Apipol Piriyagagoon 2009: Structures and Electronic Properties of Oligo(*p*-phenylenevinylene) Carboxylic Acid and Its Derivatives: Effects of Spacer and Anchor Groups by Theoretical Methods. Master of Science (Chemistry), Major Field: Chemistry, Department of Chemistry. Thesis Advisor: Associate Professor Supa Hannongbua, Dr.rer.nat. 95 pages.

A series of DPO-OPV3-COOH organic chromophore was investigated as sensitizers for DSSCs. The structures and electronic properties were studied by quantum chemical calculations. All structures were optimized using HF/6-31G* and B3LYP/6-31G* methods. The vertical excitation energies were calculated using TD-B3LYP/6-31G* method based on ground state geometry optimization. The structure obtained from HF/6-31G* method is found that coplanar conformation. Conversely, that of B3LYP/6-31G* method showed planar conformation. In addition, the electronic transitions were calculated to confirm the most reliable configuration structure from different methods. The simulated absorption spectrum of HF/6-31G* coplanar optimized structure is in well agreement with experimental absorption data than that of B3LYP/6-31G* planar optimized structure. Therefore, in this study, TD-B3LYP/6-31G*//HF/6-31G* and coplanar conformation were selected to further study on the effects of spacer and anchor groups.

For DPO-OPV3-COOH derivatives, phenylenevinylene and carboxylic acid take the role of electron donor and electron acceptor, respectively. The introduction of various thiophene spacer groups to form donor-spacer-acceptor configuration leads to superior performance over the simple donor-acceptor configuration, in terms of bathochromically extended absorption spectra and enhances the electron transfer in the molecule. Moreover, the present study of the modeling in terms of methoxy side chain, di-vinylene-thiophene spacer, and acrylic acid anchor group, the new sensitizer of DMO-OPV3-di-Vi-Th-CN-COOH is therefore suggested for the further study and synthesis.

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