Estimation of the Electric Properties of Al/Cv System

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Abstract

The electric properties of Al/Cv device system has been studied according to investigating and calculation the electron transport rate based on theoretical calculation and transition model. A classical model coupled with quantum model has been used to describe the rate of electrons at contact of Al metal with Crystal violet [Tris (4-(dimethylamino) phenyl methylium chloride] (Cv) dye has chemical formula C25H30CIN3. Two solvent Diethyl ether and Acetonitrile are used with non-homogeneous system for different absorption wave length 600,625,650,675 and 700 nm for Cv dye and the system is studied at room temperature. The effect of transition energy, potential and absorption energy on the transport rate in Al/Cv interface are studied and discussed. Rate of electrons in Al/Cv system is founded to be increasing with increasing the transition energy, increasing wave length and decreasing the potential for system in both solvents media. Our result shows that, at large transition energy and increasing wave length, the system has good electric properties and vice versa .Data show that Acetonitrile solvent is more suitable media for better electronic transfer rate in Al/Cv dye system.

Key words: Electric Properties, Al/Cv System.

Introduction

Charge transfer is a simple process which basically interaction in many biophysics, physical chemistry and Nano material for donor-acceptor systems. Transition process of electron from material to another is the most elementary reaction in solid, liquid solid and semiconductor liquid systems [1]. Electronic transition is an important basic reactions in physical properties, it can be occurs by photo induce and thermally excitation [2]. Over the past several decades, the electron transfer has been developed using different tools; time resolved, spectroscopy, analytical theory and computer simulation methods [3]. According to environmental condition reaction, the charge transfer reaction fast limited in range 1PS-1 to 1Yr-1. Charge transfer occurs in many systems such as: heterogeneous,

homogenous and molecular and homogeneous and bimolecular [4]. Charge transition reactions were occurred without breaking or reformation any bond, it can also happen within a molecule, from one group to another [5]. Charge transfer process is essentially at the interface of electronic conductors and ionic conductors in electrochemistry [6]. In contract, the energy level of molecule relative to energy level of metal is basic rule for charge transition at metal-organic system. The illustrated energy levels for this system make that reformation of potential barrier between metal and molecule interfaces [7]. Figure (1), shows charge transport at metal/molecule interface, it can introduce the barriers of charge transport due to alignment of molecular energy levels to Fermi level at metal [8].

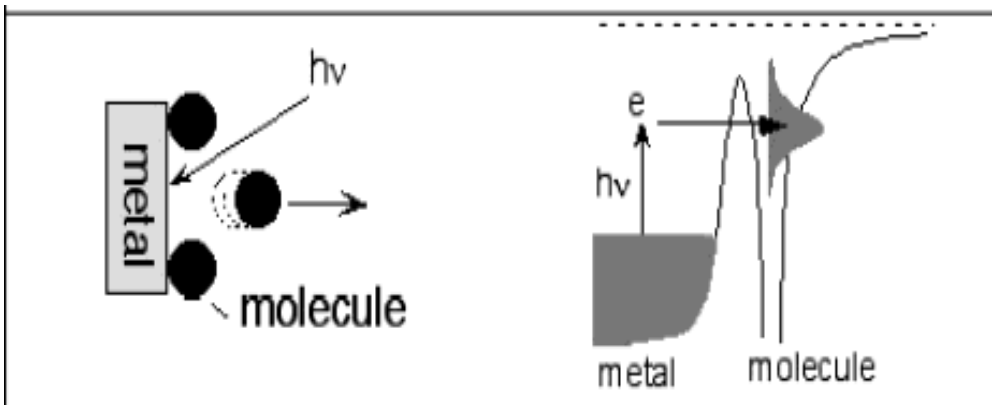

Figure (1): shows an energetic alignment formation at interface of metal-molecules structure [8].

The theoretical part

The behaviors of electron at metal-molecule system can be investigated using the probability of charge transition depending on quantum field. The metal-molecule system investigated completely independently each other at $t \leq 0$, and interacted at $t > o$. Due to Golden rule, the probability of electronic rate must be written as [9].

$$\wp_{et}(\tau) = \frac{2\pi}{\hbar}\sum|\Lambda^{ET}|^2 \int_{-\infty}^{\infty} \rho(E_M)\delta(E_M - E_m)\, dE_M \quad (1)$$

Where Λ^{ET}coupling coefficient between motel and molecule is, $\rho(E_M)$ is the density of metal state , E_M is electronic energy level state of metal and E_m is electronic energy level state of molecule. The metal density of state is given by [10].

$$\rho(E_M) = \frac{\exp^{-\frac{(\Gamma+E_o)^2}{4\Gamma k_B T}}}{\sqrt{4\pi\Gamma k_B T}} \quad (2)$$

Where Γ is transition energy and E_o is activation energy. On the other hand, the relation between transition energy Γ and activation energy E_o given by absorption energy $\hbar\omega$[11].

$$\hbar\omega = \Gamma + E_o \quad (3)$$

Where ω is frequency. Using eq.(2) in eq.(1) we find.

$$\wp_{et}(\tau) = \frac{2\pi}{\hbar}\int_{-\infty}^{\infty}\sum|\Lambda^{ET}|^2\frac{\exp^{-\frac{(\Gamma+E_O)^2}{4\Gamma k_B T}}}{\sqrt{4\pi\Gamma k_B T}}\delta(E_M - E_m)\,dE_M \quad (4)$$

Where $|\Lambda^{ET}|^2$ is the square of the electronic coupling which relatively to the density ρ(E) and given by [12].

$$\overline{|\Lambda^{ET}|^2} = \sum|\Lambda^{ET}|^2\delta(E_M - E_m) \quad (5)$$

Introduce the Fermi Dirac function F(E) to express the ocubation of electrons in state of system and given by [13].

$$F(E) = \frac{1}{[1+e^{\frac{E}{k_B T}}]} \quad (6)$$

Substitutes eq.(6) and eq.(5) in eq.(4) we gate.

$$\wp_{et}(\tau) = \frac{2\pi}{\hbar}\int_{-\infty}^{\infty}\overline{|\Lambda^{ET}|^2}\frac{\exp^{-\frac{(\Gamma+E_O)^2}{4\Gamma k_B T}}}{\sqrt{4\pi\Gamma k_B T}}[1+e^{\frac{E}{k_B T}}]^{-1}dE \quad (7)$$

After reformation eq.(7) to reach.

$$\wp_{et}(\tau) = \frac{2\pi}{\hbar}\overline{|\Lambda^{ET}|^2}\frac{\exp^{-\frac{(\Gamma+E_O)^2}{4\Gamma k_B T}}}{\sqrt{4\pi\Gamma k_B T}}\int_{-\infty}^{\infty}[1+e^{\frac{E}{k_B T}}]^{-1}dE \quad (8)$$

But the integral can be solved, by:-

$$\int_{-\infty}^{\infty}[1+e^{\frac{E}{k_B T}}]^{-1}dE \approx 2\int_{0}^{\infty}e^{\frac{-E}{k_B T}}dE \approx 2k_B T \quad (9)$$

If we inserting eq.(9) and eq.(3) in eq.(9) we get.

$$\wp_{et}(\tau) = \frac{2\pi}{\hbar}\overline{|\Lambda^{ET}|^2}\frac{2k_B T}{\sqrt{4\pi\Gamma k_B T}}\exp^{-\frac{(\hbar\omega)^2}{4\Gamma k_B T}} \quad (10)$$

The transition energy Γ (ev) is energy required orientation the structure of metal-molecule system. It is written as [14].

$$\Gamma(eV) = \frac{(\Delta e)^2}{8\pi\varepsilon_0}\left[\frac{1}{A}f(n,\varepsilon) - \frac{1}{2D}\sigma(n_M, n, \varepsilon_M, \varepsilon)\right] \quad (11)$$

Where Δe is difference in charge,ε_0 is permittivity of vacuum, A is radii of molecule, $f(n,\varepsilon) = \frac{1}{n^2} - \frac{1}{\varepsilon}$ is polarity of solvent when n and ε is refrective index and dielectric constant of solvents , D is the distance between the complex and metal electrode and $\sigma(n_M, n, \varepsilon_S, \varepsilon) = \frac{n_M^2 - n^2}{n_M^2 + n^2}\frac{1}{n^2} - \frac{\varepsilon_M^2 - \varepsilon^2}{\varepsilon_M^2 + \varepsilon^2}\frac{1}{\varepsilon^2}$ is the the polarity of metal/molecule interface ,where n_M and ε_M are refractive index and dielectric function of metal. The dielectric constant function of metal can be estimation using an expression [15].

$$\varepsilon_{M=\varepsilon_1+i\varepsilon_2} \quad (12)$$

Where $\varepsilon_1$real dielectric constant is given by [15]

$$\varepsilon_1 = {n_M}^2 - k^2 \quad (13)$$

Where $n_M$the metal refraction index and k is the extinction coefficient k,

While ε_2 is imaginary dielectric constant that computed using [15].

$$\varepsilon_2 = 2n_M k \quad (14)$$

The radii of the molecule have molecular weight M and mass density ρ is estimated from [16].

$$A = \left(\frac{3M}{4\pi N\rho}\right)^{\frac{1}{3}} \quad (15)$$

Where N is Avogadro's number.

Results

Depending on transition theory, electric properties of Al/Cv were according to calculate the rate of electrons using an expression in eq.(10). The rate of electrons have been calculated due to alignment the occupation of energy levels surface states for system and transfer of electrons cross interface of Al/CV system. One, we will be evaluation the transition energy using eq.(11) after estimation the radii of Cvdye and Al metal using eq.(15). Due inserting molecular weight $M = 361.74$[17] and the density $\rho(m) = 1.92 \frac{gm}{cm^3}$ [17] of Cv dye and molecular weight $M = 26.98$[15] and the density $\rho(m) = 2.70 \frac{gm}{cm^3}$ [15] .The result of the radii are $A = 4.21A^{\circ}$ and $1.582A^{\circ}$ for Cv dye and Al metal .The dielectric constant of metal can be estimated from Eqs.(12 to 14) using experimental data [18] for refractive index and the extinction coefficient k for Al metal [18] and evaluated using Eq.(12) with Eqs(13) and (14),results listed in table (1).

Table (1): The dielectric constant for Al metal.

Energy	Refractive index n_M[18]	Extinction coefficient k [18]	Dielectric constant of metal ε_M
2	1.304	7.48	57.636
2.4	0.826	6.28	40.158
2.6	0.695	5.8	34.123
2.8	0.598	5.39	29.356
3	0.523	5.02	25.514
3.2	0.46	4.71	22.377
3.4	0.407	4.43	19.755
3.6	0.363	0.36	0.2635
3.8	0.326	0.33	0.2126

Then , the transition energy for Al/Cv system using eq.(11) and MATLAB program with inserting the refractive index and static dielectric constant for solvent from table(2) and using refractive index and dielectric constant for Al metal from table(1), The results are shown in table(3).

Table (2): General properties of solvents [19].

Properties	Diethylether[16]	Acetonitrile [16]
Molecular weight g/mol	74	41
Empirical formula	C4H10Ol	C2H3Nl
Specific gravity	0.715	0.782
Refractive index	1.352	1.342
Dielectric Constant	4.3	37.5
Surface tension dyn/cm	17	29.1
Polarity	11.7	46
Van der Waals volume	3.39	1.87
Specific heat $(cal/mol/c^o)$	40	22
Critical temperature k	473	548

Table (3): Transition energy $\Gamma(eV)$ for Al/Cv interface system.

Energy(eV)	Refractive index n[18]	extinction coefficient k[18]	Dielectric constant of metal	Transition energy $\Gamma(eV)$	
				Diethylether	Acetonitrile
2	1.304	7.48	57.636	0.5833	0.9140
2.4	0.826	6.28	40.158	0.7258	1.0594
2.6	0.695	5.8	34.123	0.7682	1.1030
2.8	0.598	5.39	29.356	0.7987	1.1344
3	0.523	5.02	25.514	0.8217	1.1578
3.2	0.46	4.71	22.377	0.8384	1.1762
3.4	0.407	4.43	19.755	0.8518	1.1907
3.6	0.363	0.36	0.2635	0.7988	1.2016
3.8	0.326	0.33	0.2126	0.8070	1.2102

However, the electronic transition rate of Al/Cv system can be estimated according to transition energy, strength coupling and absorption energy $E = \hbar\omega$ from figure (2).

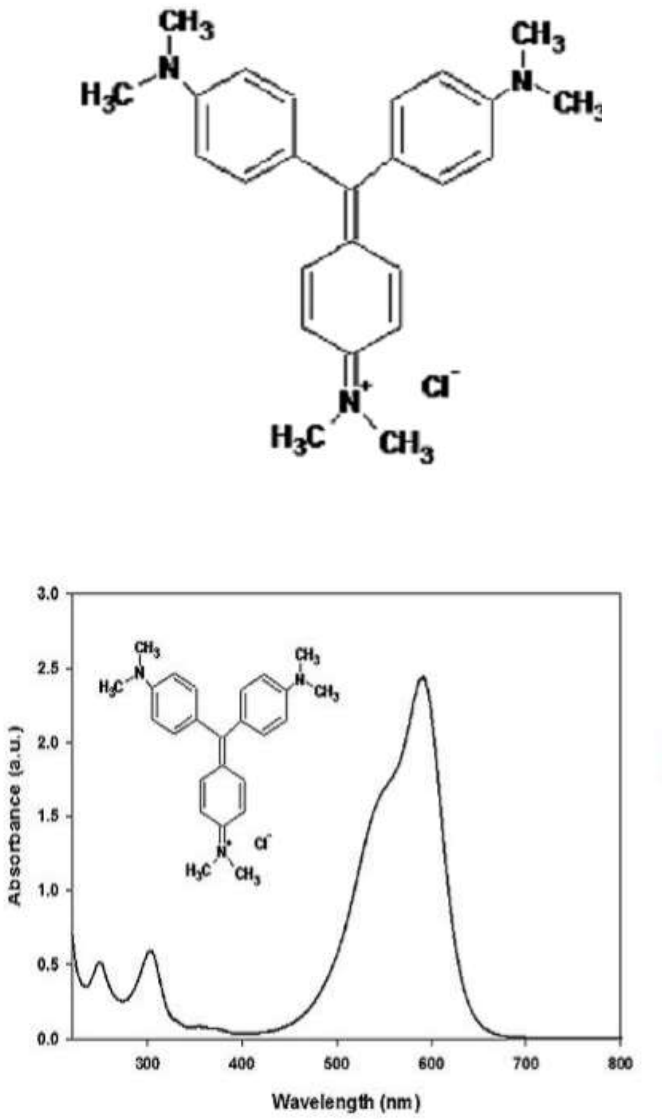

Figure (2):A) The chemical structure and spectral absorbance UV/V of Cv -dye.

The electron transfer rate has been calculated by using MATLAB program to solve the expression in eq.(10) for Al metal electrode interface with Cv dye. The strength coupling of energy levels at interface of Al metal with Cv solvent system is most important parameter has controlled the electrons transition at contact. It's determining the type of transition adiabatic or no adiabatic processes over interfaces for systems .It can be taken approximately to $\overline{\left|\Lambda^{\mathrm{ET}}\right|^2} = 5 \times 10^{-2}\ \frac{\mathrm{eV}^2}{\mathrm{state}}$[20]. The electron transfer rate calculated according to eq.(10) and estimation using MATLAB program after substituting the transition energy from table(3) and strength coupling $5 \times 10^{-2}\ \frac{\mathrm{eV}^2}{\mathrm{state}}$ under room temperature with $\hbar\omega = 600,625,650,675$ and 700 nm from absorbtion spectrum in

figure (2), , results are shown in table (4) with Diethylether and table (5) with Acetonitrile solvents respectively.

Table(4):The electron transfer rate at Al/ Cv with diethylether solvent system.

transtion energy Γ (ev)	Electron transfer rate $\wp_{et}(sec^{-1})$				
	Wave length				
	600nm	625nm	650nm	675nm	700nm
0.5833	1.188×10^{-18}	3.616×10^{-16}	6.087×10^{-14}	5.389×10^{-12}	3.166×10^{-10}
0.7258	1.762×10^{-12}	1.744×10^{-10}	1.073×10^{-8}	3.940×10^{-7}	1.040×10^{-5}
0.7682	4.351×10^{-11}	3.342×10^{-9}	1.638×7	4.930×10^{-6}	1.086×10^{-4}
0.7987	3.536×10^{-10}	2.301×10^{-8}	9.722×10^{-7}	2.569×10^{-5}	5.032×10^{-4}
0.8217	1.548×10^{-9}	8.964×10^{-8}	3.410×10^{-6}	8.222×10^{-5}	1.481×10^{-3}
0.8384	4.298×10^{-9}	2.295×10^{-7}	8.122×10^{-6}	1.839×10^{-4}	3.127×10^{-3}
0.8518	9.474×10^{-9}	4.752×10^{-7}	1.589×10^{-5}	3.425×10^{-4}	5.573×10^{-3}
0.7988	3.559×10^{-10}	2.315×10^{-8}	9.777×10^{-7}	2.582×10^{-5}	5.056×10^{-4}
0.8070	6.084×10^{-10}	3.793×10^{-8}	1.541×10^{-6}	3.939×10^{-5}	7.484×10^{-5}

Table(5):The electron transfer rate at Al/ Cv with Acetonitrile solvent system.

transtion energy Γ (ev)	Electron transfer rate $\wp_{et}(sec^{-1})$				
	Wave length				
	600nm	625nm	650nm	675nm	700nm
0.9140	2.736×10^{-7}	1.051×10^{-5}	2.770×10^{-4}	4.843×10^{-3}	6.518×10^{-2}
1.0594	1.511×10^{-4}	3.520×10^{-3}	5.919×10^{-2}	6.988×10^{-1}	0.658×10^{-1}
1.1030	7.242×10^{-4}	1.489×10^{-2}	2.240×10^{-1}	2.398×10^{0}	$2.067\times10^{+1}$
1.1344	2.076×10^{-3}	3.928×10^{-2}	5.480×10^{-1}	5.496×10^{0}	$4.463\times10^{+1}$
1.1578	4.386×10^{-3}	7.818×10^{-2}	$1.034\times10^{+0}$	9.898×10^{0}	$7.706\times10^{+1}$
1.1762	7.732×10^{-3}	1.317×10^{-1}	$1.673\times10^{+0}$	$1.546\times10^{+1}$	$1.165\times10^{+2}$
1.1907	1.193×10^{-2}	1.964×10^{-1}	$2.420\times10^{+0}$	$2.176\times10^{+1}$	$1.600\times10^{+2}$
1.2016	1.643×10^{-2}	2.636×10^{-1}	$3.174\times10^{+0}$	$2.798\times10^{+1}$	$2.021\times10^{+2}$
1.2102	2.105×10^{-2}	3.312×10^{-1}	$3.919\times10^{+0}$	$3.401\times10^{+1}$	$2.422\times10^{+2}$

Discussion

The electric properties of Al/Cv system is studied based on the electron transition rate according to quantum transition theory. In the fact, the solvents are organic polarity media a rounded the Al/Cv system, it providing more facility to transfer cross polarity solution to electrode.

Table (3) further shows the contribution of cooperation polarity of solvent and metal to the transition energy. The electron rate at nine values of transition energies are listed in tables (4) and (5) , which shows the rate increases obviously with increasing the transition energy and vice versa. Transfer rate of electrons decrease for Al/Cv with Diethylether solvent with same absorption energy indicate the potential is affected by polarity of solvent medium and large potential and decreases the driving force energy of electrons. As its more possible to transfer of electrons for system with Acetonitrile solvent because it has large transition energy and lead to reorientation the sites of molecules of dye a rounded the Al metal in the Al/Cv system . Because of the high transition energy for system with Acetonitrile solvent and similarity of wave length (600nm to 700nm) for the spectrum absorption of Cv dye , the more electrons will be transfer cross interface and have much driving force to transfer while the system with Diethylether solvent has less driving force to drive less electrons to transfer over interface. In view of transition rate for both system , the wave length 700nm is lead to more large electrons transfer cross interface comparing at 600nm indicate to less electrons transfer. Because of the polarity effect on transition energy and the electron transfer rates of the two solvents between Al and Cv dye. We show that although the two solvents are rather different in molecular weight and mass density their transition energy and electrons rate considerably. The transfer number of electrons is most probably for system has high transition energy because low potential and large driving force effective on electron. From data results in tables (4) and (5),we can find the transition rate of Al/Cv system behavior seemly approximately with absorption energy (600 nm to 700nm) this indicate the electric properties of system are same with two solvent in behavior . As shown in table (5), the Acetonitrile solvent is more available for Al metal in the Al/Cv system. Acetonitrile is suitable and greatest solvent for Al/Cv system comparing with Diethylether solvent. However, it can be noted that the electric properties dependent on the transition rate behavior.

Concussion

The electric properties are studied dependent on the kinetics of electronic transition processes in Al/Cv with two solvents systems. Different absorption energies with special strength coupling parameters tare limited the type of electron transfer between Al metal and the molecule of Cv dye. We find that the rate of electron transfer is function of electric properties.

Sufficiently, the high transfer rate indicates the system has good electric properties and low electronic transition rate indicate poor electric properties. In contrast, the Acetonitrile appears large rate compare with Diethylether solvent to be a lower rate of electronic transfer and slower transfer, this lead to suggesting that Acetonitrile is more efficient and suitable solvent with Al/Cv system compare with Diethylether has less efficient with system.

Conflict of Interests.
There are non-conflicts of interest

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الخلاصة

ان الخصائص الكهربائية لنظام نبيطة Al/Cv درس وفقا لوصف وحساب معدل الانتقال الالكتروني بالاعتماد على الحسابات النظرية والانموذج النظري. استخدم انموذج كلاسيكي مع انموذج نظري لوصف معدل الالكترونات عند ملتقى معدن الالمنيوم وصبغة Cv. اثنان من المذيبات الدایاثیر و الاسيتونترايل استعمل مع نظام هجين ولمختلف الاطوال الموجية 675,650,625,600 و 700 nm الممتصة حيث ان النظام درس في درجة حرارة الغرفة. تأثير طاقة الانتقال والجهد والطاقة الممتصة على معدل الانتقال لنظام سطحي Al/Cv درست. معدل الالكترونات لنظام Al/Cv وجد بأنه يتزايد بتزايد طاقة الانتقال وتزايد الاطوال الموجية وتناقص الجهد لكلا وسطي المذيب. نتائجنا اظهرت انه عند الطاقات العالية للانتقال وتزايد الاطوال الموجية فأن النظام له خصائص كهربائية جيدة والعكس بالعكس. ان مذيب الاستون اكثر ملائم للانتقال الالكتروني لنظام Al/Cv.

الكلمات الدالة: الخواص الكهربائية , نظام Al/Cv.