Suwannee Sriyab 2011: Experimental and Theoretical Studies of 9-octyl-3,6-di(thiophen-2-yl)-Carbazole Derivatives. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Mr. Songwut Suramitr, Ph.D. 78 pages.

The molecular structural and electronic properties of 9-octyl-3,6-di(thiophen-2-yl)-Carbazole and its derivatives were studied by quantum chemical calculations. Methyl (CH_3), formyl (CHO) and acetyl ($COCH_3$) substitutions have been applied on 9-octyl-3,6-di(thiophen-2-yl)-Carbazole to investigate the optical properties. All structures were optimized using PBE0 functional of calculations with the 6-31G(d) basis set. The electronic transition of structural geometries have been studied by PCM-TD-PBE0/6-311G(d,p) calculations based on ground state geometries at PBE0/6-31G(d) level. The obtained results indicate that calculated UV-vis absorption spectra of Th-3,6CZ-Th-H, Th-3,6CZ-Th-CH_3, Th-3,6CZ-Th-$COCH_3$ and Th-3,6CZ-Th-CHO were found at 298, 334, 393 and 402 nm with respect to the experimental data of 302, 298, 365 and 393 nm, respectively. The fluorescence quantum yield and fluorescence lifetimes of the compound in dichloromethane has been studied. The results showed Th-3,6CZ-Th-$COCH_3$ and Th-3,6CZ-Th-CHO had high quantum yield. Most of the derivative of Th-3,6CZ-Th-H molecule exhibit planar structures at excitation state. The excited state-torsion angles are more planar than the ground state geometries. The obtained results of the electronic transition of structural geometries indicate that calculated absorption and emission spectra related with the experimental data. In additional, the polarizable continuum model was successfully applied to include solvent effect in the model which plays an important role on the absorption behavior.

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