

## TiO<sub>2</sub>/N<sub>3</sub> الحسابات النظرية لثابت الانتقال الاليكتروني عبر سطح والصبغة المستضاءه للخلية الشمسية

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### الخلاصة

معدل الانتقال الاليكتروني من الصبغة المستضاءة الى شبة الموصل TiO<sub>2</sub> لانواع من المذيبات حسبت دالة لطاقة إعادة الالتحام والطاقة الحرة للفعالة وحجم شبة الموصل وثابت التوهين ثابت الشبيكه لشبه الموصل .  
الاعتماد القوي لثابت معدل الانتقال الاليكتروني على طاقة إعادة الترتيب والطاقة الحرة الفعالة. نتائج الحسابات تدل على ان شبة الموصل TiO<sub>2</sub> متاح للاستعمال مع الصبغة N<sub>3</sub> المستضاءه في الخلية الشمسية اظهرت نتائج حساباتنا تطابقا جيدا مع النتائج العملية.  
الكلمات المفتاحية: معدل الانتقال الاليكتروني، الصبغة المستضاءة N<sub>3</sub>، شبة الموصل TiO<sub>2</sub>، طاقة إعادة الالتحام.

## Theoretical Calculations of Rate Constant of Electron Transfer Across N<sub>3</sub>/TiO<sub>2</sub> Sensitized Dye Interface Solar Cell

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## Abstract

The rate of electron transfer from  $N_3$  sensitized by dye to  $TiO_2$  semiconductor in variety solvent have been calculated as a function of reorientation energy effective free energy , volume of semiconductor , attenuation and lattice constant of semiconductor .

A very strong dependence of the electron transfer rate constant on the reorientation and effective free energy .Results of calculation indicate that  $TiO_2$  is available to use with  $N_3$  dye .Our calculation results show that a good agreement with experimental result.

**Key world :**The rate of electron transfer,  $N_3$ dye sensitized,  $TiO_2$  semiconductor, reorientation energy.

## Introduction

The increase of the world's population combined with the growth per capita of energy consumption are expected to bring an explosive rise in energy consumption . To solve these problems , one need to save energy , increase the efficiency of equipment's transforming energy and develop the use of new sources of energy – solar energy is attracting a great deal of attention because it is a clean energy source and will not be depleted[1] .

For more than 16 years dye sensitized solar cells (DSSC) have been under extensive research since the (DSSC) are especially attractive building integrated photovoltaic cell .The cell concept is believed to reduce the production costs and energy pay back time significantly compared to standard silicon cells or other thin film cells [2]. The modern dye technological advancement is almost entirely dependent on the semiconductor devices .The application of the semiconductor devices fabrication commonly requires that defect would be introduced in the semiconductor lattice intentionally during processing stage [3]. The first silicon solar cell with practical energy conversion efficiency appeared in1950 until to 1990s produced cell with efficiency 24%[4]. Electron transfer processes play a key role in dye sensitized semiconductor solar cells devices work .In this paper we studied these electron transfer process through the calculation of rate constant of ET processes depending on a quantum theory. In contrast, the transfer across molecular/ bulk interfaces has gained attention only recently and is poorly understood. These interfaces play a key role in many emerging fields, creating a need for a better theoretical treatment of the interfacial electron transfer [5].

Photo induced ET at molecular/bulk interfaces is the primary step in many solar energy–conversion devices because it creates free-charge carriers on the absorption of a photon. Increased concerns with energy sources have prompted researchers to propose and test a great variety of these novel photovoltaic designs. Examples include dye-sensitized semiconductor solar cells [6].



A dye coupled to semiconductor is an excellent model for processes that occur in the above fields. This system represents one of the best-studied photovoltaic devices, the dye-sensitized semiconductor solar cell, or organic dye molecules that are adsorbed to a nanocrystalline TiO<sub>2</sub> (7). Visible light excites the dye-sensitize molecules from the ground state, which is located energetically in the semiconductor band gap, to an excited state resonant with the TiO<sub>2</sub> conduction band (CB).

The electron is then transferred to the semiconductor on an ultrafast timescale. It travels through the semiconductor to one of the electrodes, carries a load while making its way to the other electrode, and then enters an electrolyte that brings it back to the chromospheres ground state [8]. In this paper we can study the electron transfer in N<sub>3</sub> sensitized dye - TiO<sub>2</sub> semiconductor solar cell system. The chemical structure of N<sub>3</sub> dye sensitized is shown in figure (1) [9].

## Theory

For the system Dye – sensitized semiconductor solar cell setting is that introducing the donor state vector  $|D\rangle$  and acceptor state vector  $|A\rangle$  on solution side perturbs the energy between the electrode of semiconductor and molecule in solution and electron can tunnel to the acceptor state. Model Hamiltonians is used to describe the interfacial electron transfer dynamics is given by.

$$\hat{H}_{\text{mol-sem}} = \hat{H}_{\text{EL}} + \hat{H}_{\text{DA}} \dots \dots \dots (1)$$

Where  $\hat{H}_{\text{EL}}$  describes the sum of Hamiltonians for the molecules of dye state  $\hat{H}_D$ , and the Hamiltonian for the semiconductor state  $\hat{H}_A$  that is given by

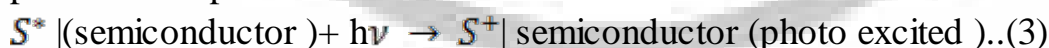
$$\hat{H}_{\text{EL}} = \hat{H}_D + \hat{H}_A.$$

The rate constant for electron transfer of the molecule dye acceptor relation to the semiconductor donor in solar cells can then be further written as [10]

$$K_{BT} = \frac{2\pi}{\hbar} \sum_k FC(\epsilon_k) f \epsilon_k |T_{DA} \epsilon(k,r)|^2 \dots \dots \dots (2)$$

For dye sensitized semiconductor solar cells devices where several electron transfer processes play a key role in dye sensitized solar cell, and it can be outlined as follows [11].

The adsorbed sensitized molecules (S) are brought into their excited state  $S^*$  by photon absorption



Electron injection dynamics from the electronically excited state of dye in conduction band of semiconductor with rate constant  $K_{et}$



The excited sensitized ( $S^*$ ) is relaxation to the ground state.



The oxidized sensitized  $S^+$  in its ground state is rapidly reduced by ions solution  $\Gamma^-$  (regeneration)



the probability reduced to the Boltzmann's equation where a change transfer from dye molecule sensitized ( donor state ) to acceptor semiconductor state , one need to integrate over all occupied state for [12]

$$K_{st} = \frac{2\pi}{\hbar} \int_{-\infty}^{\infty} \left[ \frac{1}{4\pi\lambda K_{BT}} \right]^{\frac{1}{2}} \exp \frac{-(\Delta G_0 + \lambda)^2}{4\pi\lambda K_{BT}} |T_{DA}(\epsilon_{k,r})|^2 f \epsilon_K d\epsilon \dots\dots (7)$$

The free energy of reaction is related to  $\epsilon$  by [13].

$$\Delta G = \Delta G_0 - \epsilon_k \dots\dots\dots(8)$$

And substituting  $\Delta G_0 = E_{CB} - \epsilon_{F,S/S^-}$  [13], in Eq(8), results.

$$\Delta G = (E_{CB} - \epsilon_{F,S/S^-}) - \epsilon = (\epsilon_{CB} - \epsilon_{ox}) - \epsilon_k \dots\dots\dots (9)$$

Inserting Eq (9) in (7) we gate

$$K_{eT} = \frac{2\pi}{\hbar} \left[ \frac{1}{4\pi\lambda K_{BT}} \right]^{\frac{1}{2}} \int_{-\infty}^{\infty} \exp \frac{-(\lambda + \epsilon_{CB} - \epsilon_{ox} - \epsilon_k)^2}{4\pi\lambda K_{BT}} \sum_{\epsilon}^t \rho(\epsilon) |V_{DA}(\epsilon_r)|^2 d\epsilon \dots(10)$$

Where[15].

$$|T_{DA}(\epsilon_{k,r})|^2 = \sum_{\epsilon}^t \rho(\epsilon) |V_{DA}(\epsilon_r)|^2 d\epsilon \dots\dots\dots(11)$$

The coupling by coefficient matrix element is estimated by using [10].

$$V_{Bi} = -\sqrt{\frac{\pi}{\beta a}} \frac{4}{3\pi^{\frac{3}{2}}} \epsilon_k \mu_e^k \dots\dots\dots(12)$$

Where  $\beta$  is the decay constant ,  $a$  is the lattice constant ,  $\mu_e^k$  is the factor multiplying and  $\epsilon_k$  is the energy of state k

Solving integral integrate equation to get .

$$K_{eT} = \frac{2\pi V}{9\hbar\pi^2\beta a} \left[ (4\pi\lambda K_{BT})^{\frac{3}{2}} \sqrt{\pi} + 2(4\pi\lambda K_{BT}) \frac{(\epsilon_{CB} - \epsilon_{ox} - 2\lambda)}{2} + \sqrt{4\pi\lambda K_{BT}} \frac{(\epsilon_{CB} - \epsilon_{ox} - 2\lambda)}{4} \sqrt{\pi} \right] \frac{\exp \frac{-2(\epsilon_{CB} - \epsilon_{ox})(\lambda + \epsilon_{CB} - \epsilon_{ox})}{16\pi\lambda K_{BT}}}{(4\pi\lambda K_{BT})^{\frac{1}{2}}} \dots\dots\dots(13)$$

Simplified to

$$K_{eT} = K_{eT}(0) \exp \frac{-2(\epsilon_{CB} - \epsilon_{ox})(\lambda + \epsilon_{CB} - \epsilon_{ox})}{16\pi\lambda K_{BT}} \dots\dots\dots(14)$$

Such that

$$K_{eT}(0) = \frac{2\pi V}{9\hbar\pi^2\beta a} \left[ (4\pi\lambda K_{BT})^{\frac{3}{2}} \sqrt{\pi} + 2(4\pi\lambda K_{BT}) \frac{(\epsilon_{CB} - \epsilon_{ox} - 2\lambda)}{2} + \sqrt{4\pi\lambda K_{BT}} \frac{(\epsilon_{CB} - \epsilon_{ox} - 2\lambda)}{4} \sqrt{\pi} \right] \dots\dots\dots(15)$$

Where V is the volume of semiconductor attenuation parameter, a is the lattice parameter , $\hbar$  is the Planck constant,  $K_B$  is the Boltzmann's constant and T is the temperature , $\lambda$  the reorientation energy and  $\Delta G^0$ , the effective free energy(driving force) given by [16].



$$\Delta G_o = hv - \lambda = h \left( \frac{c}{\text{wavelength}} \right) - \lambda \dots \dots \dots (16)$$

Where  $h$ , is Planck constant,  $\nu$  is the frequency,  $c$  is the velocity of light and  $\lambda$  is the reorientation energy. The reorientation energy arises from the reorientation of the charge in the medium .Its magnitude is dependent on the radius of the molecular donor and acceptor site, on its distance ( $d$ ) from the semiconductor , and on the dielectric properties of the molecule dye, the semiconductor , and the medium solvent .For electron transfer between reactant molecule dye and semiconductor , the medium reorientation energy is [17].

$$\lambda_o = \frac{(\Delta e)^2}{8\pi\epsilon_o} \left[ \frac{1}{R} \left( \frac{1}{D^{op}} - \frac{1}{D^s} \right) - \frac{1}{2d} \left( \frac{D^{op}_{se} - D^{op}}{D^{op}_{se} + D^{op}} - \frac{1}{D^{op}} \frac{D^{s^2}_{se} - D^{s^2}}{D^{s^2}_{se} + D^{s^2}} \right) \right] \quad (17)$$

Where  $\Delta e = e_D - e_A$  the difference in energy in donor and acceptor , $R$  is the radius of molecule dye,  $d$  is the distance between dye and semiconductor ,  $D^{op}$ ,  $D^s$  are the optical and static dielectric constant and  $D^{s^2}_{se}$  and  $D^{s^2}$  are the optical and static dielectric constant for semiconductor.

## Results

The theoretical calculation reported here where performed on using quantum model, and first order perturbations theory .The electron transfer rate was calculated for interface from a photo excited state molecular  $N_3$  sensitized dye to conduction band of  $TiO_2$  semiconductor depending on estimated the reorientation energy, driving force (free energy), height barrier, coupling overlap between  $TiO_2$  state and excited state molecular  $N_3$  sensitized dye.

One can be used the expression in Eq(17) to calculate the reorientation energy for  $TiO_2/N_3$  system with nine variety solvent .Inserting the values of optical  $D^{op}$ , and static  $D^s$  dielectric constant for solvent from table [1], and  $D^{op}_{se} = 2.488$  ,  $D^{s^2}_{se} = 86$  [13] for  $TiO_2$  semiconductor .  $R_{N_3} = 6.5 \text{ \AA}$  [22], and  $d = R_{N_3} + 1 \text{ \AA}$ , results are summarized in table(2).

Next we are using Eq.(17) to calculate the effective free energy (driving force), with taking the wave length of absorption light for  $N_3$  spectral (500-1000)nm, and  $h = 6.626 \times 10^{-34} \text{ J.sec}$ ,  $c = 3 \times 10^8 \text{ m/sec}$ .

The results obtained are summarized in table [3], parameters to calculate the rate of electron transfer is volume of  $TiO_2$  semiconductor that calculated using by  $V = a.b.c$  where  $a = b = 4.570 \text{ \AA}$ , and  $c = 2.989 \text{ \AA}$  [13], for  $TiO_2$  semiconductor. Result of volume of unit cell for  $V_{TiO_2} = 6.26424 \times 10^{-29} \text{ m}^3$ . For the dye/ semiconductorion , inserting of all these factors as data in a designed program to calculate the rate constant of electron transfer through the solution of the theoretical equation. These factors has been calculated with  $\beta = 0.9 \text{ \AA}^{-1}$  [10], using a Mat lab program is writing to compute the all factors that's guiding to estimate the rate constant of electron transfer in  $TiO_2/N_3$  sensitized solar cells system using Eq.(14-15), results are listed in table (4).

## Discussion

Electron transfer upon excitation rate were determined by electronic coupling coefficients between the excited state of  $N_3$  sensitized dye molecule and conduction band of the  $TiO_2$  semiconductor, the driving force energy  $\Delta G^{\circ}$ , the reorientation free energy, volume of semiconductor and attenuation parameters.

The Electron transfer upon excitation in states of molecule  $N_3$  sensitized dye when absorption a wave length (500-1000)nm and has to be rapidly injected into semiconductor before it can fall back to its ground state. The photo induce electron transfer from organic  $N_3$  dye molecule to  $TiO_2$  semiconductor is the first and most important reaction in solar cell system.

The electron transfer dynamics are determined by solvent reorientation free energy for orienting the  $N_3$  dye molecule with respect to the semiconductor. Data of results for rate electron transfer table (4) indicates that electron transfer depend on properties of the dye and  $TiO_2$  semiconductor with polar solvents.

As can be seen from table (2), the solvent controlled of reorientation energy for  $TiO_2/N_3$  system for nine solvents, the  $TiO_2/N_3$  system has large reorientation energy with most polar solvent than less polar solvent.

Consequently, the rate of Electron transfer is expected to be most favorable in more polar solvent. From table (3) and table (4) we can find the rate is strongly depending on dielectric constant. This means increasing polarity  $D^s$  for solvent leads to increase the reorientation energy and results to increase in rate constant for  $TiO_2/N_3$  system and vice versa. But the shift in the reorientation energy and rate constant results in DMF and Formamide solvent, indicate because the high value of optical dielectric constant  $D^{op} \cong 1.43$ , and 1.445 for DMF and Formamide. The results of  $TiO_2$  force free energy for electron transfer between  $N_3$  sensitized dye and  $TiO_2$  semiconductor is relative energy difference between the conduction band and oxidation. Results in table (4) show the rate constant of electron transfer is small, where the driving force due to potential different between the conduction band and the radius of dye was not enough for electron transfer to occur.

Observably, a large value of  $\Delta G_o$  would give rise a small  $K_{et}$ , however, these values continue to be large with small value of  $\Delta G_o$ .

The activation energy (height barrier) leading to the small  $K_{et}$ . The barrier created between two materials  $N_3$  sensitized dye and  $TiO_2$  semiconductor, and depending on characteristic of two materials. Near dye/semiconductor interface, due to energy level difference the barrier is formed with properties of two dye, semiconductors and caused impedance of charge transfer. Consequently the rate of electron transfer to be large when the barrier height is small and vice versa on the other hand, we can find the rate of electron transfer is proportional with volume of  $TiO_2$  semiconductor, and inversely proportional with  $\beta$ .

## Conclusion

In summary it can be concluded that rate of electron transfer is large in high polar solvent and small in the less polar solvent .This indicates that electron transfer was expected to be favorable in most polar solvents.

In order to study the oxidation and conduction band as a function of  $\Delta G_o$  for electron transfer ,the effective free energy it take for an electron to be recombined and can be determined from absorption of light for dye/semiconductor system .The rate  $K_{et}$  shift to minimum for large height barrier and small reorientation energy.

Based on this work ,we concluded the use  $TiO_2$  semiconductor with  $N_3$  dye in polar solvent is good matching system ,because of flow of electron from dye to semiconductor is large compared with less polar solvents.Also we can see the use of  $TiO_2$  semiconductor with  $N_3$  dye is attractive because it is wide band gap semiconductor with better carrier mobility, the  $TiO_2/N_3$  a good system.

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Solvent	Chemical Formula [18-19]	Dielectric constant [18- $D^s$ 19]	Optical Dielectric Constant $D^{op}$	Viscosity (cc) [18,20] $\eta$
1-Butanol	C <sub>4</sub> H <sub>10</sub> O	17.84	1.397 [20]	2.57
Methanol Ethyl Ketene	C <sub>4</sub> H <sub>8</sub> O	18.8	1.3788 [21]	
Acetone	C <sub>3</sub> H <sub>6</sub> O	21.01	1.3563 [21]	0.30



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Ethanol	C <sub>2</sub> H <sub>2</sub> O	25.3	1.359[21]	1.94
Methanol	CH <sub>4</sub> O	33.0	1.329[20]	0.55
Acetone tril	C <sub>2</sub> H <sub>3</sub> N	37.5	1.3441[20]	0.34
Formic Acid	CH <sub>2</sub> O <sub>2</sub>	51.1	1.370[21]	
DMF	C <sub>3</sub> H <sub>7</sub> NO	38.25	1.4305[21]	1.987
Formamide	CH <sub>2</sub> NO <sub>2</sub>	109	1.445[20]	3.3

Table (1): A common properties of solvent

Semiconductor	Dielectric constant $D^s$	Optical Dielectric Constant $D^{op}$	Energy gab (eV)	Lattice constant (nm)	Crystal structure
TiO <sub>2</sub> [13]	86	2.488	3.2	A=4.570c=2.989	Zinc blend

Table (2): The reorientation energies of electron transfer in TiO<sub>2</sub>/ N3 sensitized solar cell

Solvent	$\lambda$ (eV) for TiO <sub>2</sub>
1-Butanol	0.378832185
Methyl	0.39113637969367
Aceton	0.40901963694359
Ethanol	0.41616144754285
Methanol	0.44280216813319
Acetonitrile	0.43818565882596
DMF	0.39455563784532
Formicacid	0.43184397805475
Formamide	0.40641128112508

Table (3): Result of calculation of the effective free energy for electron transfer in TiO<sub>2</sub>/ N3 sensitized solar cell

ulation of the effective free energy for electron transfer in TiO<sub>2</sub>/ N3 sensitized solar cell

Wave length Solvent	Effective Free Energy $\Delta G^{\circ}$ (eV)										
	500nm	550nm	600nm	650nm	700nm	750nm	800nm	850nm	900nm	950nm	1000nm
1-Butanol	2.1028	1.8772	1.6892	1.5301	1.393	1.2755	1.1721	1.0809	0.9998	0.9272	0.8246
Ethyl	2.0905	1.8649	1.6769	1.5178	1.3814	1.2632	1.1598	1.0686	0.9875	0.9149	0.8496
Acetone	2.0726	1.8470	1.6590	1.4999	1.3635	1.2454	1.1420	1.0507	0.9696	0.8971	0.8318
Ethanol	2.0654	1.8398	1.6518	1.4927	1.3564	1.2382	1.1348	1.0436	0.9625	0.8899	0.8246
Methanol	2.0388	1.8132	1.6252	1.4661	1.3298	1.2116	1.1082	1.0169	0.9358	0.8633	0.7980
Acetonitrile	2.0434	1.8178	1.6298	1.4707	1.3344	1.2162	1.1128	1.0216	0.9405	0.8679	0.8026

DMF	2.0870	1.8614	1.6734	1.5144	1.3780	1.2598	1.1564	1.0652	0.9841	0.9115	0.8462
Formic acid	2.0498	1.8241	1.6361	1.4771	1.3407	1.2225	1.1191	1.0279	0.9468	0.8742	0.8089
Formamide	2.0752	1.8496	1.6616	1.5025	1.3661	1.2480	1.1446	1.0533	0.9722	0.8997	0.8344

Table (4): Rate constant of electron transfer  $K_{et}$  (eV.m)<sup>3</sup>/sec in N3/ SnO2 in sensitized solar cell system.

Wavelength	Rate Constant of Electron Transfer $K_{et}$ (eV.m) <sup>3</sup> /sec										
	500nm	550nm	600nm	650nm	700nm	750nm	800nm	850nm	900nm	950nm	1000nm
Solvent	X10 <sup>-47</sup>	X10 <sup>-44</sup>	X10 <sup>-40</sup>	X10 <sup>-38</sup>	X10 <sup>-35</sup>	X10 <sup>-34</sup>	X10 <sup>-32</sup>	X10 <sup>-30</sup>	X10 <sup>-29</sup>	X10 <sup>-28</sup>	X10 <sup>-27</sup>
1-Butanol	0.0139	0.0889	0.0128	0.0586	0.0109	0.0988	0.0498	0.0155	0.0323	0.0479	0.0532
Ethyl	0.0222	0.1414	0.0202	0.0925	0.0171	0.1545	0.0775	0.0240	0.0497	0.0732	0.0806
Acetone	0.0437	0.2773	0.0395	0.1792	0.0329	0.2953	0.1470	0.0451	0.0925	0.1348	0.1468
Ethanol	0.0574	0.3627	0.0516	0.2333	0.0428	0.3822	0.1896	0.0580	0.1184	0.1718	0.1861
Methanol	0.1574	0.9866	0.1391	0.6226	0.1130	0.9966	0.4880	0.1470	0.2953	0.4205	0.4462
Acetonitrile	0.1322	0.8297	0.1171	0.5253	0.0955	0.8445	0.4145	0.1252	0.2522	0.3604	0.3840
DMF	0.0253	0.1609	0.0230	0.1050	0.0194	0.1749	0.0876	0.0271	0.0560	0.0823	0.0904
Formic acid	0.1039	0.6539	0.0925	0.4160	0.0758	0.6724	0.3311	0.1004	0.2030	0.2915	0.3121
Formamid	0.0396	0.2514	0.0358	0.1627	0.0299	0.2687	0.1339	0.0411	0.0845	0.1233	0.1346

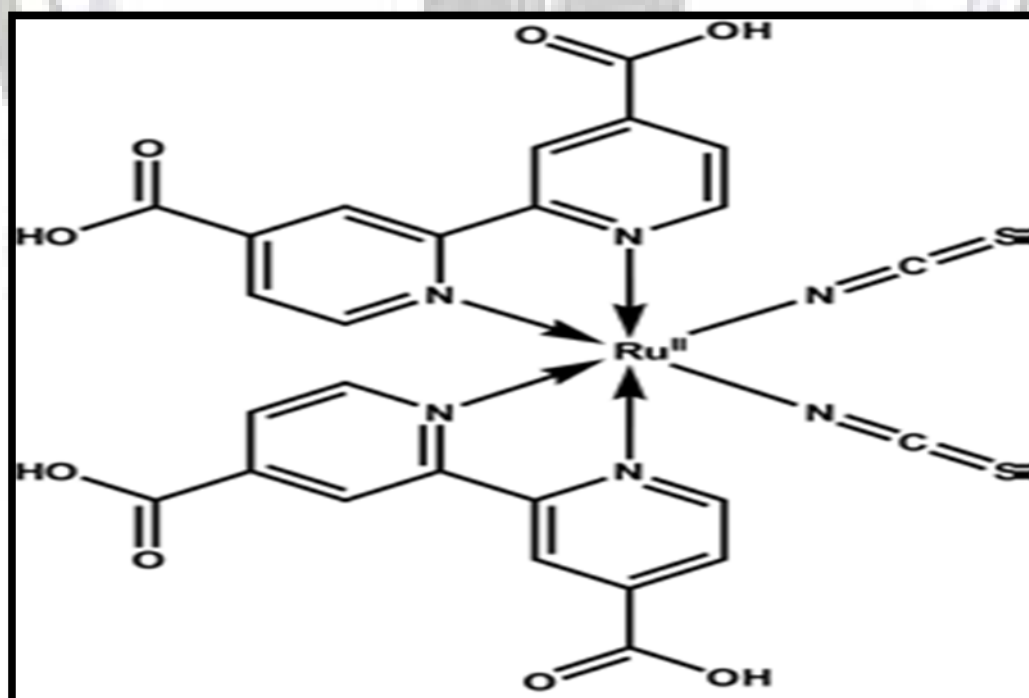


Fig.(1): Chemical structure of (N3) RuL2 (NCS) 2, L=2, 2'-bipyridyl-4, 4'-dicarboxylic acid [10].