Int. J. Electrochem. Sci., 11 **(2016)** 855 - 871

International Journal of ELECTROCHEMICAL SCIENCE
www.electrochemsci.org

Theoretical Study of Electron Transfer Process Between Fullerenes and Membrane Cells of *Helicobacter pylori*

Nargese Zolfaghar Karahrudi[1,*] *and Avat (Arman) Taherpour*[2,3,*]

[1]Chemistry Department, Faculty of Science, Islamic Azad University, P.O. Box 38135-567, Arak, Iran
[2]Department of Organic Chemistry, Faculty of Chemistry,Razi University, P.O.Box: 67149-67346, Kermanshah, Iran
[3]Medical Biology Research Center, Kermanshah University of Medical Sciences, Kermanshah, Iran
[*]E-mail: nzolfaghar@gmail.com and avatarman.taherpour@gmail.com

Received: 7 October 2015 / *Accepted:* 21 November 2015 / *Published:* 1 January 2016

The difference of the electrical potential across the membrane of *Helicobacter pylori* has applied to investigate the electron transfer between the membrane cells of *Helicobacter pylori* bacteria and the selected fullerenes C_n. The various empty carbon fullerenes as a family of carbon allotropes have been obtained and investigated. Topological descriptors were utilized to make an effective theoretical method to establish the relationship between the structural indices and the physicochemical, medicinal and biochemical properties of materials. The relationship between the ΔG_{et} (free energies of electron transfer) and the "n" descriptor (as the number of carbon atoms in fullerenes) were assessed using the *Rehm-Weller* formula for the ET-process between the membrane cells of *Helicobacter pylori* and the selected fullerenes. The oxidation potential ($^{Ox.}E$) of the fullerenes C_n were applied here. The results have applied to determine the ΔG_{et} (the free-energies of electron transfer) of the ET process of C_n molecules and the membrane cells of *Helicobacter pylori*. The free activation energies of electron transfer and the maximum wave length of the electron transfers ($\Delta G^{\#}_{et(n)}$ and λ_{et}, respectively), have determined for the experimental conditions in accordance with the *Marcus* theory. The *Hammett* type relationship was investigated between "$\Delta\Delta G_{et}^{\#}$" and "$\Delta\Delta G_{et}$" of the first free energies of the ET between the *H. pylori* bacteria in presence of urea (different pH) and the selected fullerenes.

Keywords: Fullerenes; *Helicobacter pylori*; Electrical potential; Electron transfer process; free energies of electron transfer ΔG_{et}; free activation energies of electron transfer $\Delta G^{\#}_{et(n)}$; maximum wave length of the electron transfers λ_{et}; $\Delta\Delta G_{et}^{\#}$; $\Delta\Delta G_{et}$; *Rehm-Weller* equation; *Marcus* Theory; *Hammett* type relationship; *Plank's* formula.

1. INTRODUCTION

The two basically forms of metabolic energy in microorganisms were described as: a) the ions (such as proton) gradients provide the electrochemical energy for cell of microorganisms, and b) the energy-rich phosphate bonds such as ATP molecule. A cell of bacteria includes an organized cytoplasm and the organization of the proteins particularly for those intricate and important morphogenetic processes is for the cell operations such as morphogenetic processes. One of the important requirements to survive this operations is energy.[1-12] The ΔpH and the ΔΨ (trans-membrane chemical proton gradient and trans-membrane electric potential, respectively) were constructed by the producing proton motive force (PMF).[1,2,8]

The PMF includes the chemical proton potential and the ΔΨ (in Volt). The gradient of H^+ ion can be utilized as the intermediate energy storage as an inter-convertible type of energy for the life rotations, electron potential generation, active transport, ATP synthesis/hydrolysis and the other biochemical process of cells. The energy source of ATP is created using the PMF. A couple of H^+ ion (i.e. $2H^+$) produces an ATP molecule. The gradients of H^+ ion have also run in the bacteria cells in a reversible process by running ATP syntheses.[1,2,9,10] The ΔΨ in the cell of microorganisms can be specified between the cells and the suspending media by the diffusion of lipophilic ionic molecules.

In 2002, Stingl *et al*. reported that for several hours *Helicobacter pylori* can survive with concomitant cytoplasmic pH homeostasis in the presence of urea in pH=1.[13] Stingl *et al*. have shown that without any previous adaptation, growing cells of *H. pylori* are capable of survival and cytoplasmic pH (pH_{in}) homeostasis for several hours after a shift of the medium pH (pH_{out}) to pH=1 in the presence of urea.[13,14] They reported that *H. pylori* bacteria enable to cope with fluctuating pH by the biological mechanisms, in order to overcome the gastric acid barrier.[13] Stingl *et al*. have also shown that in the pH the acidophiles exhibit a positive ΔΨ inside of the membrane [13-17]. The ΔΨ of *H. pylori* cell membrane were examined at low pH_{out} values and extended the studies to pH=1-2. [13] For the bacteria, the sign and the value of the membrane electric potential ΔΨ at low pH_{out} values is still a matter of investigations. The data is lacking for pH_{out} values of <3. [13,18] In other investigations the membrane electric potential remained negative inside of bacteria membrane to a pH=3 [13,19]. Stingl *et al*. have observed that in the presence of urea and at all of the pH_{out} values between 1.2 and 7 the ΔΨ inside of the *H. pylori* cell membrane remained negative.[13]

Ulcers in the stomach and duodenum result when the consequences of inflammation allow stomach acid. The digestive enzyme pepsin acts to overwhelm the mechanisms that protect the stomach and duodenal mucous membranes. The ammonia were produced to regulate pH is toxic to epithelial cells, as are biochemical compounds produced by *H. pylori* bacteria. *H. pylori* is a Gram-negative, micro-aerophilic bacterium found in stomach. In 1982, it was identified that the conditions not previously believed to have a microbial cause by Marshall and Warren with further research led by Goodwin.[20-30] The membrane of *H. pylori* bacteria includes of lipopolysaccharide (LPS) and phospholipids.[20-29] The bacteria outer membrane also consists cholesterol glucosides. [20-27,30] The location of colonization of *H. pylori* bacteria depends on the acidity of the stomach. [20-27,31-33]. *H. pylori* bacteria harms the stomach several mechanisms.

The different empty fullerenes (C_n) with various number of carbon atoms "n" such as C_{60}, C_{70}, C_{76}, C_{82} and C_{86}, have been obtained. [34–65] Because of the different number of the carbon atoms in their structures these molecules show different chemical, physical and mechanical properties. The compressive mechanical behaviors of the empty fullerenes C_n (n = 20, 60, 80, and 180) were investigated with using QMD (quantum molecular dynamics) technique by Shen. [36,53] The interesting stability of molecular allotropes C_{60} and C_{70} was shown in 1985. [34-36] After the discovery of C_{60} peapods by Luzzi *et al.* [37-46] the aligned structure of encapsulated molecules has been studied as a new type of hybrid material due to the molecule-molecule interactions. [42-44] Since the early 1990s, the electrochemical properties of the C_{60} were studied when these materials first became available in macroscopic quantities. [41-43]

In 2003, for the first time, the hypothesis of fullerenes acting as electron drainer which can disrupt the respiratory chain with electron leakage by Mashino et.al. [43] The report was focused on positively charged derivatives, however the behind mechanism of interactions seems to have common points. [43]

The LUMO orbital of C_{60} can accept up to six electrons (6e) to form C_{60}^{6-}, but the position of the HOMO does not allow for hole-doping under the usual reported electrochemical conditions. Haufler *et al.* [44] have demonstrated the reduction C_{60} to C_{60}^{1-} and C_{60}^{2-} electrochemically in CH_2Cl_2 media. Echegoyen *et al.* [45] electrochemically reduced C_{60} in six reversible steps for -0.97V vs. Fc/Fc^+. The irreversible electrochemical and structural reorganization of solid fullerenes in acetonitrile was reported by Bard *et al.*.[46] The experimental conditions by investigating highly organized C_{60} films on HOPG in an aqueous medium was improved by Dunsch *et al.*. [47] The reduction of the tin films induces a morphological change. They reorganized into conductive nano-clusters of ~100 nm in diameter. [47,48]

Graph theory has introduced as a high performance mathematical method in assessing the Quantitative Structure Activity Relationship (*QSAR*) and Quantitative Structure Property Relationship (*QSPR*) studies. A lot of studies in different areas have applied the topological descriptors.[49-79] The extrapolation of the physical and chemical properties from one molecule to other molecules must account the considerations based on the *QSAR* studies. To make good correlations between several properties of chemicals should utilize the effective mathematical methods. Several interesting applications of the descriptors carbon atoms of the fullerenes have reported. [53-79]

The *Arrhenius* equation is one of the main foundations of *Marcus* theory. The *Arrhenius* equation has utilized to measure the rates of chemical reactions in two pathways: a) This formula constructs an equation to calculate the activation energy based on a parameter called the *reorganization energy* (RE) and the *Gibbs* free energy. The reorganization energy has defined as the energy required reorganizing the structure of the system from initial to the final coordinates without changing the electronic states, b) this theory constructs another formula to construct the exponential factor in the *Arrhenius* equation, based on the electronic coupling between the initial and final state of the electron transfer reaction. [80-87]

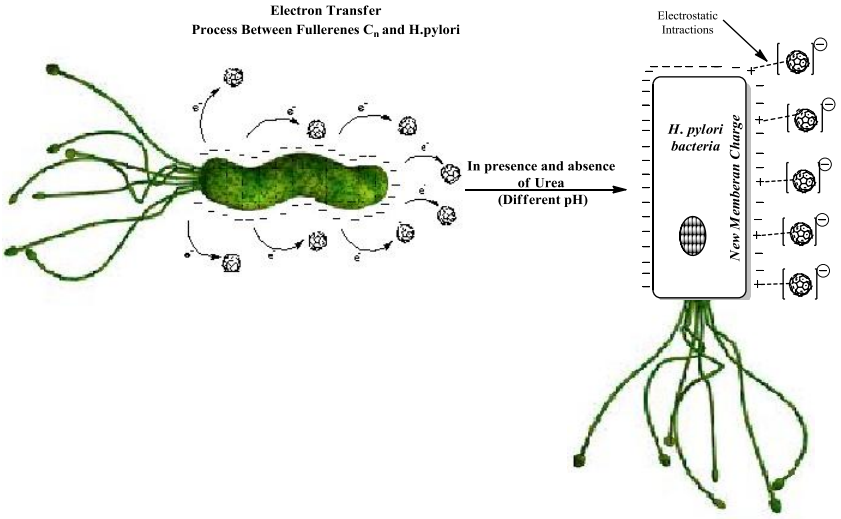

Figure 1. The imaginary ET-process between *Helicobacter pylori* bacteria in the presence and absence of Urea (in the different pH) and the selected fullerenes C_n to construct the dipolar complexes.

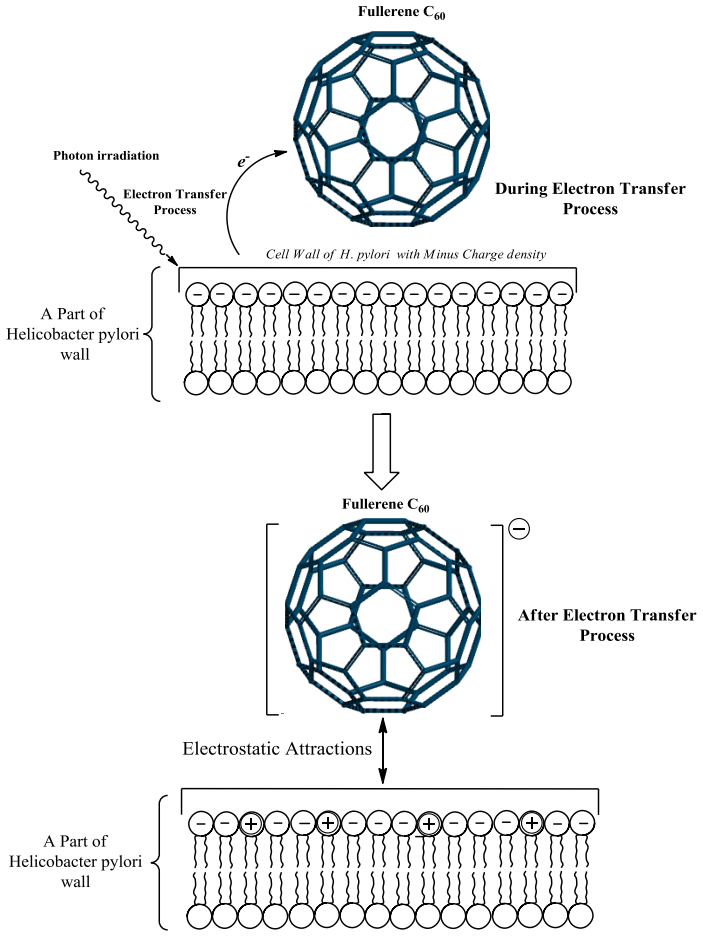

Figure 2. The imaginary ET-process between the cell wall of *H. pylori* bacteria and the selected fullerenes to construct the dipolar complexes by electrostatic attraction.

Electrons have described as residing in electron orbitals in electron bands and molecules. An electron can be excited from a ground state orbital to a higher energy orbital level when a photon

irradiates to a molecule and excites it. This mechanism constructs a vacancy in the lover energy orbital levels. This vacancy can be occupied by an electron donor agent. The electron that it is produced in a higher-energy orbital can be donated electron to an electron acceptor molecule with lower-energy orbital. A Photo-induced electron transfer is a type of ET-process. It occurs when certain photoactive materials interact with light irradiation, including semiconductors. The phenomenon can be also named as photo-activated process. This phenomenon can be occurred in some chemical and biological systems like those applied in photosynthesis, small molecules with many solar cells, suitable absorptions and redox states. [80-88]

This study elaborates on the electron transfer process between the selected fullerenes C_n (n = 60, 70, 76, 82 and 86) and the membrane cells of *Helicobacter pylori*. The relationship of the free energies of electron transfer (ΔG_{et}) between the cell wall of *H. pylori* bacteria and the number of carbon atoms of the selected fullerenes C_n (n=60, 70, 76, 82 and 86) were investigated, on the basis of the oxidation potentials ($^{Ox.}E_1$) of the fullerenes as assessed by applying the *Rehm-Weller* equation.[89] The results were extended to calculate the free energies of electron transfer (ΔG_{et}) of the other fullerenes C_{78}, C_{84} and C_{120} and the introduced conditions and *H. pylori* bacteria. See the equations 1 to 12, Tables 1 to 6 and Figures 1-3 and Scheme-1.

In this study, were also calculated the activate free energies of electron transfer and the maximum wave length of the electron transfers ($\Delta G^{\#}_{et(n)}$ and λ_{et}), applying *Marcus* theory and the polynomial equations on the basis of the oxidation potentials of the selected fullerenes C_n (n=60, 70, 76, 82 and 86) to predict the data of the ET-process between the membranes of *H. pylori* and the fullerenes. See the equations, Tables and Figures. One of the aspects in this study was the determination of the relationship between the number of carbon atoms descriptor in the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}) and the data values on the electron transfer (ΔG_{et}, in kcal mol^{-1}) between the *H. pylori* bacteria cell wall in presence of Urea (in different pH) with the fullerenes. The linear relationship was investigated between "$\Delta\Delta G_{et}^{\#}$" and "$\Delta\Delta G_{et}$" (*Hammett* type equation) of the first free energies of the electron transfer between the *H. pylori* bacteria in presence of Urea (different pH) and the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}).

It has supposed that the electron transfer process between *Helicobacter pylori* bacteria and the selected fullerenes construct the dipolar complexes to perform a condition for *H. pylori* bacteria damage. It is assumed that the results of this study and the phenomenon of photoelectron transfer can be applied in some biological and medical treatments, such as irradiation of he selected wavelengths (calculated λ_{et}) on *H. pylori* in the presence of the fullerenes through endoscopy, during the stomach diseases, to destruct the membrane cells of *H. pylori* bacteria.

It was also assumed that the discussed ET-process has also stopped some phenomena related to restriction in bacteria growth by perturbation on the membrane charge of *H. pylori* bacteria cell wall.

2. MATHEMATICAL METHODS AND GRAPHING:

All of the mathematical operations and graphing have performed using *Microsoft Office Excel-2003* and *MATLAB-7.4.0(R2007a)* programs. By using the descriptor of the number of carbon atoms

contained within the C_n fullerenes can be calculated several valuable properties of the fullerenes. The values were used for calculating the free energies of electron transfer (ΔG_{et}), according to the *Rehm-Weller* formula for the electron transfer process between the selected fullerenes and the cell wall of *Helicobacter pylori* bacteria.

Equations 1 and 5-21 have applied to measure the values of ΔG_{et} for the dipolar complexes that have yet to be reported in the literature. Some of the other descriptors were examined, and the best results and equations for extending the physicochemical data have selected. [53-66]

The free energy changes between an electron donor (*D*) and an acceptor (*A*) estimates by *Rehm-Weller* equation estimates, as: [89]

$$\Delta G^{\circ} = e[E_D^{\circ} - E_A^{\circ}] - \Delta E^{*} + \omega_1 \qquad \text{(Eq.-1)}$$

In this equation *"e"* is the unit electrical charge, E_D^{o} and E_A^{o} are the reduction potentials of the electron donor and acceptor, respectively, ΔE^{*} is the energy of the singlet or triplet excited state and ω_1 is the work required to bring the donor and acceptor to within the electron transfer (ET) distance. If an electrostatic complex constructs before the ET process, the work term in this expression is equal to zero.[89]

The *Marcus* theory of ET-process implies rather weak (<0.05eV) electronic coupling between the initial (locally excited, LE) and final (electron transfer, CT) states and presumes that the TS (transition state) is close to the crossing point of the LE and CT terms. The value of the ET-rate constant k_{et} is controlled by $\Delta G^{\#}_{et}$, which is a function of the *reorganization energy* (*l*/4) and electron transfer driving force ΔG_{et}:

$$\Delta G^{\#}_{et} = (l/4)(1+\Delta G_{et}/l)^2 \qquad \text{(Eq.-2)}$$

$$k_{et} = k_0 \exp(-\Delta G^{\#}_{et}/RT) \qquad \text{(Eq.-3)}$$

The reorganization energy of organic molecules ranges from 0.1-0.3 eV. In this study, was utilized the minimum amount of the reorganization energy.[80-87]

The maximum wavelength (λ_{et}) of the electromagnetic photon for the electron transfer process in the dipolar complexes, was calculated by *Planck's* formula:

$$\Delta G^{\#}_{et} = \Delta E = h.c/\lambda_{(n)} \qquad \text{(Eq.-4)}$$

In this study, has also applied this equation to measure the activation free energy of the ET-process.[80-88]

To investigate the linear relationship between "$\Delta\Delta G_{et}^{\#}$" and "$\Delta\Delta G_{et}$" of the first free energies of the ET-process between the *H. pylori* cell wall bacteria in presence of Urea (in different pH) and the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}) was utilized the *Hammett* type equation [90]:

$$\Delta\Delta G_{et}^{\#} = m.\Delta\Delta G_{et} \qquad \text{(Eq.-5)}$$

3. RESULTS AND DISCUSSION:

The potential of membrane or cell wall in a microorganism is generated by extrusion of protons (H^+) coupled to oxidative reactions in the membrane of the cell.[1] The H^+ extrusion process constructs a PMF as a term that it was introduced by Mitchell. [1,3-9] The PMF includes an electrical component $\Delta\Psi$ (membrane potential) and a proton concentration component given by the difference in

pH_{out}. The data of ΔΨ of *H. pylori* at different pH_{out} has reported by Stingl *et al*..[13] The basis of this measurement was the movement of permeable lipophilic ions TPP^+ and SCN^- across the membrane in response to ΔΨ until electrochemical equilibrium has established.[13] Stingl *et al*. have reported that cells of *H. pylori* survive for several hours in pH=1 and in the presence of urea, when the pH_{in} is in a value near to neutral, that indicates homeostasis of pH_{in}.[13-15] As their experiments have shown this process is crucial for the cells at low pH_{out} values with both acidophiles and *H. pylori*, since at low pH_{in} values cytoplasmic enzymes become inactive.[13-15]

The reported oxidation potentials ($^{Ox.}E$) of fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}) are: 1.21, 1.19, 0.81, 0.72 and 0.73 Volt, respectively.[50]

Table 2 includes the calculated data of ΔG_{et}, $\Delta G^{\#}_{et(n)}$ and λ_{et} for the ET-process between the membranes of *Helicobacter pylori* in presence and absence (in different pH_{out}) of Urea and the selected fullerenes. These data have measured using the *Rehm-Weller* formula, *Marcus* theory and *Plank*'s equation (see the equations 1 to 4 in section 2). Figures-1 and -2 depict the imaginary ET-process between the membrane of *Helicobacter pylori* bacteria with the selected fullerenes and the dipolar complexes by electrostatic attractions.

Table 1. The ΔΨ (in Volt) in different pH_{out} of *H. pylori* bacteria cell walls. The data of this table were obtained directly from the reference [13].

Condition*	Urea	pH_{out}	ΔΨ (in Volt)
1	Presence	1.2	-0.026
2	Presence	2.4	-0.053
3	Presence	3.3	-0.064
4	Presence	4.8	-0.047
5	Presence	5.8	-0.056
6	Presence	6.3	-0.108
7	Presence	7.2	-0.143
8	Absence	6.1	-0.102
9	Absence	7.1	-0.132

*See the reference [13].

Table-2 shows equations 6-14 which indicate the second order polynomial relationship between "C_n" descriptor of the selected fullerenes and the free energies (ΔG_{et}) of the ET-process between the *H. pylori* bacteria cell wall in presence and absence (in different pH_{out}) of Urea and the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}). These equations show good correlations between the index C_n of the fullerenes and the ΔG_{et} of electron transfer process between the bacteria cell wall and the fullerenes. It is possible to apply the results to extend the calculations for other fullerenes by equations 6-14.

Figure-3 (the combined graphs) demonstrates the correlations between the number of carbon atoms of the selected fullerenes "n" and the free energies of electron transfer (ΔG_{et}) of *Helicobacter pylori* in presence (in different pH_{out}=1.2, 2.4, 3.3, 4.8, 5.8, 6.3 and 7.2) of Urea and the selected

fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}). The equations 6 to 12 correspond to Figure-3 and the related combined graphs. These values were regressed with a second-order polynomial equation. The R^2 (R-squared) values for the graphs were obtained about 0.99. By using Equations 6 to 14, it is possible to calculate the values of ΔG_{et} for this ET-process between the membranes of *Helicobacter pylori* in presence and absence (in different pH_{out}) of Urea and the selected fullerenes. Table-2 exhibits the measured values of these free energies of electron transfer ($\Delta G_{et;}$ in kcal mol^{-1}).

Table 2. The Eq. 6-14 have indicated the second order polynomial correlations between "C_n" descriptor of the selected fullerenes and the free energies of the electron transfer (ΔG_{et}) between the *H. pylori* bacteria in presence and absence (in different pH_{out}) of Urea and the C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86})

Equations	**ΔΨ (in Volt)**	**pH**	**Urea**	**R^2**	$\Delta G_{et} = a(n)^2 + b(n) + c$		
					a	***b***	***c***
Eq.6	-0.026	1.2	Presence	0.987	-0.023	2.920	-65.98
Eq.7	-0.053	2.4	Presence	0.987	-0.023	2.919	-66.57
Eq.8	-0.064	3.3	Presence	0.987	-0.023	2.919	-66.80
Eq.9	-0.047	4.8	Presence	0.987	-0.023	2.919	-66.80
Eq.10	-0.056	5.8	Presence	0.987	-0.023	2.919	-66.64
Eq.11	-0.108	6.3	Presence	0.986	-0.024	3.121	-75.03
Eq.12	-0.143	7.2	Presence	0.986	-0.024	3.121	-75.03
Eq.13	-0.102	6.1	Absence	0.987	-0.023	2.920	-67.73
Eq.14	-0.132	7.1	Absence	0.987	-0.023	2.920	-68.42

The good agreement between the theoretical calculation and the predicted values were seen. In lieu of increasing the "n" index in the fullerenes, the values of ΔG_{et} were decreased in different pH_{out}. So, because of the electron population increasing in the C_n structures the electron transfer increased. See the Tables 2 and 3. These results may relate to the HOMO-LUMO gap ($\Delta E_{HOMO\text{-}LUMO}$) of the fullerenes and the membrane potential (ΔΨ) of the cell wall of *Helicobacter pylori* in presence and absence of Urea (in different pH_{out}). See the reported conditions in Table-1 by Stingl *et al*..[13]

The *Marcus* theory is currently the dominant theory of ET in chemistry. This theory constructed surprising predictions about ET-rates that have been nonetheless supported experimentally over the several decades. The most significant prediction by this theory is that the ET-rate will increase as the ET reaction becomes more exergonic, but only to a point.[80-87]

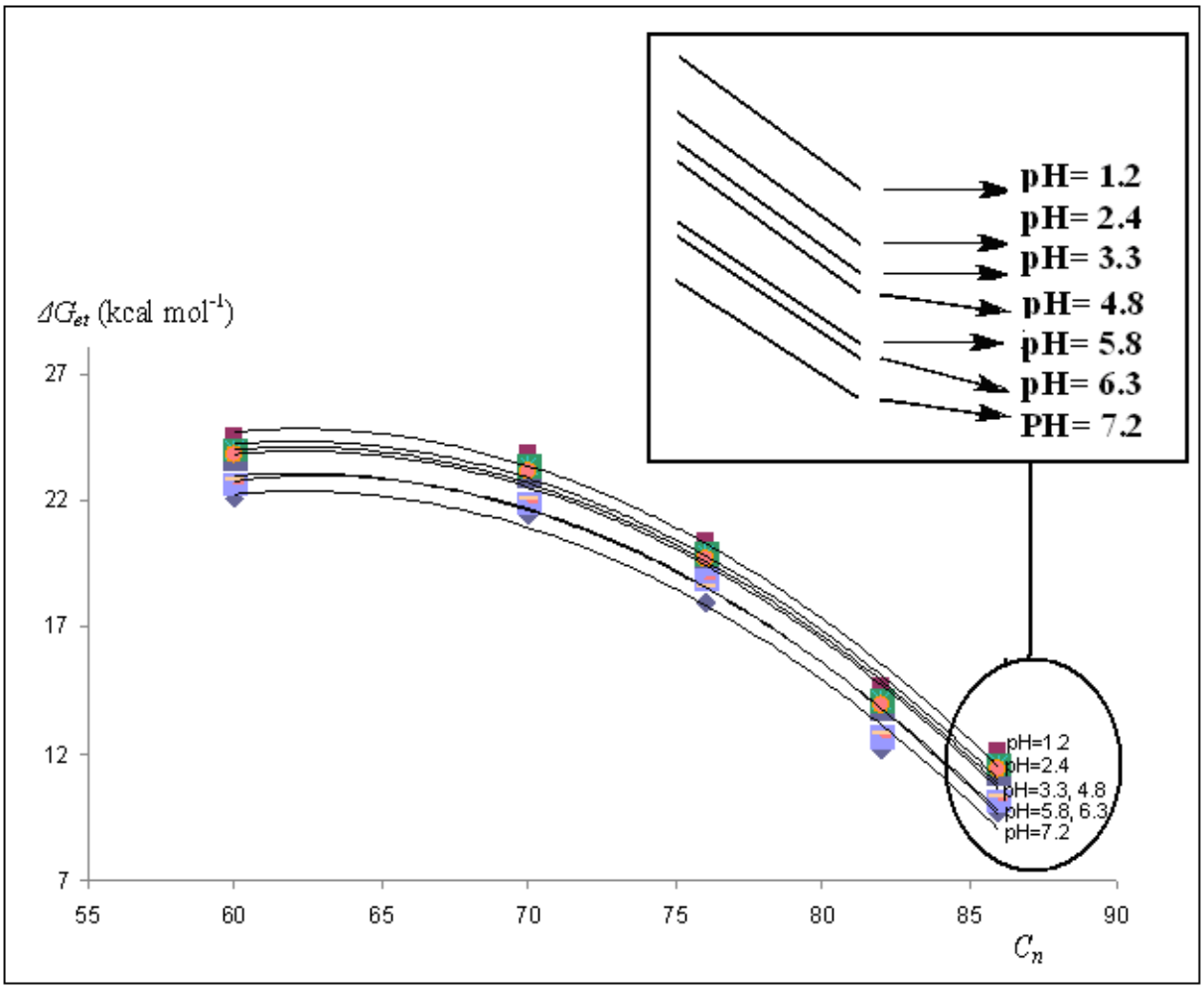

Figure 3. The second order polynomial correlations between the "n" values in the fullerenes C_n (C_{60}, C_{70}, C_{76}, C_{82} and C_{86}) and the data on the ET-process (ΔG_{et}, in kcal mol^{-1}) between the *H. pylori* bacteria in presence of Urea (in different pH_{out}) with the fullerenes. The values of ΔG_{et} have predicted by the *Rehm-Weller* formula (Eq. 1).

The Electron transfer (ET) plays a central role in many physical, chemical (both organic and inorganic) and biological systems. The new area of molecular electronics depends critically on the understanding and the control of the transfer of electrons in and between molecules and nanostructures. The solid state electronics relates to the control of the ET in semiconductors. One of the other reasons to study ET is that it is a very simple kind of chemical reaction. In understanding it one can gain insight into other kinds of chemistry and biochemistry. After all the important point is the chemistry of the transfer of electrons from one place to another and one donor agent to the other molecules. [80-87]

The ΔG_{et} is the difference between the free energy reactants on the left and the products on the right of an ET-reaction, and $\Delta G_{et}^{\#}$ is the activation energy of this reaction. As explained before the energy it would take to force the reactants to have the same nuclear configuration as the products without permitting the electron transfer were called reorganization energy. The free energy becomes energy or potential energy, if the ΔS changes are ignored.[80-87]

Table 3. The data of the ET-process (ΔG_{et}) between the membrane of *H. pylori* bacteria in the presence and absence (in different pH_{out}) of Urea and the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}). The data of ΔG_{et} in parentheses were predicted by using the *Rehm-Weller* equation (Eq. 1).

***Helicobacter pylori* with C_n**	**pH & ΔΨ** (V)	ΔG_{et} (in *kcal mol*$^{-1}$)								
		In the presence of Urea							**In the absence of Urea**	
	pH	**1.2**	**2.4**	**3.3**	**4.8**	**5.8**	**6.3**	**7.2**	**6.1**	**7.1**
	ΔΨ	**-0.026**	**-0.053**	**-0.063**	**-0.047**	**-0.056**	**-0.108**	**-0.143**	**-0.102**	**-0.132**
C_{60}		24.53	23.91	23.68	24.05	23.84	22.64	21.83	22.78	22.09
C_{70}		23.84	23.22	22.99	23.35	23.15	21.95	21.14	22.09	21.40
C_{76}		20.38	19.76	19.53	19.90	19.69	18.94	17.68	18.63	17.94
C_{82}		14.62	13.99	13.76	14.13	13.92	12.72	11.92	12.87	12.18
C_{86}		12.08	11.46	11.23	11.60	11.39	10.19	9.39	10.33	9.64

* The free energy of electron transfer (ΔG_{et}) for the *Helicobacter pylori* bacteria with C_n were not reported previously.

Table 4. The data of the ET-process ($\Delta G^{\#}_{et}$) between the membrane of *H. pylori* bacteria in the presence and absence of Urea (in different pH_{out}) and the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}).

**** Helicobacter pylori* with C_n**	**pH & ΔΨ** (V)	$\Delta G^{\#}_{et}$ (in *kcal mol*$^{-1}$)								
		In the presence of Urea							**In the absence of Urea**	
	pH	**1.2**	**2.4**	**3.3**	**4.8**	**5.8**	**6.3**	**7.2**	**6.1**	**7.1**
	ΔΨ	**-0.026**	**-0.053**	**-0.063**	**-0.047**	**-0.056**	**-0.108**	**-0.143**	**-0.102**	**-0.132**
C_{60}		30.89	29.76	29.34	30.01	29.63	27.52	26.15	27.76	26.57
C_{70}		29.63	28.53	28.13	28.77	28.41	26.34	24.99	26.57	25.42
C_{76}		23.76	22.77	22.41	22.99	22.66	20.82	19.62	21.03	20.00
C_{82}		15.41	14.62	14.32	14.78	14.52	13.06	12.11	13.22	12.41
C_{86}		12.31	11.59	11.33	11.75	11.52	10.22	9.38	10.36	9.64

* The free energy of electron transfer $\Delta G^{\#}_{et}$ for the *Helicobacter pylori* bacteria with C_n were not reported previously.

Tables 3 and 4 show the calculated values of $\Delta G^{\#}_{et}$ and λ_{et} by utilizing equations 2 and 3. It is possible, through the use of Equations 2 and 3, to calculate the values of $\Delta G^{\#}_{et(n)}$ and λ_{et} in the ET-process between the membranes of *Helicobacter pylori* in presence and absence (different pH_{out}) of Urea with the selected fullerenes in accordance with *Marcus* theory.

Table 5. The data on the maximum wave length of ET-process (λ_{et}) between the membrane of *H. pylori* bacteria in the presence and absence of Urea (in different pH_{out}) and the selected fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}).

*** *Helicobacter pylori* with C_n**	**pH & ΔΨ** (V)	λ_{et} (in *nm*)								
		In the presence of Urea							**In the absence of Urea**	
	pH	**1.2**	**2.4**	**3.3**	**4.8**	**5.8**	**6.3**	**7.2**	**6.1**	**7.1**
	ΔΨ	**-0.026**	**-0.053**	**-0.063**	**-0.047**	**-0.056**	**-0.108**	**-0.143**	**-0.102**	**-0.132**
C_{60}		925	960	974	952	964	1038	1092	1029	1075
C_{70}		964	1005	1015	993	1006	1084	1143	1075	1124
C_{76}		1202	1254	1275	1242	1261	1372	1456	1359	1429
C_{82}		1854	1955	1994	1932	1966	2187	2358	2160	2302
C_{86}		2322	2463	2519	2431	2480	2796	3044	2756	2963

* The λ_{et} values of the *H. pylori* bacteria electron transfer process with C_n were not reported previously.

Table 6. The values of $\Delta\Delta G_{et}$ for the electron transfer process between the membrane of *H. pylori* bacteria in the presence (in different pH_{out}) of Urea and the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}).

*** *Helicobacter pylori* with C_n**	**In the presence of Urea $\Delta\Delta G_{et}$ (kcal mol^{-1})**							
	pH	**1.2**	**2.4**	**3.3**	**4.8**	**5.8**	**6.3**	**7.2**
	ΔΨ	**-0.026**	**-0.053**	**-0.063**	**-0.047**	**-0.056**	**-0.108**	**-0.143**
C_{60}		12.45	12.45	12.45	12.45	12.45	12.45	12.44
C_{70}		11.76	11.76	11.76	11.75	11.76	11.76	11.75
C_{76}		8.30	8.30	8.30	8.30	8.30	8.75	8.29
C_{82}		2.54	2.53	2.56	2.54	2.53	2.53	2.53
C_{86}		0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 7. The values of $\Delta\Delta G_{et}^{\#}$ for the electron transfer (ET) process between *H. pylori* bacteria in the presence (in different pH_{out}) of Urea and the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}).

*** *Helicobacter pylori* with C_n**	**In the presence of Urea $\Delta\Delta G_{et}^{\#}$ (kcal mol^{-1})**							
	pH	**1.2**	**2.4**	**3.3**	**4.8**	**5.8**	**6.3**	**7.2**
	ΔΨ	**-0.026**	**-0.053**	**-0.063**	**-0.047**	**-0.056**	**-0.108**	**-0.143**
C_{60}		18.58	18.17	18.01	18.26	18.11	17.30	16.77
C_{70}		17.32	16.94	16.80	17.02	16.89	16.12	5.61
C_{76}		11.45	11.18	11.08	11.24	11.14	10.60	10.24
C_{82}		3.10	3.03	2.99	3.03	3.00	2.84	2.73
C_{86}		0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table 8. The equations 15-21 indicate the linear relationship between "$\Delta\Delta G_{et}^{\#}$" and "$\Delta\Delta G_{et}$" (Hammett type equation) of the free energies of the electron transfer between the membrane of *H. pylori* in the presence of Urea (in different pH_{out}) and the fullerene C_{60}.

Equations	ΔΨ (in Volt)	pH	Urea	R^2	$\Delta\Delta G_{et}^{\#} = a(\Delta\Delta G_{et}) + b$	
					a	***b***
Eq.15	-0.026	1.2	Presence	0.997	1.4988	0.4163
Eq.16	-0.053	2.4	Presence	0.997	1.4651	0.4036
Eq.17	-0.064	3.3	Presence	0.997	1.4546	0.4263
Eq.18	-0.047	4.8	Presence	0.997	1.4734	0.4126
Eq.19	-0.056	5.8	Presence	0.997	1.4618	0.4132
Eq.20	-0.108	6.3	Presence	0.997	1.3854	0.4614
Eq.21	-0.143	7.2	Presence	0.997	1.3542	0.4118

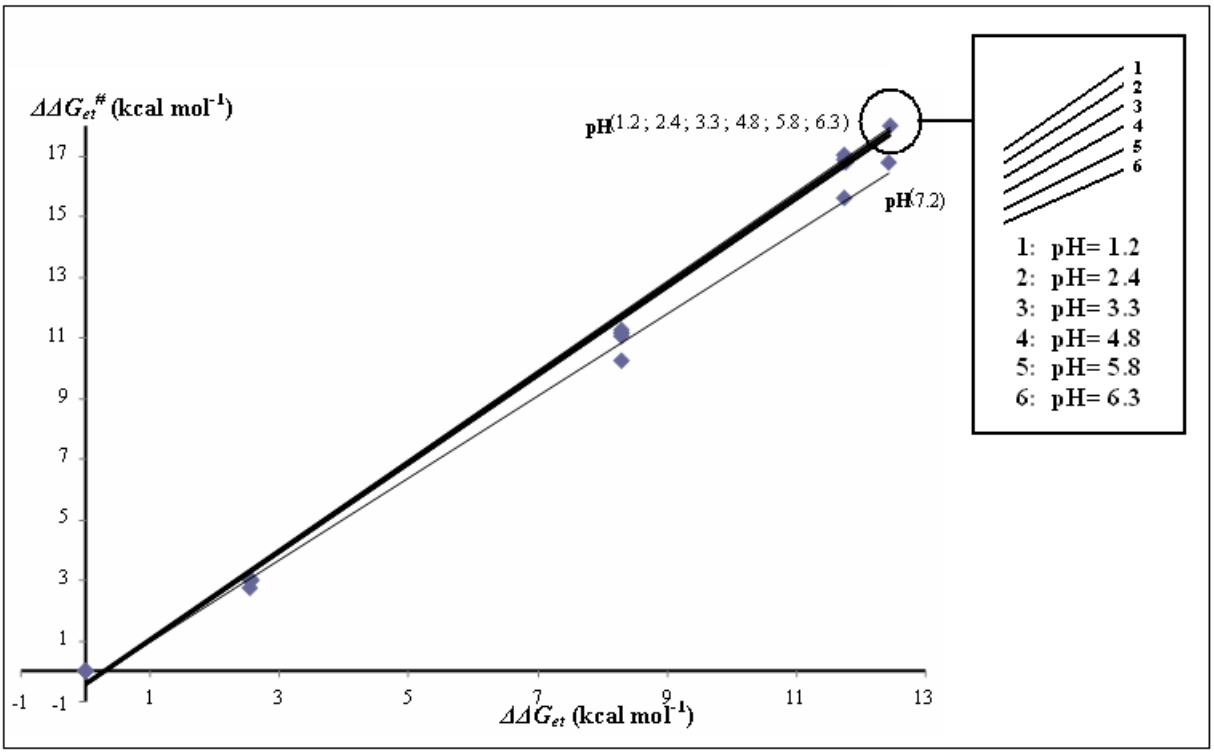

Figure 4. The linear relationship between "$\Delta\Delta G_{et}^{\#}$" and "$\Delta\Delta G_{et}$" (Hammett type equation) of the free energies of the ET-process between the cell wall of *H. pylori* bacteria in presence of Urea (in different pH_{out}) and the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}).

In Table-6 could see the data values of $\Delta\Delta G_{et}$ for electron transfer (ET) process between *H. pylori* bacteria in the presence (in different pH_{out}) of Urea and the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}). Table-7 has shown the data values of $\Delta\Delta G_{et}^{\#}$ for electron transfer (ET) process between *H. pylori* bacteria in the presence (in different pH_{out}) of Urea and the fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}) as well. Table-8 shows the equations 15-21 that indicates the linear relationships between "$\Delta\Delta G_{et}^{\#}$" and "$\Delta\Delta G_{et}$" (*Hammett* type equations) of the free energies of the ET-process between the membrane of *H. pylori* bacteria in the presence of Urea (in different pH_{out}) and the fullerene C_{60}. This data was

regressed with linear relationships. The R^2 (R-squared) values for the graphs were obtained about 0.997. The results for other selected fullerenes have demonstrated same results of fullerene C_{60}. Figure-4 demonstrated the graphs of the linear *Hammett* type relationship equations between "$\Delta\Delta G_{et}^{\#}$" and "$\Delta\Delta G_{et}$" of the free energies of the electron transfer between the *H. pylori* bacteria in presence of Urea (in different pH_{out}) and the selected fullerenes C_n. The results show that in pH_{out}=7.2 the slop of the linear relationship between "$\Delta\Delta G_{et}^{\#}$" and "$\Delta\Delta G_{et}$" of the free energies of the electron transfer between the membrane of *H. pylori* bacteria in presence of Urea and the selected fullerenes to construct the dipolar complexes by electrostatic attraction is obviously different with the other pH_{out} conditions. The kinetic of the ET-process is much faster in pH_{out}=7.2 in accordance with the results of the $\Delta G_{et}^{\#}$ and $\Delta\Delta G_{et}^{\#}$ of ET-process between the *H. pylori* bacteria in the presence of Urea and the selected fullerenes. See Tables 3-8 and Figures -4 and -5.

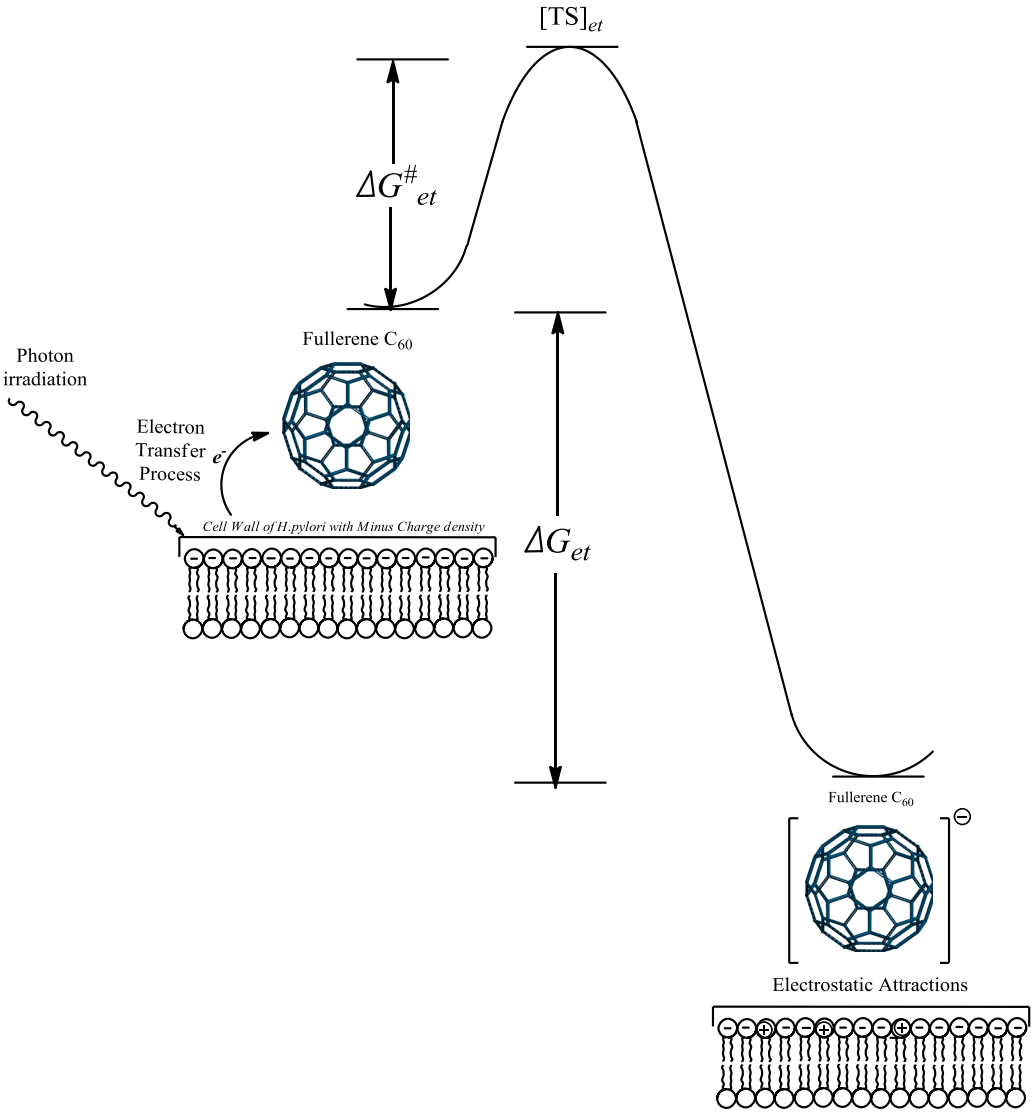

Figure 5. The imaginary surfaces of the free energies of the ET-process ΔG_{et} and $\Delta G^{\#}_{et}$ between the cell wall of *H. pylori* bacteria in presence of Urea (in different pH_{out}) and the fullerenes. See Tables-3 and -4.

Figure 5 exhibits the levels of the free energies of electron transfer ΔG_{et} and $\Delta G_{et}^{\#}$ in the ET-process. The values of the $\Delta G^{\#}_{et}$ for this ET-process, increase by increasing the $\Delta G_{et(n)}$ and the number of carbon atoms index in the dipolar complexes, while the values of λ_{et}, decrease by increasing the values of $\Delta G_{et(n)}$ and $\Delta G_{et(n)}^{\#}$ for the ET-process. See Tables 2-5 and Figure 5.

By applying the equation 1 (*Rehm-Weller* formula), the equations 2 and 3 (*Marcus* theory) and equations 6-14, the ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} values have calculated for the electron transfer process between the membrane of *Helicobacter pylori* in presence and absence (in different pH_{out}) of Urea and the selected fullerenes. The "n" descriptor has a good relationship with the values of the free energies of electron transfer ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} . It is possible to calculate the free energies of electron transfer (ΔG_{et} in kcal.mol^{-1}), the activated free energies of electron transfer and the maximum wave length for the electron transfers, $\Delta G^{\#}_{et}$ and λ_{et}, respectively, by using the appropriate equations for the ET-process between the membranes of *H. pylori* in presence and absence (in different pH_{out}=1.2, 2.4, 3.3, 4.8, 5.8, 6.3 and 7.2) of Urea and the selected fullerenes C_n ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}), in close accordance with the results of *Marcus* theory.

In this study, the values of the maximum wavelengths (λ_{et}) for the ET-process between the selected fullerenes and the bacteria cell wall in the dipolar complexes by *Planck*'s formula were demonstrated. The photonic energy of the ET- process was also determined by the use of this formula. Most of the values were found in the range of Visible to IR (900–3050 nm) range of the electromagnetic spectrum. The λ_{et} depends on the $\Delta G^{\#}_{et}$ value in each state. The values of λ_{et} have increased by decreasing of the $\Delta G^{\#}_{et}$ value in each state. In this study, the photo-electron transfer process was investigated to find medicinal and antibiotic activities for the selected fullerenes by performing the complexes between fullerenes and the bacteria membrane in presence and absence (in different pH_{out}=1.2, 2.4, 3.3, 4.8, 5.8, 6.3 and 7.2) of Urea. The structures of the dipolar complexes between fullerenes and *H. pylori* bacteria membrane and the calculated values of ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} corresponding to these complex structures have not been reported before.

The results of this study may be applied in some medical treatment operations, such as irradiation of the appropriate λ_{et} through endoscopy for the stomach diseases to destruct the membrane cells of *H. pylori* bacteria in presence of the fullerenes in stomach media. The results discussed here and the calculated values of ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} corresponding to the electron transfer process have neither predicted nor reported before. It is supposed that the ET-process between the membrane of *H. pylori* bacteria with the selected fullerenes prepare the conditions to restrict the bacteria (*H. pylori*) growing by perturbation in the cell wall charges of *H. pylori*.

4. CONCLUSION

The ET-process of the membrane of *Helicobacter pylori* and fullerenes have exhibited the important effects to restrict the microorganism growing by perturbation in the cell wall charges of *H. pylori*. The electrochemical data of this electron transfer process were reported here. The data have included the values of ΔG_{et} calculated using the *Rehm-Weller* equation and $\Delta G^{\#}_{et}$ as well as the values of λ_{et} applying equations of the *Marcus* theory for the ET-process. Using the "n" descriptor, along with

the obtained equations of this model, one can derive sound structural correlations between the aforementioned the physicochemical data. The structure of this model allow one to calculate ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} for the ET-process between the *H. pylori* and the selected fullerenes (C_{60}, C_{70}, C_{76}, C_{82} and C_{86}). The linear *Hammett* type relationship equations were discussed between "$\Delta\Delta G_{et}^{\#}$" and "$\Delta\Delta G_{et}$" of the first free energies of the electron transfer between the *H. pylori* bacteria in presence of Urea (different pH_{out}) and the fullerenes C_n. The described ET-process could stop some of the phenomena related to the microorganism (*H. pylori* bacteria) growing by perturbation in the cell wall charges of *H. pylori*.

ACKNOWLEDGEMENT
The authors also gratefully acknowledge Theoretical and Computational Research Center of Chemistry and Nano Sciences, Faculty of Chemistry, Razi University, Kermanshah, Iran and Medical Biology Research Center, Kermanshah University of Medical Sciences. Nargese Zolfaghar Karahrudi gratefully acknowledges from the colleagues in Chemistry Department of Razi University-Kermanshah-Iran for their useful suggestions during her research opportunity at research group of Prof. A. A. Taherpour.

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