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Study of Electron Transfer Process Between Fullerenes and Membrane Cells of *E-coli* in Presence of Dihydrostreptomycin in NaCl and Sucrose Medias

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The electrical potential difference on the *Escherichia coli* membrane was utilized for theoretical study of electron transfer (ET) process between fullerenes and the membrane cells of *Escherichia coli* bacteria. The strains of *Escherichia coli* which they are selected in this study are: FRAG-5, TK-1207, TK-1208 and TK-1235. The NaCl and *sucrose* medias in presence of dihydrostreptomycin (an aminoglycoside) are the reported experimental conditions which is selected in this study. Fullerenes are the main group of carbon allotropes, which they constructed entirely of C-atoms, that take the different geometrically shapes like spheres, ellipsoids and cylinders. The empty fullerene carbon allotropes with different number of C-atoms have been studied. Topological descriptors are numerical parameters of a graph which characterize its topology and are usually graph invariant. They were applied to construct effective mathematical (QSAR and QSPR) methods to establish the relationships between structural data of the different molecules and their chemical and/or physical properties. The relationship between the number of C-atoms and the ΔG_{et} (free energies of electron transfer) are evaluated using the *Rehm-Weller* equation for ET-process between fullerenes and the membrane cells of *Escherichia coli* with strains FRAG-5, TK-1207, TK-1208 and TK-1235 in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin. The calculations are shown for the oxidation potential ($^{Ox.}E_1$) of the selected fullerenes. The results have applied to calculate ΔG_{et} of the ET-process for the fullerenes. In this study, the first $\Delta G^{\#}_{et(n)}$ (free activation energies of electron transfer) and λ_{et} (the maximum wave length of the electron transfers) were also calculated for the selected conditions agree with the *Marcus* theory.

Keywords: Fullerenes; *Escherichia coli*; Antibiotics; Electrical potential; Free energy of electron transfer; Electron transfer properties; Activated free energies of electron transfer; Rehm-Weller equation; Marcus Theory.

1. INTRODUCTION

In microorganisms, there are basically two forms of metabolic energy. These two types are: 1) energy-rich phosphate bonds such as ATP and 2) electrochemical energy which it provides by ion gradients (such as proton). The bacterial cell has a well known cytoplasm and the localization of protein molecules is essential for their function, particularly for those involved in morphogenetic processes. Survive of this order requires energy.[1-9] The producing the PMF (proton motive force) is constructed of the ΔpH (trans-membrane chemical proton gradient) and the ΔΨ (trans-membrane electric potential).[1,5] ATP is created using the PMF as an energy source. Each pair of H^+ yields one ATP molecule. Proton (H^+) gradients have also constructed in bacteria cell by running ATP syntheses in reverse. The proton gradient can be applied as intermediate energy storage for heat production and life rotation. It is an inter-convertible type of energy in electron potential generation, active transport, ATP synthesis/hydrolysis and the other biochemical process of cells. A pair of protons ($2H^+$) are generated the PMF by expell at each coupling site.[1,6,7] The trans-membrane electric potential (ΔΨ) in cells can be specified by the diffusion of lipophilic ionic molecules between the cells and the suspending media. The proton motive force (PMF) consists of the ΔΨ (in Volt) and the chemical proton potential. The ΔΨ across the membrane of *E.coli* was determined by the distribution measurement of lipid-soluble cations and correlated with resistance to dihydrostreptomycin, where resistance was assumed due to reduced uptake of the medicine by Damper and Epstein.[1] Their results were investigated to support a model in which the perception of the polycationic aminoglycosides electrogenic was driven by ΔΨ.[1,5] They have progressed a model which reports the MIC (minimal inhibitory concentration) to the rate of aminoglycoside cognition and the measure of growth.[1] Damper and Epstein had studied a number of conditions that alter ΔΨ in *E. coli* bacteria and they found a relationship between susceptibility to aminoglycosides and ΔΨ. Their results introduce that the amount of ΔΨ is an important determinant of aminoglycosides resistance.[1,5,7-9] Some of the selected strains of *Escherichia coli* were FRAG-5, TK-1207, TK-1208 and TK-1235 by Damper and Epstein.[1]

The empty fullerenes with different numbers of C-atoms such as C_n (n=60, 70, 76, 82 and 86), with different mechanical and physicochemicalproperties have been obtained before.[10–33] Shen have studied the compressive mechanical properties of the fullerenes C_n (n = 20, 60, 80 and 180) in detail by using QMD (quantum molecular dynamics) technique.[11,24] In 1985, the interesting stabilities of the carbon allotropes such as C_{60} and C_{70} was shown.[10,11] Luzzi *et al.* discovered of fullerene C_{60} peapods [12-17]. After that the aligned structure of encapsulated molecules due to the molecule-molecule and/or molecule-SWNT interactions were studied as the new hybrid materials.[14,15] Zhang *et al.* have investigated the evidences for the thermal stability of C_{60} peapods.[12-16] Since the early 1990s, the electrochemical properties of the C_{60} were studied, when these materials became available in macroscopic quantities.[13,14] In 1990, was reported that CH_2Cl_2

electrochemically reduces C_{60} to C_{60}^{1-} and C_{60}^{2-} by Haufler *et al.*[15] Xie et al. cathodically reduced C60 in six reversible one-electron steps for -0.97 V vs. Fc/Fc^{+}(Fc = ferrocene).[16] This result, along with the inability to perform anodic electrochemistry on fullerenes, revealed the electronic structure of fullerenes, the LUMO orbitals of C_{60} can accept up to six electrons to form C_{60}^{6-}, but the position of the HOMO orbitals does not allow for hole-doping under the usual reported electrochemical conditions. Jehoulet et al. [17] reported on the irreversible electrochemical and structural reorganization of solid fullerenes in acetonitrile. Janda et al. [18] improved upon the experimental conditions by investigating highly organized C60 films on highly oriented pyrolytic graphite (HOPG) in an aqueous medium. The reduction of these films induces a morphological change; they re-structure into conductive nano-clusters of about 100 nm in diameter [18,19].

Graph theory is important to utilize effective mathematical methods to make good correlations between several activities and properties of different molecules. Graph theory (GT) is an effective tool for studying the Quantitative Structure Activity Relationship (*QSAR*) and Quantitative Structure Property Relationship (*QSPR*). A lot of investigations in various aspects have applied the topological descriptors.[34-42] Any extrapolation of the investigations from one chemical molecule to other similar chemical molecules must take into account considerations based on the *QSAR* studies. The correlation depends on how close the chemical properties are of the compounds in question. Several applications of the topological indices (descriptors) have been reported.[24-44] The number of carbon atoms in the various fullerene structures was determined with these applications.

This study consider the electron transfer (ET) process between the selected fullerenes $C_{60,}$ C_{70}, C_{76}, C_{82} & C_{86} and the membrane cells of *Escherichia coli* with strains FRAG-5, TK-1207, TK-1208 and TK-1235 in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin. The relationship between the descriptor of the number of C-atoms and ΔG_{et} of selected fullerenes ($C_{60,}$ C_{70}, C_{76}, C_{82} & C_{86}) with strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin were investigated, on the basis of the ${}^{Ox.}E_1$ (oxidation potentials) of the fullerenes, as investigated by utilizing the *Rehm-Weller* equation. [45] The results can applied to calculate the ΔG_{et} of the other fullerenes and the selected conditions and strains of *Escherichia coli* bacteria. See the scheme 1, equations 1 to 20, Tables 1 to 6, Figures 1-3.

In this study, also were calculated the $\Delta G^{\#}_{et(n)}$ (free activation energies of electron transfer) and λ_{et} (the maximum wave length of the electron transfers), as assessed applying the *Marcus* theory and the related equations on the basis of the ${}^{Ox.}E_1$ potentials of the selected fullerenes to calculate the data of the ET process between the membranes of the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias, in the presence of dihydrostreptomycin and the fullerenes. See the equations, Tables and Figures.

Electrons are explained as residing in electron orbital levels in molecules and electron bands in bulk materials. While a photon irradiates to a molecule and excites it, one electron can be excited from a ground state orbital to a higher energy orbital level. This excited state (ES) makes a vacancy in the lover energy orbital levels. This vacancy can be filled again by an electron donor molecule (agent). The electron that is produced in a high-energy orbital can be donated electron to an electron acceptor agent. Photo-induced ET is an ET-process, which it occurs when certain photoactive materials interact

with light, including semiconductors. This phenomenon can be named as photo-activated process. photo-activated process can be occurred in some devices such as chemical and biological systems like those applied in photosynthesis, small molecules with suitable absorptions, redox states and many solar cells.[45,46a-h,47]

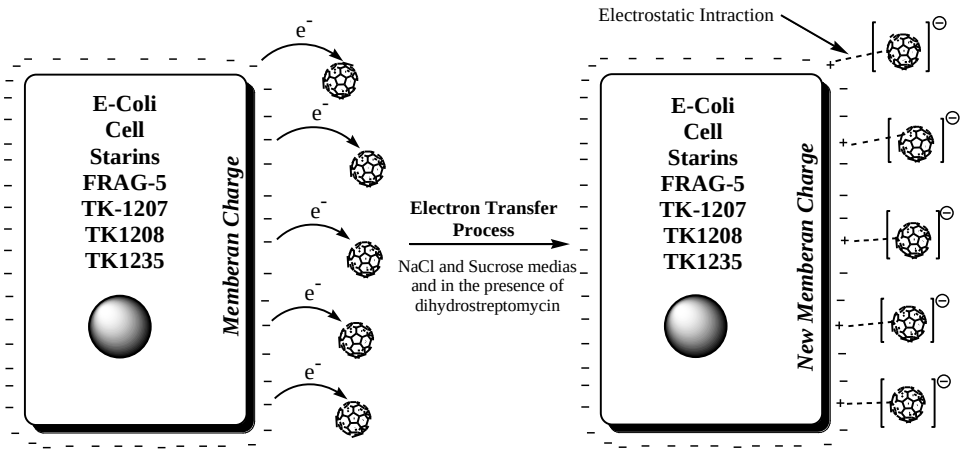

Figure 1. The schematic electron transfer process between the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria at the predicted experimental conditions and the fullerenes to construct the dipolar complexes.

One of the main basis of Marcus theory is the *Arrhenius* equation. This equation is utilized to measure the rates of chemical reactions in two pathways: 1) It constructs an equation to calculate the *Gibbs* free energy and the activation energy based on a parameter called the *reorganization energy* (RE). The RE has defined as the energy required reorganizing the structure of the system from initial to the final coordinates without changing the electronic states. 2) It constructs another equation to make the pre-exponential factor in the *Arrhenius* equation, based on the electronic coupling between the initial and final state of the ET reaction.[46a-h]

It has supposed that the electron transfer process between the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin and the selected fullerenes construct the dipolar complexes to perform a condition for bacteria (*E-coli*) damage. It seems that the discussed electron transfer has also stopped some phenomena related to restriction in bacteria (*E-coli*) growth by perturbation on the membrane charge of *E-coli*.

2. CALCULATION METHODS:

All of the operations on the calculations and graphing were carried out by using *MATLAB-7.4.0(R2007a)* and *Microsoft Office Excel-2003* programs. Several valuable properties of C_n can be calculated by the use of the number of C-atoms of the fullerenes as a useful descriptor. The data were used to calculate ΔG_{et}, according to the *Rehm-Weller* equation for the ET-process between the strains

FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin and the fullerenes.

The equations 1 and 5-20 were applied to determine the amounts of ΔG_{et} for the studied complexes. Some of the other structural descriptors were examined. The best results and equations to extend the physicochemical data were selected. [38-42,44]

By the use of the equation of *Rehm-Weller* can estimate the free energy changes between an electron donor (*D*) and an acceptor (*A*) as: [45]

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

In this equation, ΔE^{*} is the energy of the singlet or triplet excited state, E_D^{o} and E_A^{o} were introduced as the reduction potentials of the electron donor and acceptor, respectively, the terms "*e*" and "ω_1" are: the unit electrical charge and the work required to bring the donor (D) and acceptor (E) agents to within the ET distance, respectively. The ω_1 term in this expression is equal to zero, if an electrostatic complex forms before the ET process. [45]

In accordance with the Marcus theory ET-process is rather weak (<0.05eV) electronic coupling between the locally excited "LE" (initial) and electron transfer "CT" (final) states and assumes that the transition state)TS) is near to the crossing point of the "LE" and "CT" items. The value of the ET-rate constant k_{et} is controlled by the $\Delta G^{\#}_{et}$ (activation free energy), which it is a function of the reorganization energy (RE=l/4) and ET-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 range of RE (reorganization energy) for organic molecules was determined as 0.1-0.3 eV. In this study, was utilized the minimum amount of RE.[46a-h]

To compute the maximum $\lambda_{(n)}$ of the for the photoelectron transfer process in the nanostructure supramolecular complexes, was utilized *Planck's* formula:

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

In this study, was also used this equation to compute the $\Delta G^{\#}_{et}$ of the ET-process.[46a-h-48]

3. RESULTS AND DISCUSSION

The membrane potential ($\Delta\Psi$) in *Escherichia coli* bacteria is produced by extrusion of H^+ coupled to oxidative reactions in the membrane of the bacteria cell.[1] This process produces a PMF for the membrane of the bacteria cell. The PMF term was introduced by Mitchell.[1,6] The proton motive force consists of an electrical component that demonstrated by $\Delta\Psi$ and the H^+ concentration given by the difference in pH. The internal pH of bacteria is maintained near 7.5. In notice to this point there is little difference in the pH across the membranes of the bacteria cells in medium at this pH.[1] Because of that, the almost all of the PMF is expressed membrane potential ($\Delta\Psi$).[1,7] Damper and Epstein had reported the membrane potential ($\Delta\Psi$ in Volt) of the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin with its minimum inhibitory concentrations (MIC, μg/ml).[1] Their report about the experimental data were extracted directly from reference.[1] It was known that the addition of salt

increase the resistance of *Escherichia coli* bacteria to aminoglycosides (dihydrostreptomycin) and to inhibit gentamycin uptake.[1,3,8,9] Damper and Epstein had shown that such resistance was associated with a reduction in the ΔΨ (membrane potential) in different strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria. [1] They had also found that in some of the strains 0.5 M NaCl allowed reasonable rates of growth and generated over a 10-fold increase in MIC and reduction in ΔΨ of 0.22 to 0.48 Volt.[1] They reported that the concentration of sucrose about 0.3 M was the osmotic equivalent of 0.17 M NaCl, indicating that osmotically equivalent concentrations of sucrose are at least effective as NaCl in producing resistance.[1] It has founded that reducing external pH (media)increases resistance to aminoglycosides. [1,9]

The values reported of the oxidation potentials ($^{Ox.}E$) of fullerenes C_n (C_{60}, C_{70}, C_{76}, C_{82} & C_{86}) are: 1.21, 1.19, 0.81, 0.72 and 0.73 Volt, respectively. [21]

Table 2 contains the summarized data (ΔG_{et}, $\Delta G^{\#}_{et(n)}$ and λ_{et}) of the electron transfer process between the membranes of the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin and the fullerenes. These data have computed by using the equation of *Rehm-Weller* (Eq. 1), *Marcus* theory and *Plank*'s formula (equations 1 to 4). Figure-1 depicts the schematic electron transfer process between the strains of *Escherichia coli* bacteria and the fullerenes.

Table 1. The membrane potential (ΔΨ in Volt) of the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of with its minimum inhibitory concentrations (MIC, μg/ml). The experimental data of this table were extracted directly from reference [1].

Strain of *E-coli**	Solute	Concn. (M)	ΔΨ (Volt)	MIC (μg/ml)
FRAG-5	–	–	-0.142	0.5
	NaCl	0.5	-0.120	7
	Sucrose	0.3	-0.114	10
TK-1207	–	–	-0.120	12
	NaCl	0.2	-0.096	28
	Sucrose	0.3	-0.162	22
TK-1208	–	–	-0.114	0.3
	NaCl	0.5	-0.106	5
	Sucrose	0.3	-0.114	0.6
TK-1235	–	–	-0.106	5
	NaCl	0.2	-0.055	24
	Sucrose	0.3	–	14

*See the reference [1].

The figure-2 (graphs *a-c*) demonstrate the correlations between the C-atoms descriptor (n) of the fullerenes and the free-energies of the ET-process (ΔG_{et}) of the strain FRAG-5 of *Escherichia coli* bacteria in ordinary solution, NaCl (0.5 M) and *sucrose* (0.3 M) medias in the presence of

dihydrostreptomycin (with minimum inhibitory concentrations MIC, 0.5, 7 and 10 μg/ml, respectively) and the fullerenes. Equations 5-7 were related to the Figure-2 (graphs *a-c*).

Table 2. The equations 5-15 indicate the relationship between the C-atom counts (n) as the descriptor for the fullerenes and the ΔG_{et} (free energies) of the ET-process between the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin and the fullerenes.

Strains of *E-coli*	Equations	Solute	R^2	$\Delta G_{et} = a(n)^2 + b(n) + c$		
				a	*b*	*c*
FRAG-5	Eq.5	–	0.9876	-0.0235	2.9245	-68.8010
	Eq.6	NaCl	0.9875	-0.0235	2.9241	-68.2690
	Eq.7	Sucrose	0.9876	-0.0234	2.9152	-67.8190
TK-1207	Eq.8	–	0.9875	-0.0235	2.9241	-68.2690
	Eq.9	NaCl	0.9876	-0.0235	2.9245	-68.7410
	Eq.10	Sucrose	0.9875	-0.0235	2.9201	-68.7300
TK-1208	Eq.11	–	0.9875	-0.0235	2.9241	-69.2390
	Eq.12	NaCl	0.9876	-0.0235	2.9197	-67.9790
	Eq.13	Sucrose	0.9876	-0.0235	2.9245	-67.9710
TK-1235	Eq.14	–	0.9876	-0.0235	2.9245	-67.9710
	Eq.15	NaCl	0.9875	-0.0235	2.9241	-66.7690

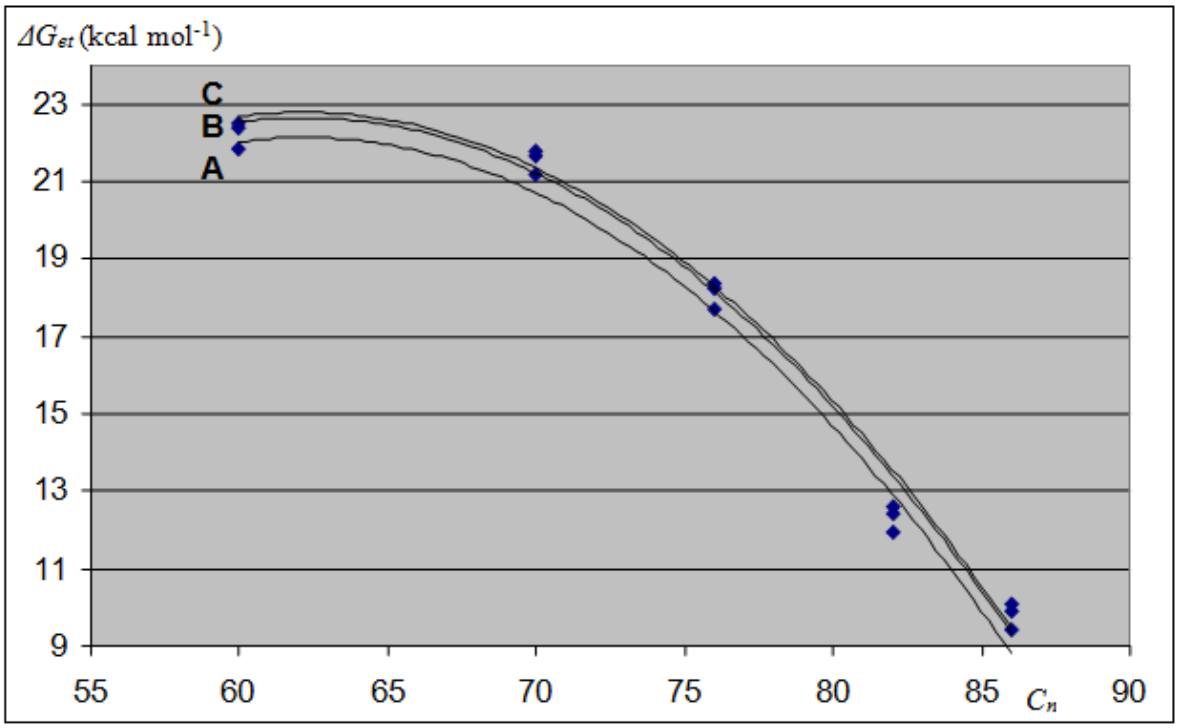

Figure 2. The second order polynomial correlations between the C-atom counts (n) in the selected fullerenes and the values on the electron transfer (ΔG_{et}) between the strain FRAG-5 of *Escherichia coli* bacteria in neutral media (A), NaCl (B) and *Sucrose* (C) medias with the presence of dihydrostreptomycin and the fullerenes. The data of ΔG_{et} were predicted by Eq. 1 (the equation of *Rehm-Weller*).

This results was regressed with a second-order polynomial equation. The R^2 values (R-squared) for the graphs (*a-c*) of Figure-2 are: 0.987, 0.992 and 0.947, respectively. By applying Equations 5-7, it is possible to calculate the values of ΔG_{et} for the ET-process. Table 2 shows the computed values of the free-energies of the ET-process ($\Delta G_{et;}$ in kcal mol^{-1}) between the membrane of the strain FRAG-5 of *E.coli* bacteria in ordinary solution, NaCl (0.5 M) and *sucrose* (0.3 M) medias in the presence of dihydrostreptomycin (with minimum inhibitory concentrations MIC, 0.5, 7 and 10 μg/ml, respectively) and the fullerenes.

Table 3. The data values on the electron transfer (ΔG_{et}) between the strain FRAG-5 of *Escherichia coli* bacteria in NaCl and *sucrose* medias with the presence of dihydrostreptomycin and the fullerenes. The data of ΔG_{et} were calculated by Eq. 5 to Eq. 7. The data in parentheses have calculated by using Eq. 1 (*Rehm-Weller* equation).

*The Strain FRAG-5 with C_n	ΔG_{et} (in *kcal* mol^{-1})			$\Delta G^{\#}_{et}$ (in *kcal* mol^{-1})			λ_{et} (in *nm*)		
	ΔG_{et}	ΔG_{et}	ΔG_{et}	$\Delta G^{\#}_{et}$	$\Delta G^{\#}_{et}$	$\Delta G^{\#}_{et}$	λ_{et}	λ_{et}	λ_{et}
	–	NaCl	Sucrose	–	NaCl	Sucrose	–	NaCl	Sucrose
C_{60}	21.59 (21.86)	22.09 (22.37)	22.23 (22.51)	26.19	27.05	27.29	1091	1056	1047
C_{70}	20.65 (20.91)	21.41 (21.68)	21.54 (21.81)	25.04	25.88	26.11	1141	1104	1094
C_{76}	17.49 (17.71)	17.99 (18.22)	18.12 (18.35)	19.66	20.41	20.22	1453	1400	1386
C_{82}	11.80 (11.95)	12.30 (12.45)	12.43 (12.59)	12.15	12.73	12.90	2352	2244	2215
C_{86}	9.28 (9.40)	9.79 (9.91)	9.93 (10.05)	9.41	9.93	10.07	3037	2878	2837

*The data of ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} related to the ET-process for the strain FRAG-5 of *E-coli* with C_n had not been reported before.

Table 4. The data on the electron transfer (ΔG_{et}) between the strain TK-1207 of *Escherichia coli* bacteria in NaCl and *sucrose* medias with the presence of dihydrostreptomycin and the fullerenes. The data of ΔG_{et} were were calculated by Eq. 5 to Eq. 7. The data in parentheses have calculated by using Eq. 1 (*Rehm-Weller* equation).

*The Strain TK-1207 with C_n	ΔG_{et} (in *kcal* mol^{-1})			$\Delta G^{\#}_{et}$ (in *kcal* mol^{-1})			λ_{et} (in *nm*)		
	ΔG_{et}	ΔG_{et}	ΔG_{et}	$\Delta G^{\#}_{et}$	$\Delta G^{\#}_{et}$	$\Delta G^{\#}_{et}$	λ_{et}	λ_{et}	λ_{et}
	–	NaCl	Sucrose	–	NaCl	Sucrose	–	NaCl	Sucrose
C_{60}	22.09 (22.37)	22.64 (22.92)	22.50 (22.78)	27.05	28.01	27.77	1056	1020	1029
C_{70}	21.41 (21.68)	21.95 (22.23)	21.82 (22.09)	25..88	26.81	26.58	1104	1066	1075
C_{76}	17.99 (18.22)	18.54 (18.77)	18.40 (18.63)	20.41	21.24	21.03	1400	1345	1359
C_{82}	12.30 (12.45)	12.85 (13.01)	12.71 (12.87)	12.73	13.39	13.33	2244	2133	2160
C_{86}	9.79 (9.91)	10.33 (10.46)	10.20 (10.33)	9.93	10.51	10.36	2878	2718	2757

*The data of ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} related to the ET-process for the strain FRAG-5 of *E-coli* with C_n had not been reported before.

Equations 8-10 show the correlations between the C-atoms descriptor (n) of the fullerenes and the free-energies of the ET-process (ΔG_{et}) of the strain TK-1207 of *Escherichia coli* bacteria in ordinary solution, NaCl (0.2 M) and *sucrose* (0.3 M) medias in the presence of dihydrostreptomycin (with minimum inhibitory concentrations MIC, 12, 28 and 22 μg/ml, respectively) with the selected fullerenes: $C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}.

Equations 11-13 and 14-15, are related to the relationships between the number "n" of carbon atoms in the fullerenes and the first free-energies of electron transfer (ΔG_{et}) of the strain TK-1208 and TK-1235 of *Escherichia coli* bacteria, respectively, with the mentioned conditions of Table-1 in the presence of dihydrostreptomycin and the fullerenes ($C_{60,}$ C_{70}, C_{76}, C_{82} and C_{86}). The R^2 values for the equations were good and demonstrated in Table 2.

There is good compromise between the computed values with two methods. The values of ΔG_{et} were decreased by increasing the number of carbons atoms (n) in the structure of the fullerene. The ET-rate increases as the electron population in the C_n structures increases. See Tables 3-6. These results could interpret by the HOMO-LUMO gaps and the MO energy levels of the fullerenes and the membrane potential (ΔΨ) of the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin. See the reported conditions in Table-1 by Damper and Epstein.[1]

The *Marcus* theory is widely accepted and applied. This theory makes surprising predictions about ET-process that have been nevertheless supported experimentally over the last several decades. The most important prediction is that the ET-rate will increase as the ET reaction becomes more exergonic, but only to a point.[46a-h]

The ET-process is one of the significant chemical processes in nature and acts as an important role in many chemical, medicinal, biological, physical and semiconductors systems and the new area of molecular electronics. The ET process is a very simple kind of chemical reaction and in understanding it, one can reach insight of the other kinds of biochemistry and chemistry. What is important is the chemistry of the ET-process from one place to another part of one or between the molecules. [46a-h]

The ΔG_{et} (free energy of ET) is the difference between the energy levels of the reactants and the products and $\Delta G_{et}^{\#}$ is the free activation energy of a reaction. If the entropy changes (ΔS) were ignored the free energy becomes energy or potential energy.[45,46a-h,47]

Table 5. The values on the electron transfer (ΔG_{et}) between the strain TK-1208 of *Escherichia coli* bacteria in NaCl and *sucrose* medias with the presence of dihydrostreptomycin and the fullerenes. The data of ΔG_{et} were calculated by Eq. 5 to Eq. 7. The data in parentheses have calculated by using Eq. 1 (*Rehm-Weller* equation).

*The Strain TK-1208 with C_n	ΔG_{et} (in *kcal mol*$^{-1}$)			$\Delta G^{\#}_{et}$ (in *kcal mol*$^{-1}$)			λ_{et} (in *nm*)		
	ΔG_{et}	ΔG_{et}	ΔG_{et}	$\Delta G^{\#}_{et}$	$\Delta G^{\#}_{et}$	$\Delta G^{\#}_{et}$	λ_{et}	λ_{et}	λ_{et}
	–	NaCl	Sucrose	–	NaCl	Sucrose	–	NaCl	Sucrose
C_{60}	21.13 (21.40)	22.23 (22.51)	22.41 (22.69)	25.42	27.29	27.61	1124	1047	1035

C_{70}	20.45 (20.71)	21.54 (21.81)	20.74 (21.00)	24.28	26.11	26.42	1177	1094	1081
C_{76}	17.04 (17.25)	18.13 (18.36)	18.31 (18.54)	18.99	20.62	20.89	1504	1386	1368
C_{82}	11.34 (11.48)	12.43 (12.59)	12.62 (12.78)	11.62	12.90	13.12	2458	2215	2178
C_{86}	8.83 (8.94)	9.93 (10.05)	10.10 (10.23)	8.95	10.07	10.27	3193	2837	2783

*The data of ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} related to the ET-process for the strain FRAG-5 of *E-coli* with C_n had not been reported before.

Table 6. The data on the electron transfer (ΔG_{et}) between the strain TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias with the presence of dihydrostreptomycin and the fullerenes. The data of ΔG_{et} were calculated by Eq. 5 to Eq. 7. The data in parentheses have calculated by using Eq. 1 (*Rehm-Weller* equation).

*The Strain TK-1235 with C_n	ΔG_{et} (in *kcal mol*$^{-1}$)			$\Delta G^{\#}_{et}$ (in *kcal mol*$^{-1}$)			λ_{et} (in *nm*)		
	ΔG_{et}	ΔG_{et}	ΔG_{et}	$\Delta G^{\#}_{et}$	$\Delta G^{\#}_{et}$	$\Delta G^{\#}_{et}$	λ_{et}	λ_{et}	λ_{et}
	–	NaCl	Sucrose	–	NaCl	Sucrose	–	NaCl	Sucrose
C_{60}	22.40 (22.69)	23.49 (23.87)	–	27.61	29.68	–	1035	963	–
C_{70}	21.73 (22.00)	22.89 (23.18)	–	26.42	28.45	–	1081	1004	–
C_{76}	18.31 (18.54)	19.48 (19.72)	–	20.89	22.70	–	1368	1259	–
C_{82}	12.62 (12.78)	13.78 (13.95)	–	13.12	14.56	–	2178	1963	–
C_{86}	10.10 (10.23)	11.27 (11.41)	–	10.27	11.54	–	2783	2475	–

*The data of ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} related to the ET-process for the strain FRAG-5 of *E-coli* with C_n had not been reported before.

In Tables 2-5 were shown the calculated data of $\Delta G^{\#}_{et}$ and λ_{et} by utilizing Eq. 2 and Eq. 3. By using Eq. 2 and Eq. 3, it is feasible to compute the activate free energies ($\Delta G^{\#}_{et(n)}$) of the ET process and the maximum wave length (λ_{et}) for the electron transfers process between the membranes of the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *E. coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin and the fullerenes agree with *Marcus* theory.[45,46a-h,47] In Figure 3 has shown the levels of ΔG_{et} and $\Delta G_{et}^{\#}$ in this ET-process. The values of the activated free energies of electron transfer ($\Delta G^{\#}_{et}$) for this ET-process, increase by increasing the $\Delta G_{et(n)}$ and the C-atom counts in the complexes, while the amounts of λ_{et} for the electron transfers, decrease by increasing $\Delta G_{et(n)}$ and $\Delta G_{et(n)}^{\#}$ for the electron transfer process. See Tables 2-5 and Figure 3. By using *Rehm-Weller* equation (Eq. 1), Eq. 2 and *Marcus* theory (Eq. 3) and the equations 5-15, the values of ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} were calculated for the ET-process between the membranes of the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin and the fullerenes. The C-atom counts (n descriptor) show a good correlation with the values of ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et}.

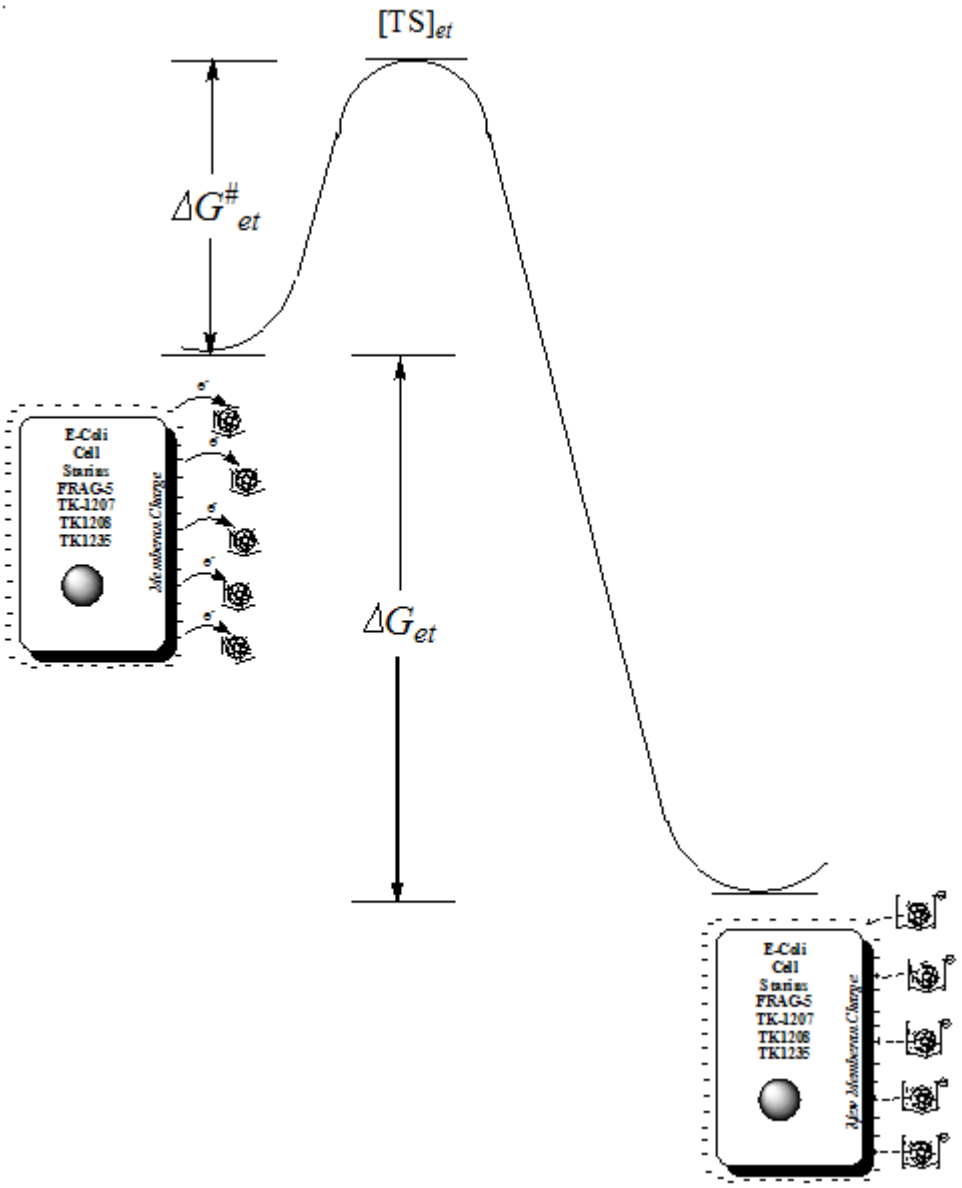

Figure 3. The levels of the amounts of ΔG_{et} and $\Delta G^{\#}_{et}$ between the strain TK-1235 of *Escherichia coli* bacteria in NaCl and *Sucrose* medias with the presence of dihydrostreptomycin and the fullerenes.

With the equations of this model, it is possible to calculate ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et}, for the ET process between the membranes of the strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin and the fullerenes, in close accordance with the results of the *Marcus* theory.

The discussed results and the computed data of ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} corresponding to the ET-process were neither predicted nor reported before. It has supposed that the electron transfer process between the strains of *Escherichia coli* bacteria with the fullerenes make conditions to restrict the bacteria (*E-coli*) growing by perturbation in the membrane charges of *E-coli*.

4. CONCLUSION

The electron transfer process between the selected strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin and fullerenes have shown important effects to restrict the bacteria (*E-coli*) growing by perturbation in the *E-coli* membrane charges. The electrochemical data of this electron transfer between the membranes of he selected strains of *Escherichia coli* bacteria and fullerenes were reported in this study. These included ΔG_{et} computed by using the *Rehm-Weller* equation and $\Delta G^{\#}_{et}$ as well as λ_{et} using the equations of the *Marcus* theory for the ET-process. Using the C-atom counts (n descriptor), along with the obtained equations in this modeling, one can derive sound structural correlations between the expressed physicochemical data. These equations allow to calculate ΔG_{et}, $\Delta G^{\#}_{et}$ and λ_{et} for the ET-process between the selected strains FRAG-5, TK-1207, TK-1208 and TK-1235 of *Escherichia coli* bacteria in NaCl and *sucrose* medias and in the presence of dihydrostreptomycin and the fullerenes (C_{60}, C_{70}, C_{76}, C_{82} and C_{86}). It seems that the discussed electron transfer could stop some of the phenomena related to the bacteria (*E-coli*) growing by perturbation in the membrane charges of *E-coli*.

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References

1. P. D. Damper and W. Epstein, *Antimic. Agen. Chemother.*, 20(6) (1981) 803.
2. a) B. I. Kanner, D. L. Gutnick, *J. Bacteriol*., 111 (1972) 187. b) L. E. Rryan, S. K. Kowand and H. M. Van Den Elzen, *Antimicrob. Agents Chemother*., 15 (1979) 7. c) L. E. Rryan and H. M. Van Den Elzen, *Antimicrob. Agents Chemother*., 9 (1976) 928.
3. B. D. Campbell and R. J Kadner, *Biochem. Biophys. Acta,* 593(1980) 1.
4. H. Taber and Halfenger G. M., *Antimic. Agen. Chemother.*, 9 (1976) 251.
5. P. D. Damper and W. Epstein, *Mechanism of low-level aminoglycoside resistance in Escherechia coli, p. 706-708*. In J. D. Nelson and C. Grassi (ed.), current chemotherapy and infectious disease, vol 1. 1980, American Society for Microbiology, D.C. Washington.
6. P. Mitchell, *Biol. Rev.,* 41 (1966) 445.
7. E. Padan, D. Zilberstein and H. Rottenberg, *Eur. J. Biochem.,* 63 (1976) 533.
8. A. A. Medeiros, T. F. O'Brien, W. E. C. Wacker and N. F. Yulug , *J. Infect. Dis.*, 124 (1971) S59.
9. G. P. Youmans and M. W. Fischer, *Action of stereptomycin on microorganisms in vitro, p.91-111*. In S. A. Waksman (ed.), Streptomycin, nature and practical applications. 1949, Williams & Wilkins Co., Baltimore.
10. (a) H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl and R. E. Smalley, *Nature,* 318 (1985) 162. (b) H. W. Kroto, *Nature*., 329 (1987) 529.
11. H. Shen, *Molecular Physics*., 105(17-18) (2007) 2405.

12. (a) K. Kimura, N. Ikeda, Y. Maruyama, T. Okazaki, H. Shinohara, S. Bandow, S. Iijima, *Chem. Phys*. Letters., 379 (2003) 340. (b) B. W. Smith, M. Monthioux, D. E. Luzzi, *Nature*, 396 (1998) 3239. (c) T. Miyak, S. Saito, *Solid State Commun*., 125 (2003) 201. (d) M. Zhang, M. Yudasaka, S. Bandow, S. Iijim, *Chem. Phys*. *Lett*., 369 (2003) 680.
13. L. Kavan, L. Dunsch, H. Kataura, *Carbon*., 42 (2004) 1011.
14. B. S. Sherigara, W. Kutner, F. D'Souza, *Electroanalysis*., 15 (2003) 753.
15. R. E. Haufler, J. Conceicao, L. P. F. Chibante, Y. Chai, N. E. Byrne, S. Flanagan, et al., *J. Phys. Chem*., 94 (1990) 8634.
16. Q. Xie, E. Perez-Codero, L. J. Echegoyen, *Am. Chem. Soc*., 114 (1992) 3978.
17. C. Jehoulet, Y. O. Obeng, Y. T. Kim, F. Zhou, A. J. Bard, *J. Am. Chem. Soc.*, 114 (1992) 4237.
18. P. Janda, T. Krieg, L. Dunsch, *Adv. Mater*., 17 (1998) 1434.
19. A. Touzik, H. Hermann, P. Janda, L. Dunsch, K. Wetzig, *Europhys. Lett*., 60 (2002) 411.
20. T. Tsuchiya, T. Shimizu, and N. J. Kamigata, *J. Am. Chem. Soc*., 123 (2001) 11534. (and the literature cited therein).
21. T. Suzuki, K. Kikuchi, F. Oguri, Y. Nakao, S. Suzuki, Y. Achiba, K. Yamamoto. H. Funazaka, and T. Takahashi, *Tetahedron*., 52(14) (1996) 4973. (and the literature cited therein).
22. M. R. Anderson, H. C. Dorn and S. A. Stevenson, *Carbon*, 38 (2000) 1663.
23. S. R. Cooper, *Acc. Chem. Res*., 21 (1998) 141.
24. A. A. Taherpour, *Full. Nanotu.Carb. Nanostruc.*, 16 (2008) 196.
25. A. A. Taherpour, *Full. Nanotu.Carb. Nanostruc.*, 15 (2008) 279.
26. A. A. Taherpour, *Full. Nanotu.Carb. Nanostruc.*, 15 (2007) 405.
27. (a) A. A. Taherpour and T. Asadi, *Full. Nanotu.Carb. Nanostruc.*, 19 (2011) 166. (b) A. A. Taherpour and Z. Talebi-Haftadori, *Internat. Nano Letters*, 3(22) (2013) 1.
28. A. A. Taherpour and M. Maleki, *Analytical Letters*, 43 (2010) 658.
29. A. A. Taherpour, *Phosphorus, Sulfur, and Silicon*, 185 (2010) 422.
30. A. A. Taherpour, *Int. J. Green Nanotech. : Phys. & Chem.*, 1(2) (2010) 97.
31. A. A. Taherpour, and F. Keyvan, *Phosph. Sulf. Silic. & Relat. Elem.*, 185(8) (2010)1604.
32. A. A. Taherpour, *Chem. Phys. Lett.*, 483 (2009) 233.
33. (a) A. A. Taherpour, D. Narian and A. Taherpour, *J. Nanostruct. Chem.*, 5(2), (2015) 153. (b) A. A. Taherpour and P. Lajevardi, *Int. J. Electrochem. Sci.*, 6 (2011) 5482. (c) A. A. Taherpour, M. Tayebi-Suraki and N. Mahdizadeh, *Eur. J. Chemistry*, 3(3) (2012) 340.
34. Y. P Du, Y. Z. Liang, Y. Li and C. J. Xu, *J. Chem. Inf. Cmput. Sci*., 42 (2002) 1128.
35. M. J. Randic, *J. Am. Chem. Soc*., 97 (1975) 6609.
36. S. D. Bolboaca, and L. Jantschi, *Int. J. Mol. Sci*., 8 (2007) 335.
37. Z. Slanina, F. Uhlik, S. L. Lee, E. Osawa, *MATCH Commun. Math. Comput. Chem*., 44 (2001) 335.
38. A. A. Taherpour, F. Shafiei, *J. Mol. Struct*. *THEOCHEM*, 726 (2005) 183.
39. (a) A. A. Taherpour, *Full. Nanotu. Carb. Nanostruc.*, 17(1) (2009) 26. (b) A. A. Taherpour and M. Maleki-Nureini, *Full. Nanotu. Carb. Nanostruc.*, 21(6) (2013) 485. (c) A.A.Taherpour and R. Jalajerdi, *Full. Nanotu. Carb. Nanostruc.*, 21(7) (2013) 653.
40. A. A. Taherpour, *Chem. Phys. Lett*., 469 (2009) 135.
41. A. A. Taherpour, *J. Phys. Chem*. *C*., 113(14) (2009) 5402.
42. A. A. Taherpour, and E. Mohammadinasab, *Full. Nanotu.Carb. Nanostruc.*, 18 (2010) 72.
43. Z. Slanina, M. C. Chao, S. L. Lee and I. Gutman, *J. Serb. Chem. Soc*., 62(3) (1997) 211.
44. D. Plavsic, S. Nikolic, N. Trinajstic and Z. Mihalic, *J. Math. Chem*., 12 (1993) 235.
45. D. Rehm and A. Weller, *Isr*. *J. Chem*., 8 (1970) 259.
46. (a) R. A. Marcus, *Rev. Modern Physics*, 65(3) (1993) 599. (b) M. Andrea Marcus Theory for Electron Transfer a short introduction MPIP-Journal Club-Mainz-January 29, 2008 (c) P. F. Barbara, *J. Phys. Chem*., 100 (1996) 13148. (d) M. D. Newton, *Chem. Ren*, 91 (1991) 767. (e) J. Jortner and K. F. Freed, *J. Chem. Phys*. 52 (1970) 6272. (f) R. A. Marcus, *J. Chem. Phys*., 43

(1965) 679. (g) R. A. Marcus, N. Sutin, *Biochim. Biophys. Acta.*, 811 (1985) 265. (h) M. G. Kuzmin, *XVIIth IUPAC Symposium on Photochemistry, Dresden, German, July 22-27, 2000, Book of Abstracts*, p. 372.
47. P. W. Atkins, *Physical Chemistry*, 6th ed., Oxford University Press, Oxford 1998& http://en.wikipedia.org/wiki/Photoinduced_electron_transfer.
48. a) G. S. Hammond, *J. Am. Chem. Soc.*, 77 (1955) 334. b) F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry*, 4th Ed., Kluwer Academic/Plenum Publishers, New York, USA, P.217.