TAQIAH BINTI KAMARUDDIN MASTER OF SCIENCE 2017

SYNTHESIS, CHARACTERIZATION AND ELECTRICAL PROPERTIES OF FERROCENAMIDE DERIVATIVES AS POTENTIAL ORGANIC SOLAR CELLS

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DEDICATION

Dedicated to

My beloved parents (mak and ayah) and siblings

My hero, Khairil

Thanks for the endless love and support

Abstract of thesis presented to the Senate of Universiti Malaysia Terengganu in fulfillment of the requirement for the degree of Master of Science.

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School : School of Fundamental Science

The unique redox properties of ferrocene have made it an excellent candidate in the application of molecular electronics. In this study, five new ferrocenamide-based derivatives were synthesized and their electrical properties as potential organic solar cells were evaluated. All of the synthesized compounds (**1-5**) were characterized via Nuclear Magnetic Resonance (NMR), Fourier transform Infrared spectroscopy (FTIR), elemental analysis, Mass Spectrometer (MS), Ultraviolet-Visible (UV-Vis) spectrophotometer and electrochemical analysis. In elemental analysis, the experimental values of C, H, and N were comparable to the calculated theoretical values. This indicated that, the synthesized compounds were reasonably pure.

The infrared spectra for compounds **1-5** showed significant absorption bands within the expected range. In UV-Vis spectra, the presence of π-π* and n-π* electronic transitions which referred to C=O chromophore, azo (pseudo-stilbene), phenyl and naphthalimide moieties were found. The *d-d* transition for compounds **1, 3** and **4** were displayed *ca*. 430 nm. However, for compounds **2** and **5,** the *d-d* transition could not be observed as they were obscured by the azo (pseudo-stilbene) π-π* and charge-transfer (CT) transitions. The ^{1}H NMR spectra showed the presence of all of

the expected resonances. To note, proton signals for NH, Fc-H_α and Fc-H_β were observed in the range of δ_H 7.80-9.63, 4.78-5.06 and 4.33-4.49 ppm, respectively. Whilst, ^{13}C NMR spectra exhibited the expected resonances of C=O, Fc-C_α and Fc-C_α in the range of δ_C 168.33-168.85, 67.52-69.18 and 69.27-71.09 ppm, respectively, which proved that these compounds are definitely ferrocenamide derivatives.

The synthesized compounds were fabricated on Indium Thin Oxide (ITO) substrates using electrochemical deposition method. All compounds (**1-5**) exhibited the reversible one-electron oxidation process of the ferrocenyl moiety. The electrical conductivity for compounds **1-5** were observed in the range of semiconductor materials. Characteristic graph (I-V) for all thin films **1**-**5** showed promising performance of compounds as organic solar cell devices with power conversion efficiency (PCE) value at ~0.30 %.

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SINTESIS, PENCIRIAN DAN SIFAT ELEKTRIK TERBITAN FEROSENAMIDA BERPOTENSI SEBAGAI SEL SOLAR ORGANIK

TAQIAH BINTI KAMARUDDIN

MEI 2017

Penyelia Utama : Tei Woo Chiat, Ph.D

Pusat Pengajian : Pusat Pengajian Sains Asas

Ferosena mempunyai ciri redoks yang unik yang menjadikan ferosena berpotensi digunakan dalam aplikasi elektronik. Di dalam kajian ini, lima terbitan ferosenamida yang baru telah disintesis dan sifat elektriknya dikaji bagi menentukan prestasinya sebagai Sel Solar Organik. Semua sebatian yang disintesis (**1-5**) telah dicirikan melalui Resonans Magnetik Nuklear (NMR), Spektrometer Infra-merah (FTIR), analisis unsur, Jisim Spektrometer (JS), ultralembayung-cahaya nampak dan analisis elektrokimia. Di dalam analisis unsur, nilai yang diperolehi dari eksperimen bagi unsur C, H dan N menunjukkan kadar yang hampir sama dengan nilai teori. Ini membuktikan sebatian yang disintesis adalah tulen.

Spektra inframerah untuk sebatian **1**-**5** menunjukkan serapan penting dalam julat yang dijangkakan. Daripada spektra ultralembayung-cahaya nampak, kehadiran peralihan elektronik π-π* dan n-π* ditunjukkan kepada kromofor C=O, azo(pseudo-stilbena) dan naftalimida moieti. Bagi sebatian **1**, **3** dan **4** peralihan elektronik *d-d* ditunjukkan pada lingkungan 430 nm. Bagaimanapun, bagi sebatian **2** dan **5**, peralihan elektronik *d-d* tidak dapat dilihat kerana ia dikaburi oleh peralihan elektronik π-π* azo (pseudo-stilbena) dan peralihan elektronik pertukaran cas.

Spektra ^{1}H NMR telah menunjukkan semua resonan yang dijangkakan. Signal bagi proton NH, Fc-H_{α} dan Fc-H_{β} dapat dilihat di dalam julat bacaan masing-masing pada δ_H 7.80-9.63, 4.78-5.06 dan 4.33-4.49 ppm. Manakala, ^{13}C NMR juga mempamerkan resonan yang dijangkakan iaitu C=O Fc-C_{α} dan Fc-C_{β} di dalam julat bacaan masing-masing pada δ_C 168.33-168.85 ppm, 67.52-69.18 ppm dan 69.27-71.09 ppm yang membuktikan bahawa sebatian ini adalah terbitan ferosenamida.

Semua sebatian difabrikasikan ke atas substrat ITO dengan menggunakan kaedah pengenapan elektrokimia. Sebatian **1-5** menunjukkan proses berbalik pengoksidaan satu elektron bagi motif ferosena. Kekonduksian elektrik bagi sebatian **1-5** menunjukkan bacaan di dalam julat bahan semikonduktor. Graf pencirian I-V menunjukkan kesemua filem nipis **1-5** berprestasi sebagai sel solar organik dengan nilai kecekapan penukaran kuasa (PCE) ~0.30%.