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Junction properties and conduction mechanism of new terbium complexes with triethylene glycol ligand for potential application in organic electronic device

N.K. Za'aba[1,*], M.A. Mohd Sarjidan[1], W.H. Abd. Majid[1,*], Eny Kusrini[2], Muhammad I. Saleh[3]

(1. Low Dimensional Materials Research Centre, Physics Department, University Malaya, 50603, Kuala Lumpur, Malaysia; 2. Department of Chemical Engineering, Faculty of Engineering, Universitas Indonesia, 16424 Depok, Indonesia; 3. School of Chemical Sciences, Universiti Sains Malaysia, 11800 Penang, Malaysia)

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Abstract: Terbium-picrate triethylene glycol (EO3-Tb-Pic) complex was prepared in thin film and single layer device structure of ITO/EO3-Tb-Pic/Al, using spin coating technique. The UV-Vis absorption spectroscopy analysis was performed to evaluate the electronic molecular transition of the complex. The optical band gap, E_g estimated from the Tauc model revealed that EO3-Tb-Pic thin film exhibited a direct transition with E_g of 2.70 eV. The electronic parameters of the ITO/EO3-Tb-Pic/Al device such as the ideality factor n, barrier height Φ_b, saturation current I_o, and series resistance R_s, were extracted from the conventional ln*I-V*, Cheung's functions and Norde's method. It was found that the evaluated parameters calculated from Norde's and Cheung's methods were consistent with those calculated from the conventional *I-V* method. In the double logarithmic *I-V* plot, three distinct regions based on the slope were identified, and the conduction mechanisms were discussed and explained. The mobility, μ value was estimated from SCLC region as 2.58×10^{-7} $cm^2/(V\cdot s)$. This newly obtained lanthanide complex may be potentially utilized in electronic devices.

Keywords: terbium-picrate complex; triethylene glycol; Tauc model; optical band gap; current-voltage; rare earths

Lanthanide complexes are one type of optoelectronic functional material that has been used in the organic semiconductor application, especially in organic light emitting devices (OLED)[1]. Their attractive features that offer nearly monochromatic luminescent emitters with emission peaks covering a broad spectral range in the visible region have fascinated researchers for decades[1–3]. The excellent pure emission possessed by these materials is known to originate from their specific electronic structure that is due to the f-f transitions in the 4f orbitals which is well shielded by closed 5s and 5p shells[2–4]. Therefore, the emission characteristic from these materials is expected to be very narrow and leads to the high radiative quantum yield. This particular property makes lanthanide complexes, especially europium (Eu) and terbium (Tb) attractive candidates employed as an electroluminescence emitter in OLED[3].

Terbium-picrate triethylene glycol (abbreviated hereafter as EO3-Tb-Pic) is of special interest to many researchers. It is because the acyclic polyether ligands possess a pseudo-cyclic like crown ether conformation which will provide greater stability for the complexes[5]. Moreover, the ability of the triethylene glycol (EO3) ligand to satisfy the coordination requirements of the Ln(III) center with a high coordination number is an important criterion in the design of a green emitter center for applications associated with organic light emitting diodes (OLEDs)[6]. The promising result from photoluminescence reported from our previous work indicated that EO3-Tb-Pic is a suitable candidate as organic semiconductors, especially in OLED application[5]. However, the previous research on EO3-Tb-Pic focuses mainly on the innovations in crystallography, structural and photoluminescence properties. Less attention has been paid on the electrical properties, despite the fact that they are the main factors that affect the device characteristics of an OLED. Moreover, a comprehensive knowledge regarding the electrical behavior of metal/organic semiconductor and charge conduction mechanism at an interface is essential as it is among the main factors that will also reflect and influence the device behavior.

Current-voltage (*I-V*) measurement plays an important role in characterization of device parameters. It has been proven to be one of the techniques for identifying and characterizing the charge conductions phenomenon in various organic semiconductor materials. Moreover, the various electronic parameters of electrical behavior of EO3-Tb-Pic/Al interface may lead to the estimation of several electronic parameters such as the ideality factor, n, barrier height, Φ_b, saturation current, I_0 and series resistance, R_s.

As an extension of this work, the optical behavior of

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* **Corresponding authors:** N.K. Za'aba, W.H. Abd. Majid (**E-mail:** khairiah85@gmail.com, q3haliza@um.edu.my; **Tel.:** +603-796704088)

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EO3-Tb-Pic in the thin film form was further analyzed by assessing the UV-Vis absorption measurement. Their band gap transition and optical band gap, E_g was determined by using the Tauc model. The electrical behavior and device characteristic of ITO/EO3-Tb-Pic/Al were evaluated by means of current-voltage measurement. The charge conduction mechanism was predicted through the double logarithmic *I-V* plot according to the power law relation whereas the estimation of the electronic parameters was made via the well-known modified Shockley equation by assuming the thermionic model. Three different methods which are the conventional ln *I-V* method, the Cheung's function and the modified Norde's function are utilized to extract these electronic parameters.

1 Experimental

1.1 Device fabrication and measurement

The molecular structure of EO3-Tb-Pic compound is shown in Fig. 1(a)[5] and details on the synthesisation method employed were similar to those described elsewhere[5]. In order to fabricate the organic semiconductor device, the EO3-Tb-Pic thin film was spin coated to an overall of 330.6±0.1 nm over the glass and indium tin oxide (ITO) coated glass substrates. Consequently, top contact aluminium (Al) electrode was thermally evaporated on top of the EO3-Tb-Pic thin film at a pressure of approximately 10^{-3} Pa with a deposition rate of 0.5 A/s. The schematic diagram of the single-layer device configuration, ITO/EO3-Tb-Pic/Al, is shown in Fig. 1(b). Analysis of the optical properties of EO3-Tb-Pic thin film was performed using UV-VIS/NIR Spectrometer (model Jasco 570). The electrical properties of ITO/EO3-

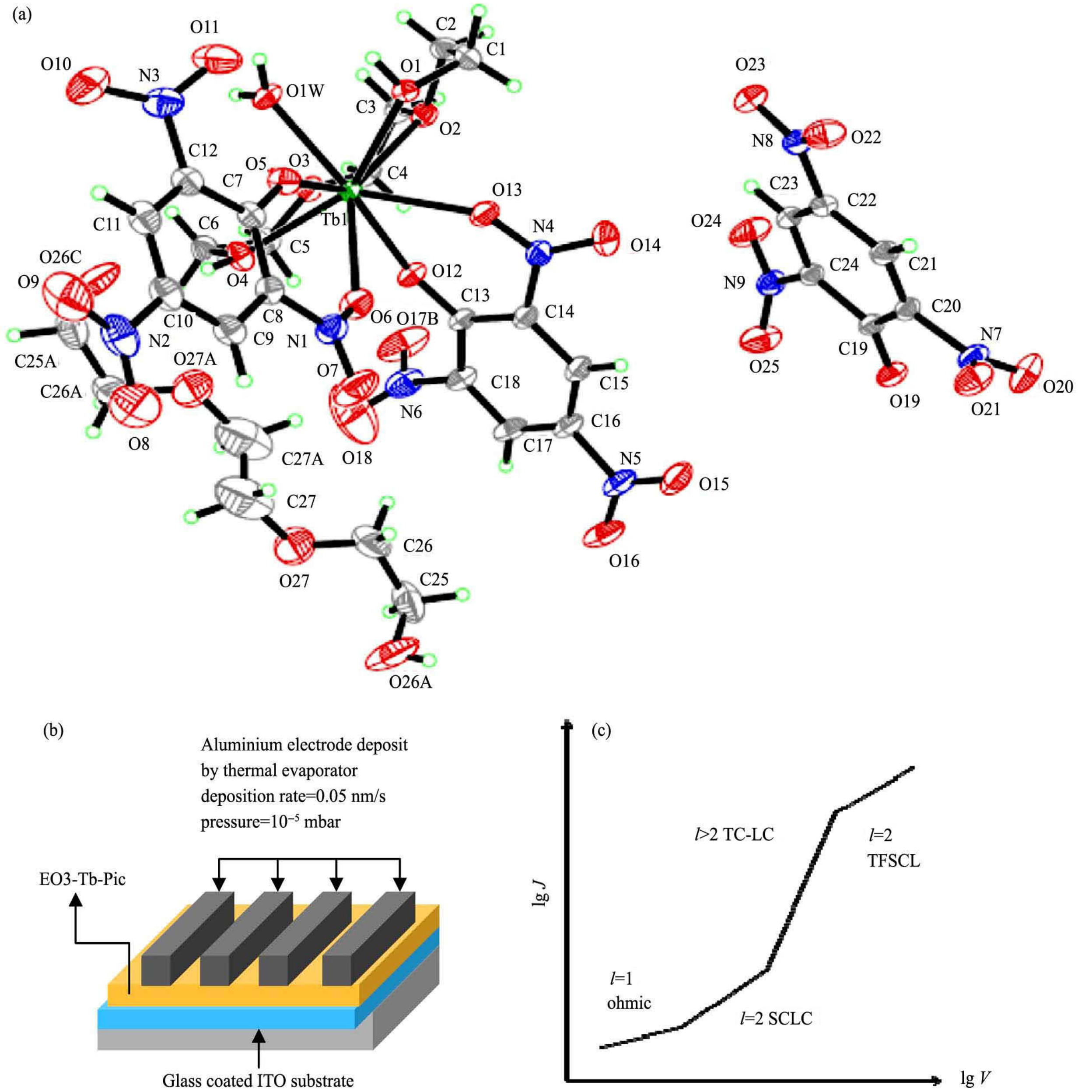

Fig. 1 Molecular structure of EO3-Tb-Pic compound (a), device structure of ITO/EO3-Tb-Pic/Al (b) and three different regime of charge transport in the organic semiconductor layer (c)