

## Single Molecule Thin Film Featuring Disubstituted Thiourea (TU) Doped with Chlorophyll as Potential Active Layer in Photovoltaic Cell

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The versatility of conjugated thiourea compound enhances the development of molecular wire architectures due to the overlapping of  $\pi$ -electrons which can be applied as potential organic solar cell (OSC). Hence, new innovational and breakthrough are needed for OSC molecules to become competitive in the future since they represent lower cost and more flexible devices, tunable electronic properties and easier processing compared to other organic molecules. Due to this interest, a study on the performance of essentially linear conjugated organic compound based on Donor (D)- $\pi$ -Acceptor (A) system which featuring D-ArNHC=SNH-A-NHC=SNHAr-D to act as potential active layer in OSC was carried out. The synthesized compound was successfully designed, prepared, and characterized prior to form thin film. The compound was then spectroscopically and analytically characterized via <sup>1</sup>H and <sup>13</sup>C Multi-Nuclear Magnetic Resonance (NMR), Fourier Transform Infrared (FT-IR), UV-Visible Analysis (UV-Vis), Thermogravimetric Analysis (TGA), Scanning Electron Microscopy (SEM), CHNS Elemental Microanalysis as well as Cyclic Voltammetry (CV) analysis. In turn, it was fabricated on Indium Tin Oxide (ITO) substrate before its conductivity behaviour, efficiency and OSC parameter were evaluated by Four Point Probe. From the electrical conductivity study, it revealed that it performed better and higher conductivity with the presence of chlorophyll (CHLO) under maximum light intensity of 100 Wm<sup>-2</sup>. The result shows the electrical conductivity increases with the increasing of the light intensity. The electrical conductivity of the thin films shows the conductivity of 0.2040 Scm<sup>-1</sup> (with CHLO) compares to 0.1472 Scm<sup>-1</sup> (without CHLO) under maximum light intensity. From the result obtained, it clearly shows the synthesized compound has great potential to act as an active layer in photovoltaic cell. Therefore, further investigation on

photovoltaic studies on the similar molecular system should be seriously considered for further development in molecular electronics application.

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**Keywords:** Organic Solar Cell, Thiourea, Thin film.

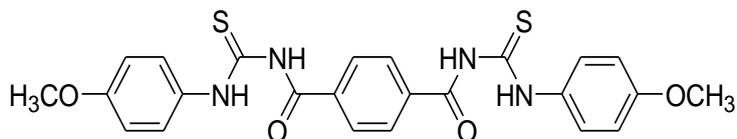
## 1. INTRODUCTION

Nowadays, climate changes are threatening our life, and non-renewable resources which are a primary energy that predicted to decrease terrifically over years which can affect human health and environment. Hence, it is important to take serious actions on energy issues by reducing energy consumption and increase the production of energy originating from inexpensive renewable sources such as sun energy [1-2] where the devices can convert sun's energy to electrical energy via chlorophyll [3-4]. The process of converting light into electrical current in an organic photovoltaic cell is accomplished by four consecutive steps begin with absorption of photon excitation, charge separation, and finally the formation of current [5]. Development in the field of organic solar cells has been growing due the system of roll-to roll manufacturing on flexible substrate [6-7]. This field becomes as an exciting approach for efficient, low-weight, and low-cost photovoltaic devices to grab the challenge of the rising demand for green and clear electricity supply [8-10].

Within these concerns, molecular electronic materials are becoming as one of the great potential for further applied in solar cell studies due to their molecular framework and electronic behaviours. Since Aviram and Ratnam proposed that an unimolecular obeying system donor-spacer-acceptor structure would behave like electronic device, then molecular electronic has attracted great attention as replacements for silicon technology to facilitate nanoscale electronic devices [11-12]. In addition, one of the advantage of using synthesized molecules is it can be tolerate to the need of their electrical properties which potentially allowed for the development of novel electronic devices. [13]. Undoubtedly, in the active layer of organic solar cell, the conjugated system that presence in organic molecules play the crucial key role of absorbing light, creating excitons for charge separations and transporting hole to the anode [14-17] and currently, ITO coated substrate has been developed and the coating is used as part of the organic solar cells materials [18-19].

In previous occasions, we have introduced so-called mono-substituted linear [20] and 'V'-shaped systems [21] of conjugated thiourea for single molecule solar cell with proven promising conductivity in high intensities of light especially in dark conditions [22]. However, the report on ideal organic materials and investigation on suitable fabrication method to be applied in organic solar cell (OSC) are rather limited. Thus, in the light of these previous works, herein we reported the synthesis and characterization of disubstituted thiourea (TU) derivative with linear configuration in the form of thin-film based using Electrochemical Impedance Spectroscopy (EIS). The compound that contains TU moiety emerges as  $\pi$ -conjugated system that can be a good charge transport for current flow. The presence of chlorophyll that doped on the TU compound will be then coated on ITO substrate in order to increase the ability of light absorption [23-25]. Thus, this study focuses on the preparation,

characterization, and its promising potential to act as organic solar cell featuring TU derivatives as shown in Figure 1 below.



**Figure 1.** Molecular structure of disubstituted thiourea (TU) as active layer in photovoltaic cell synthesized in the study.

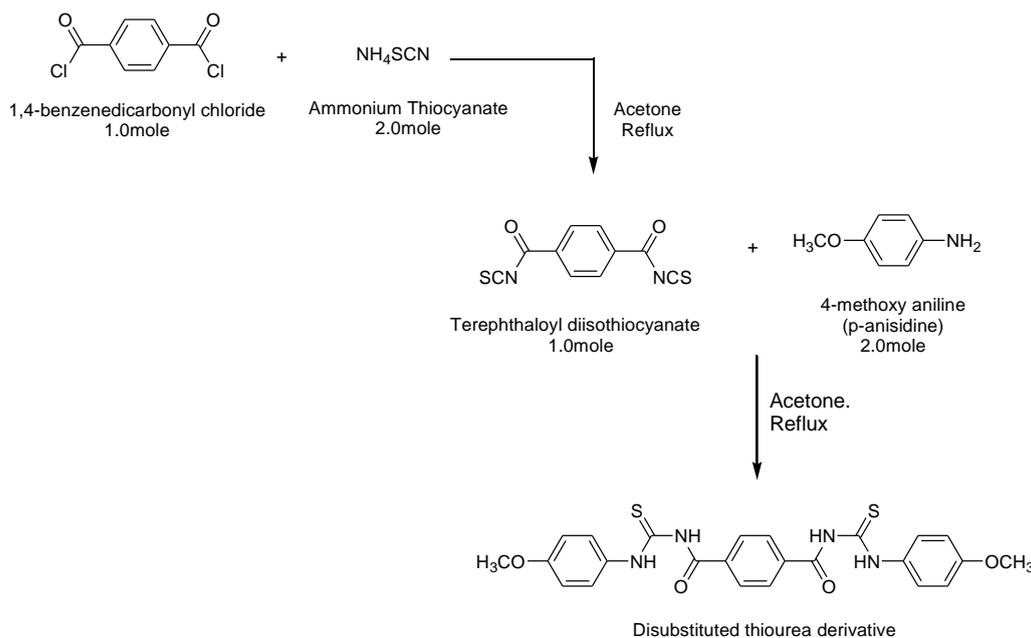
## 2. EXPERIMENTAL

### 2.1 Material and General Methodology

All reactions were carried out under an ambient atmosphere and no special procedures were taken to exclude air or moisture during work-up. The chemicals and reagents used were purchased from standard commercial suppliers (Fisher Scientific, Merck, Sigma Aldrich, R&M Marketing and Acros organic) and used as received without further purification. The infrared (IR) spectra were recorded by a Fourier Transform-Infrared Spectrometer (FTIR), Perkin Elmer Spectrum 100 in the range of 4000-400  $\text{cm}^{-1}$  using Potassium Bromide (KBr) pellets. Electronic absorption spectra of sample were recorded in the range of 200-400 nm using Shimadzu UV-Vis Spectrophotometer in 1  $\text{cm}^3$  cuvette in methanolic solution. The proton Nuclear Magnetic Resonance ( $^1\text{H}$  NMR, 500.16 MHz) and carbon Nuclear Magnetic Resonance ( $^{13}\text{C}$  NMR, 125.77 MHz) spectra were recorded via Joel NMR Spectrometer in deuterated dimethyl sulfoxide (DMSO) as solvent and chemical shift values were given in parts per million (ppm) relative to solvent resonances as internal standard. For CHNS elemental analysis, it was carried out by CHNS-O Analyzer Flash EA 1112 series. Thermogravimetric analysis was performed using Perkin-Elmer TGA Analyzer from 0  $^{\circ}\text{C}$  to 700  $^{\circ}\text{C}$  at a heating rate of 10  $^{\circ}\text{C}/\text{min}$  under nitrogen atmosphere. While, the surface morphology of the compound was scanned by JSM 6360 Joel Scanning Electron Microscopy (SEM) with accelerated voltage 20 kV and magnification from 3500x until 5500x. To assess intrinsic redox potential of the synthesized compound as active layer material, the electrochemical study was investigated using Electrochemical Impedance Spectroscopy (EIS) PGSTAT302. Afterwards, ITO/Thiourea (TU) thin films were deposited by electrochemical deposition (ECD) method and followed by chlorophyll (CHLO) via spin coating technique by using Spin Coater Model WS-400B-6NPP-LITE. Investigation of the energy bandgap of the compound also was measured and calculated from the Cyclic Voltammetry (CV) and UV-Vis Optical spectrum. Finally, the electrical conductivity of the thin film was measured in dark and under various intensity of light by using Four-point Probe which consists of Jandel Universal Probe combined with a Jandel RM3 Test.

## 2.2 General Overview of Synthetic Work

The synthesis of TU involved a reaction between corresponding chloride with equimolar amount of ammonium thiocyanate to form analogue of isothiocyanate after being stirred and put at reflux for *ca.* 4 hours. Afterwards, amine in equivalent molar was added to the reaction mixture and continuously stirred and put at reflux for another *ca.* 4 hours. The reaction was carried out in acetone as solvent to obtain desired precipitate as well as inorganic salt as by product. The filtrate was then poured into a beaker containing some ice cube. The resulting precipitate was then filtered and recrystallized from hot methanol to afford the desired compound. The synthetic route is shown in Scheme 1.



**Scheme 1.** General outline for synthesis of disubstituted thiourea (TU) derivative

### 2.2.1 Synthesis of disubstituted thiourea (TU) derivative

The synthesis of disubstituted thiourea (TU) derivative was conducted by adding stoichiometric amount of 1,4-benzenedicarbonyl chloride (5.0g, 24.6 mmol) and ammonium thiocyanate (3.75g, 49.2 mmol) with *ca.* 100ml of acetone in a 250ml two-necked round bottom flask. The reaction mixture was then heated at reflux condition with constant stirring for *ca.* 4 hour to attain a pale yellow solution with white inorganic salt as by products at the end of the reaction. The progress of the reaction was monitored by using TLC in the ratio of solvent used was (hexane: ethyl acetate; 2:3).

Afterwards, p-anisidine (6.06 g, 49.2 mmol) in *ca.* 50ml acetone was added into the solution of terephthaloyl diisothiocyanate. After adjudged completion by TLC (hexane : ethyl acetate) (2 : 3), the reaction mixture was filtered and the filtrate was left to cool at room temperature. Next, 3 ice cubes were added into the yellow filtrate and yellow precipitate was obtained at the end of the reaction. Then,

the yellow precipitate was recrystallized from hot methanol to attain the thiourea compound (6.67 g, 65 %). The physical properties with analytical data of the synthesized compound is shown in Table 1.

**Table 1.** Physical properties and analytical data of the synthesized compound.

Molecular formula of compound	Appearance	Yield (%)	Percentage of weight element			
			%C	%H	%N	%S
C <sub>24</sub> H <sub>22</sub> N <sub>4</sub> O <sub>4</sub> S <sub>2</sub>	Pale yellow solid	65	65.316 (65.863)	8.681 (7.569)	8.465 (8.091)	10.287 (9.236)

\* In bracket: theoretical percentage of element

### 2.3 Electrochemical Measurement

The electrochemical study of the synthesized compound was performed using Electrochemical Impedance Spectroscopy (EIS) PGSTAT 302 in order to investigate the redox reaction and potential range of different electrochemical processes of the compound to act as active material in organic solar cell. A typical electrochemical impedance experimental set-up consists of an electrochemical cell, a potentiostat/galvanostat and a General Purpose Electrochemical System (GPES). A conventional three-electrode configuration used for an electrochemical cell which most common for electrochemical applications. It consists of platinum, Pt electrode acts as working electrode.

Then, second functional electrode is the platinum wire as counter electrode which serves as a source sink for the electrons, so that the current can pass from the external circuit through the cell. While, Ag/AgCl electrode was used as reference electrode, in which the potential is constant enough and can be taken as the reference standard. The acetonitrile (CH<sub>3</sub>CN) and 0.5 M sulphuric acid (H<sub>2</sub>SO<sub>4</sub>) were used as solvents and supporting electrolyte with concentration of (1x10<sup>-5</sup>M). By using the General Purpose Electrochemical System (GPES) method software, Cyclic Voltametry (Staircase) method set to be in Normal procedure which is shown in Table 2.

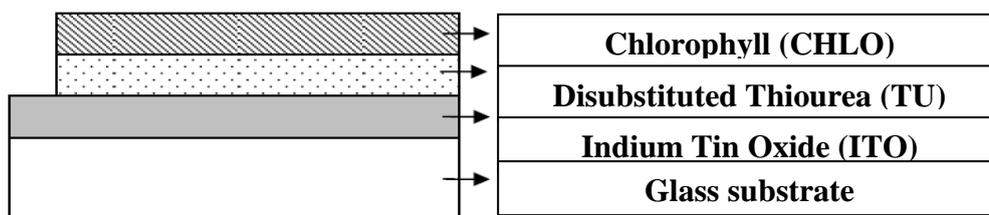
**Table 2.** Procedure set for electrochemical deposition process

Parameter Setup	Value of Parameter
Start Potential (V)	0
First Vertex Potential (V)	2
Second Vertex Potential (V)	0
Step Potential (V)	0.03007
Scan Rate (Vs <sup>-1</sup> )	0.050005

### 2.4 Thin Film Preparation

The thin films were prepared by different techniques for each layer. The synthesized compound had been deposited on the ITO substrate via electrochemical deposition (ECD) method and second

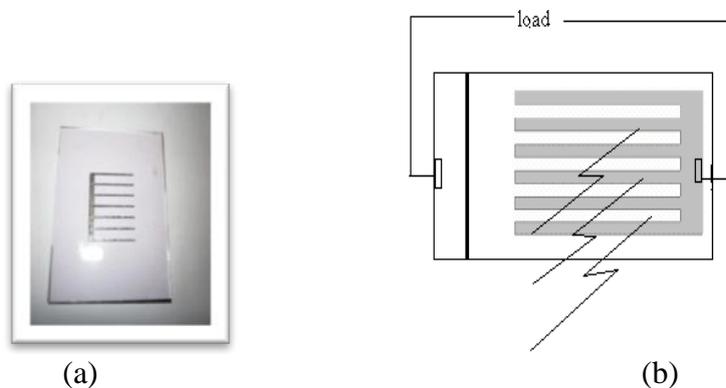
layer was deposited with chlorophyll (CHLO) on the top layer of compound by using spin coating technique. The compound was deposited on the ITO substrate in the following conditions: 0.05V, 0.05 V/S, potential range: -0.5V until 3.5V in acetonitrile and 0.5M sulphuric acid (as supporting electrolyte) with concentration of the compound ( $1 \times 10^{-5} \text{M}$ ). In turn, CHLO thin film was prepared by using spin coating technique via Spin Coater Model WS-400B-6NPP-LITE. In this study, four stages of spin were used (500 rpm for 10 seconds, 1000 rpm for 15 seconds, 1500 rpm for 20 seconds, and 2000 rpm for 30 seconds) to complete a cycle. Figure 2 shows the general illustration of layer arrangement in thin film prepared by different techniques for each layers.



**Figure 2.** The general illustration of layer arrangement in thin film

### 2.5 Deposition of the Electrodes

The thin film fabrication was completed via thermal evaporation of aluminum for inverted architecture process which known as masking process. The mask was designed same as the ITO sample size and then the electrode was deposited on the active area surface. In this study, the aluminium electrode must be deposited on the chlorophyll surface as shown in Figure 3. The efficiency of a flexible device with an active area with a grid is much higher than a similar device based on ITO.



**Figure 3.** The schematic diagram (a) Thin film fabrication with aluminium grid (b) Solar cell under radiation of light

### 2.6 Electrical Conductivity Study

Four Point Probe was used to determine the conductivity of thin films. In this study, the sheet resistivity in produced film was measured with complete four point probe system consists of Jandel Universal Probe combined with a Jandel RM3 Test Unit. The electrical conductivity of thin film was measured in the dark condition and light condition with intensity of  $10 \text{ Wm}^{-2}$ ,  $30 \text{ Wm}^{-2}$ ,  $50 \text{ Wm}^{-2}$ , and  $100 \text{ Wm}^{-2}$  respectively by using Four Point Probe and LI-200 Pyranometer Sensor with LI-1400 Data Logger. Current output, which is directly proportional to solar radiation, was calibrated against Eppley Precision Spectral Pyranometer (PSP) under natural daylight conditions in units of watts per square meter ( $\text{Wm}^{-2}$ ). Under most conditions of natural daylight, the error is  $< 5 \%$ . LI-1400 is a multipurpose data logger that functions both as a data logging device and a multichannel auto ranging meter.

## 3. RESULT AND DISCUSSIONS

### 3.1 IR spectroscopy Analysis

As expected, the infrared (IR) spectrum of disubstituted thiourea (TU) shows five absorption bands of interest namely;  $\nu(\text{N-H})$ ,  $\nu(\text{C=O})$ ,  $\nu(\text{C-N})$ ,  $\nu(\text{C-O})$ , and  $\nu(\text{C=S})$ . It is clearly stated that, the absorption at  $3467\text{cm}^{-1}$  represents stretching vibration for secondary thioamide (N-H) group with broad intensity which is believed due to inter and intra molecular hydrogen bonding. This result was supported by previous literature describing on similar structured framework [26-27] where the frequency for (N-H) was reported at wavenumber  $3400\text{cm}^{-1}$  and above. Moreover, the carbonyl (C=O) band is clearly observed at  $1657\text{cm}^{-1}$  which might be related to the resonance effect of phenyl rings and intermolecular hydrogen bonding towards N-H moiety [28-31]. In addition, the (C-N) stretching frequencies has been assigned at  $1323\text{cm}^{-1}$  with medium intensity and the results was supported by previous work where the assignments of (C-N) for thiourea derivatives can be obtained within frequencies  $1400\text{-}1000\text{cm}^{-1}$  [32]. Besides, strong absorption band of (C-O) observed at  $1251\text{cm}^{-1}$ . From this IR result, it can be concluded that there is an addition of absorption band of interest of (C=S) which has been assigned at  $724\text{cm}^{-1}$  [33] and it is proven to be thiourea derivatives compound [34].

### 3.2 UV-Visible Spectroscopy Analysis

In UV-vis analysis, the compound was dissolved in methanol ( $1 \times 10^{-5} \text{ M}$ ) with cut-off point at 205 nm. Two important peaks can be observed in the electronic spectra of this compound. The first band observed at 243 nm is attributed as mixture of  $n\text{-}\pi^*$  and  $\pi\text{-}\pi^*$  electronic transition of C=O chromophores. The first band is weaker than second electronic transition band due to highly conjugated system of this molecule [35]. The broad absorption band at 273 nm is assigned as  $n\text{-}\pi^*$  and  $\pi\text{-}\pi^*$  electronic transition of C=S chromophores. The electronic transitions of  $n\text{-}\pi^*$  and  $\pi\text{-}\pi^*$  in this study are expected to be produced from lone pairs of electron at oxygen and sulphur atoms of C=O and C=S moieties [36].

### 3.3 $^1\text{H}$ and $^{13}\text{C}$ Nuclear Magnetic Resonance (NMR) Analysis

Based on the result, the  $^1\text{H}$  NMR spectrum showed the expected resonances in the appropriate regions. A methoxy resonance is found at  $\delta_{\text{H}}$  3.78 ppm as singlet which is different from typical methyl moiety. This is due to deshielding effect of oxygen atom and intermolecular hydrogen bonding which decreases the electron density of the group, thus moving the methyl peak to downfield position [37]. At higher chemical shift, aromatic protons of the molecule can be clearly seen as pseudo-doublet in range of  $\delta_{\text{H}}$  6.97-7.57 ppm. This is may due to the different electron withdrawing groups attached at para position of phenyl rings which cause the protons to be magnetically non-equivalent [20,37]. This result was supported by previous literature describing on similar structured framework [20,21,38] where the phenyl rings are strongly influenced by the o, m and p-substituent methyl group at the phenyl ring and due to the overlapping proton signals in the aromatic. At  $\delta_{\text{H}}$  7.98-8.04 ppm, unresolved multiplet resonance can be observed which is assigned as resonance of aromatic protons [20,39-40]. For N-H moieties, the signal for proton observed as two distinctive singlet resonances from two N-H groups can be clearly observed at  $\delta_{\text{H}}$  11.64 ppm and 12.39 ppm respectively. The presence of electron-withdrawing carbonyl and thione will decrease electron density around the protons and thus, deshield the proton resonances to higher chemical shift [41]. Data of  $^1\text{H}$  NMR of this compound is tabulated in Table 3.

**Table 3.**  $^1\text{H}$  NMR data for the disubstituted thiourea (TU) compound

Moiety	Chemical Shift, $\delta_{\text{H}}$ (ppm)
(s, 6H, OCH <sub>3</sub> )	3.78
(pseudo-d, $^3J_{\text{HH}}=10$ Hz, 2H, CH, Ar)	6.97-6.99
(pseudo-d, $^3J_{\text{HH}}=10$ Hz, 2H, CH, Ar)	7.55-7.57
(m, 2H, CH, Ar)	7.98-8.04
(s, 1H, NH)	11.64
(s, 1H, NH)	12.39

**Table 4.**  $^{13}\text{C}$  NMR data for the synthesized compound of disubstituted (TU) compound.

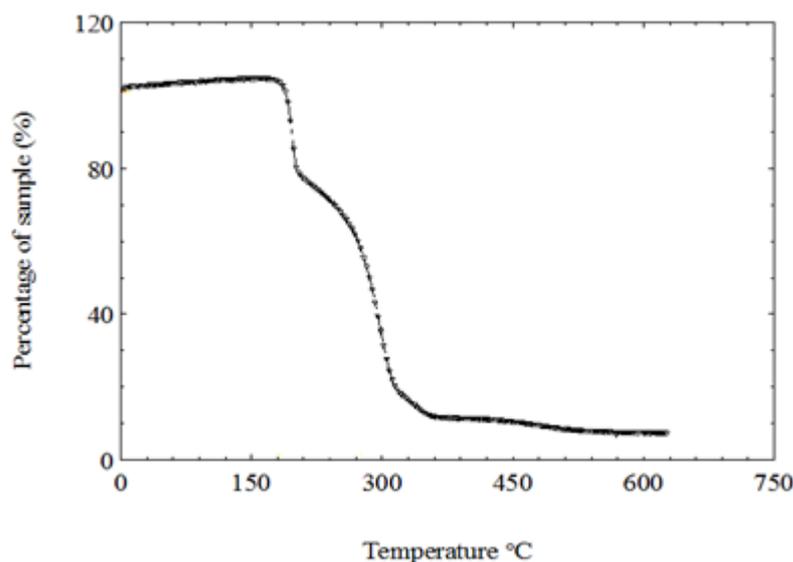
Moiety	Chemical Shift, $\delta_{\text{C}}$ (ppm)
(O-CH <sub>3</sub> )	55.31
(Ar-C)	113.81, 125.98, 127.41, 130.83, 138.03, 157.47
(C=O)	167.66
(C=S)	179.04

$^{13}\text{C}$  NMR analysis also exhibits the resonances at expected regions. The most deshielded signals in the  $^{13}\text{C}$  NMR spectrum are from the carbons of carbonyl and thiocarbonyl groups which are at  $\delta_{\text{C}}$  167.66 ppm and  $\delta_{\text{C}}$  179.04 ppm respectively. Meanwhile, resonances of aromatic protons of this

molecule can be found between  $\delta_C$  113.81-157.47 ppm which corresponds to three phenyl groups in the compound. All data of  $^{13}\text{C}$  NMR is shown in Table 4.

### 3.4 Thermogravimetric Analysis (TGA) Analysis

Thermal decomposition of thiourea derivatives studies has shown various correlations of decomposition temperature with moiety in the ligand [42]. Thermal stability of the material fabricated onto solar cell is one of the major tasks for solar cell application. Long term stability of solar cell should be stable under high temperature environment over long period of time. The thermal property of the sample was investigated by TGA at a heating rate of  $10\text{ }^\circ\text{C}/\text{min}$  under nitrogen atmosphere. The thermogram result for the synthesized compound is presented in Figure 4.



**Figure 4.** TGA thermograms of the synthesized disubstituted thiourea.

**Table 5.** The thermogravimetric analysis data for disubstituted thiourea (TU)

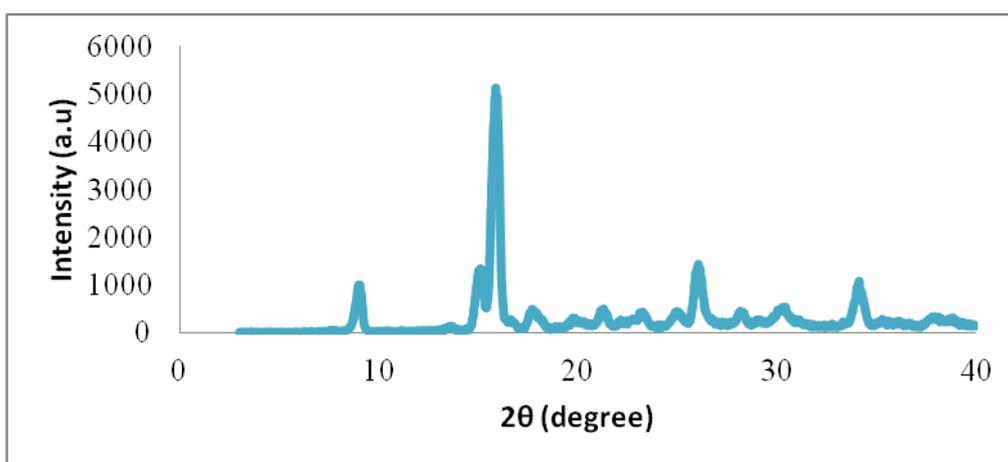
Compound	Stage	Temperature ( $^\circ\text{C}$ )	Weight loss (%)
TU	I	202	64.88
	II	306	22.97

From the thermograms, the synthesized compound shows two stages of degradation. The initial degradation takes place at  $202^\circ\text{C}$  with 64.88% of weight loss and followed by another weight loss at about 22.97% at  $306^\circ\text{C}$ . The thermogravimetric analysis data for the synthesized compound is shown in Table 5 below. The thermal stability of compound increases as the temperature of degradation increases due to the increase molecular weight [43]. The thermal stability of the modified photovoltaic

cell (PVC) increases as the decomposition temperature increases due to the increase in glass transition temperature ( $T_g$ ). [44]. The material with high glass transition temperature will significantly improve the thermal stability of the PVC [45].

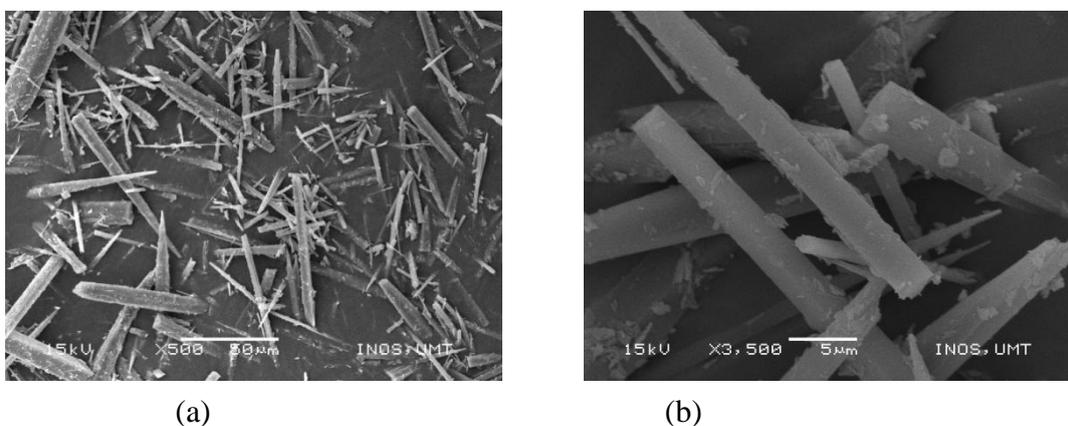
### 3.5 X-Ray Diffraction (XRD) Analysis

Figure 5 shows XRD pattern for the synthesized compound. The obtained XRD pattern indicated that disubstituted thiourea (TU) derivative have polycrystalline structure. The synthesized compound exhibited crystalline peaks at about  $2\theta = 8.9, 15.88, 26, 34$  which shows that it have  $\pi$ -conjugated molecule packing. Crystalline structure gives high efficiency to the solar cell as it has lower band gap compared to the amorphous structure compound [46]. Thus, this compound gives positive indicator for the potential of organic solar cell.



**Figure 5.** XRD pattern the synthesized compound.

### 3.6 Scanning Electron Microscopy (SEM) Analysis



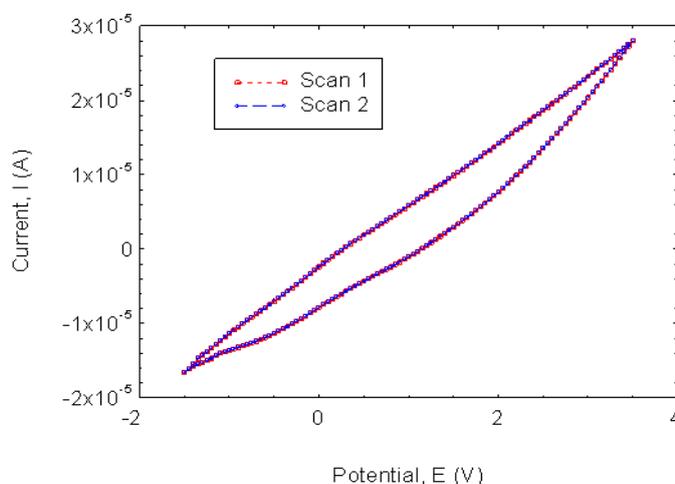
**Figure 6.** Surface morphology of the compound by (a) (500x magnification) and (b) (3,500x magnification).

By using SEM, the surface morphology of the synthesized compound was viewed and exhibited as rod-like, smooth and solid surface. This image clearly indicates that the surface was compact and smooth, as shown in Figure 6.

With this surface, it helps the compound to dissolve easily in the solvent and once the compound is completely dissolved, the distribution of the compound will be smooth on the ITO surface. The smooth surface will enhance the maximum absorption of the sun energy with high electrical conductivity and it has potential to act as photovoltaic cell [20,21].

### 3.7 Cyclic Voltammetry (CV) Analysis

The interest of the electrochemical study of disubstituted thiourea (TU) is to determine the redox reaction and potential range of different electrochemical processes [47]. Besides, the focus is to investigate the dynamic electrochemical interface during the anodisation of thiourea containing supporting electrolyte [48]. In this study, the initial electrochemical study of  $1 \times 10^{-5}$  M of the compound in acetonitrile has been studied using cyclic voltammetry (CV) as shown in Figure 7.

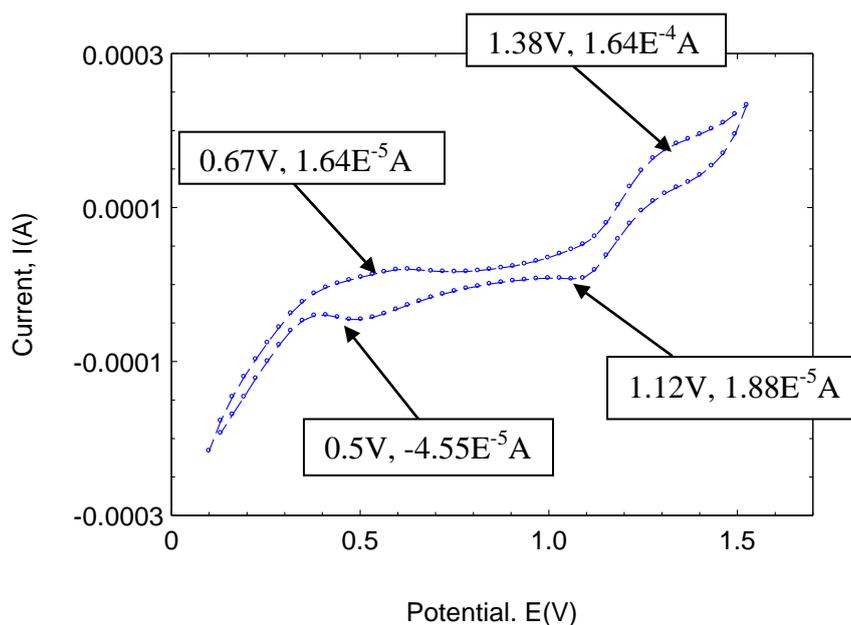


**Figure 7.** The cyclic voltammogram of disubstituted thiourea (TU) in  $\text{CH}_3\text{CN}$  on Pt electrode run at 0.05 V,  $0.03 \text{ Vs}^{-1}$

A typical cyclic voltammogram (blank) of the synthesized compound in acetonitrile ( $\text{CH}_3\text{CN}$ ) on Pt electrode was run at 0.05 V,  $0.03 \text{ Vs}^{-1}$ . From the voltammograms curve in Figure 7, it seems unobvious to observe any redox peaks in this electrochemistry process. Thus, it can be stated that electro-oxidation of disubstituted thiourea (TU) on platinum did not occur in the solvent individually. This is due to TU is a fairly large polarizable molecule which is most likely to be solvated poorly in aqueous solution exhibiting acid-base properties [49]. Meanwhile, in aqueous solution, TU decomposes slowly at room temperature but only limited information about the stability of this solution in different environment is available [50]. In addition, there are a number of questions still open to particular issue of thiourea containing solution include the corresponding electrochemical

kinetics, the electrical behaviour and equivalent circuit accounting for electrodisolution conditions [48].

However, when supporting electrolyte was introduced using 0.5 M sulphuric acid, the cyclic voltammogram of the compound reveals a redox reaction with the presence of oxidation and reduction peaks respectively. This result was supported by previous literature describing on similar structured framework [20, 21] where the redox potential appears in the positive region with the electro-oxidation stage and formamide disulphide (FDS). For this purpose, the cyclic voltammetry characterization obtained TU was performed in acetonitrile solutions containing only sulphuric acid as supporting electrolyte. For the forward scan, two signals are observed which the first shoulder located at about 0.67V and 1.38V. For the first peak, it appears at high frequency, involving the electro-oxidation of the TU to formamide disulphide (FDS). Formamidine disulphide,  $(\text{H}_2\text{N})_2(\text{HN})_2\text{C}_2\text{S}_2$ , (FDS) is the first electro-oxidation product from thiourea that produced at potentials lower than the threshold potential for electrodisolution [51]. It has been reported that formamidine disulphide (FDS) ions are formed as a product from thiourea electro-oxidation in acidic solutions on platinum, by either chemical or electrochemical methods [20,21,52]. In addition, Jiang and co-workers claimed that FDS is one of the products of thiourea oxidation path on platinum in the presence of chloride ions using cyclic voltammetry. There was a report claimed that the first oxidation of thiourea is defined around 0.7 V which represents to the formation of formamidine disulphide (FDS) [53].



**Figure 8.** The cyclic voltammogram of disubstituted thiourea (TU) derivative ( $1 \times 10^{-5}$  M) in  $\text{CH}_3\text{CN}$  + 0.5 M sulphuric acid, 298 K at 0.05 V, 0.03  $\text{Vs}^{-1}$

Thus, from the voltammogram, it can be concluded that the oxidation peak occurs at  $\Delta E_{pa} = 0.67\text{V}$  with  $I_{pa} = 1.64 \times 10^{-5}$  A and  $\Delta E_{pa} = 1.38\text{V}$  with  $I_{pa} = 1.64 \times 10^{-4}$  A while the reduction peak

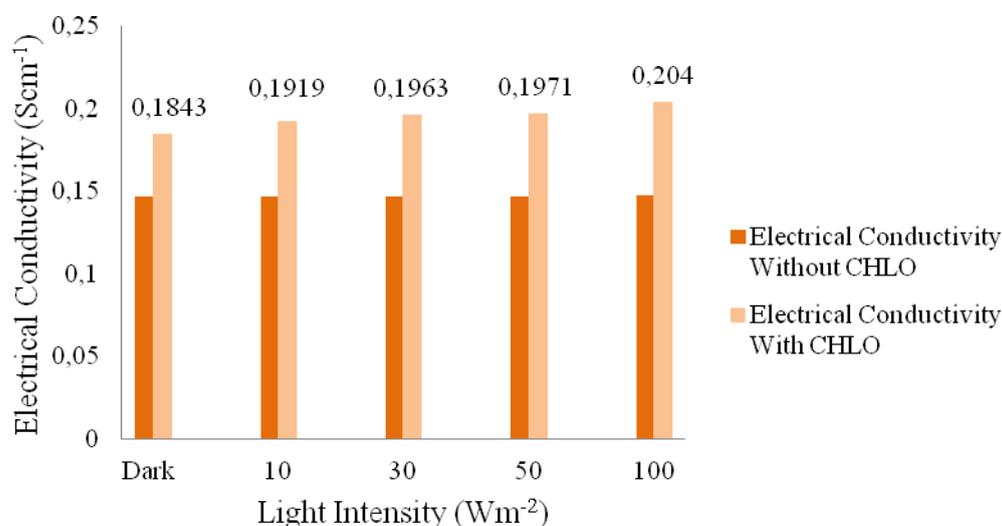
occurs at  $\Delta E_{pc} = 1.12V$  with  $I_{pc} = 1.88 \times 10^{-5}A$  and  $\Delta E_{pc} = 0.50V$  with  $I_{pc} = -4.55 \times 10^{-5}A$ , as shown in Figure 8. Therefore, it shows that the peak becomes better defined when the potential scan goes from 0 to 1.5V. Obviously, there are two pairs of peaks exist as the synthesized compound is made of disubstituted system and appears in the positive region with its electro-oxidation stage.

### 3.8 Electrical Conductivity Study

The electrical conductivity of TU/ITO and TU/CHLO/ITO thin film was measured in the dark and under various intensities of light conditions ( $Wm^{-2}$ ) by using Four-Point Probe. Table 6 and bar chart in Figure 9 show the electrical conductivity values in the dark and various light conditions with and without presence of chlorophyll (CHLO).

**Table 6.** The electrical conductivity values of TU/ITO with and without presence of chlorophyll (CHLO) in following condition.

Light Intensity ( $Wm^{-2}$ )	Electrical Conductivity $\sigma$ ( $Scm^{-1}$ )	
	Without CHLO	With CHLO
Dark condition ( $0 Wm^{-2}$ )	0.1464	0.1843
Light condition ( $10 Wm^{-2}$ )	0.1466	0.1919
Light condition ( $30 Wm^{-2}$ )	0.1469	0.1963
Light condition ( $50 Wm^{-2}$ )	0.1470	0.1971
Light condition ( $100 Wm^{-2}$ )	0.1472	0.2040



**Figure 9.** The electrical conductivity of ITO/TU/CHLO in both conditions with and without chlorophyll

From the data analysis, it shows the electrical conductivity increases by the increasing of light intensities. The highest conductivity is observed under maximum light intensity ( $100 \text{ Wm}^{-2}$ ) with the conductivity value of  $0.1472 \text{ Scm}^{-1}$ . Besides, it is obviously clarify that the compound can conduct electricity even in dark conditions without obtaining energy from sunlight which show its uniquely of compound to other solar cell system which need sufficient solar energy to perform at its best. Hence, it can be concluded that thiourea compound has great potential to act as active and conducting material in organic solar cell.

As expected, when chlorophyll layer combined with thin film of the synthesized compound to form ITO/TU/CHLO, it shows the electrical conductivity increased in the same conditions. It shows the conductivity of  $0.2040 \text{ Scm}^{-1}$  (with CHLO) compared to  $0.1472 \text{ Scm}^{-1}$  (without CHLO) under maximum light intensity of  $100 \text{ Wm}^{-2}$ . In this case, it can be concluded that the introduction of chlorophyll thin film affects the performance of the ITO/TU/CHLO thin film, whereas the ability of the thin film to conduct electricity could be better with existence of chlorophyll thin film. In addition, the electrical conductivity under influence of intensity of light increase with the increasing values and the positive result obtained showed that the thin films were successfully coated on the ITO substrate. Thus, from the promising conductivity result obtained, it is revealed that disubstituted thiourea has great potential to act as an active layer and conducting material in photovoltaic cell.

#### 4. CONCLUSION

A novel linear conjugated disubstituted molecule featuring thiourea compound has been successfully designed, prepared and characterized to act as potential material for application as solar cell. The compound was spectroscopically and analytically characterized via structural, thermal and electrical properties. The electrical conductivity of the thin film ITO/TU/CHLO formed fall in the range of  $0.1843 \text{ Scm}^{-1}$  to  $0.2040 \text{ Scm}^{-1}$ . Based on the spectroscopy and analytical result obtained, thiourea compound shows a promising material for future research which brings the new prospective in molecular electronic application.

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