, chemical hardness and electrophilicity index were also calculated. They were calculated as described earlier (Parlak et al., 2016; Parlak et al., 2017).

All the calculations were performed in both gas and water environment to evaluate the solvent effect on the stabilities of the systems. Polarizable continuum model was used to investigate the solvent effect. Gaussian 09 was performed for the computations whereas structural illustrations of the molecular systems were done with GaussView and GaussSum programs (Dennington et al., 2009; Frisch et al., 2009; O'Boyle et al., 2008). The calculation of QTAIM analysis was performed using Multiwfn software (Lu and Chen, 2012).

4 Conclusions

To explore the interaction between favipiravir with the silicon doped and undoped C₂₀ fullerenes, quantum mechanical calculations and topological analysis by DFT/QTAIM were carried out with the M062X/6-31G(d) method in the gas phase and water. The possible interaction edges were proposed for the drug molecule and their stabilities shows dependence on the medium (gas or water). It is observed that SiC₁₉...Drug system gains more stability and more negative binding energies in water compared to the gas phase. SiC₁₉...(OH) in water and SiC₁₉...(C=O) in gas systems are found as the most stable structures. The physical and chemical adsorptions determined with binding energies were also supported by QTAIM topological study. For the adsorption energy and interaction site in the gas phase and water, Si-doped C20 fullerene with favipiravir has similar trend with C60 fullerene. All systems have large dipole moment (12-30 Debye for SiC₁₉...Drug) and this is an essential criterion for drug-receptor interaction (Parlak et al., 2014). The electrical band gaps are ~3 eV which is sufficiently large to meet the viability criterion (Hoffmann et al., 2008).

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