Suphawarat Phalinyot 2010: Experimental and Theoretical Studies of 2-Methoxy-5-(2'-ethylhexyloxy)-1,4-phenylene-vinylene Derivatives. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Mr. Songwut Suramitr, Ph.D. 110 pages.

The light-emitting organic materials are prepared as the emissive layer to improve OLEDs device. Thus, the main objective of this work are to synthesize and characterize the organic molecules of [1',4'-Bis(thienyl-vinyl)]-2-methoxy-5-(2'-ethylhexyloxy)-1,4-phenylene-vinylene with and without cyano group on the vinylene moiety and the two thiophene rings are linked with a conjugated phenylene group through -C=C- double bond *via* Knoevenagel condensation. The characteristic of its structures were confirmed with ^{1}H-NMR, ^{13}C-NMR, FTIR, TGA, LC-MS, EA, UV-vis and fluorescence spectrometre. Thermal stability of MEH-ThV and MEH-ThV-CN (T_d > 300 °C) enough to be used as electroluminescence materials in light-emitting devices. The absorption spectrum of PTVMEH-ThV is red-shifted and broadened in comparison with that of MEH-ThV-CN. The photophysical properties of both structures exhibited as green light emission. It is noteworthy that can be used as new luminescence materials in the fabrication of OLED-based full-color displays.

Moreover, quantum chemical calculations are investigated the structural, electronic, optical and emission properties of MEH-ThV and MEH-ThV-CN molecules by HF and DFT methods. The effect of substituents on strctures with electron donating (thiophene ring) and withdrawing groups (cyano group) are compared between the experimental and theroretical results. The calculated ground state geometry of *EE*-MEH-ThV-CN is non-planar because of the sterical hindrance of the electron-withdrawing cyano groups effect.The optical and emission properties of *EE*-MEH-ThV is red-shifted, as compared to the *EE*-MEH-ThV-CN, due to there is stronger interchain interactions in *EE*-MEH-ThV, which leads to more coplanar backbone structure than that *EE*-MEH-ThV-CN molecule.

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