

Supporting information

Synthesis and properties of the derivatives of triphenylamine and 1,8-naphthalimide with the olefinic linkages between chromophores

Dalius Gudeika,^a Gjergji Sini,^b Vygintas Jankauskas,^c Galyna Sych,^a Juozas V. Grazulevicius^{a,*}

^a Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu pl. 19, LT-50254 Kaunas, Lithuania Fax: +37037 300152; tel: +37037 300193; e-mail: juozas.grazulevicius@ktu.lt

^b Laboratoire de Physicochimie des Polymères et des Interfaces, EA 2528 Université de Cergy-Pontoise, 5 mail Gay-Lussac, 95031 Cergy-Pontoise

^c Department of Solid State Electronics, Vilnius University, Sauletekio aleja 9, LT-10222 Vilnius, Lithuania

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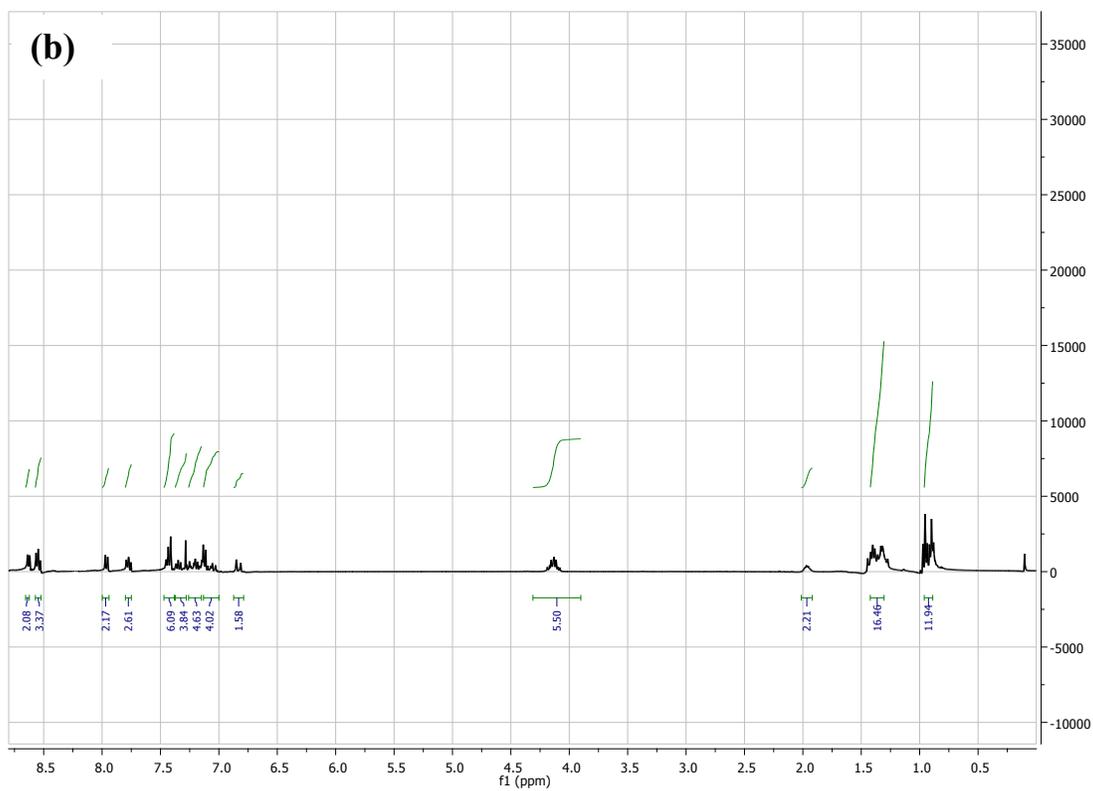
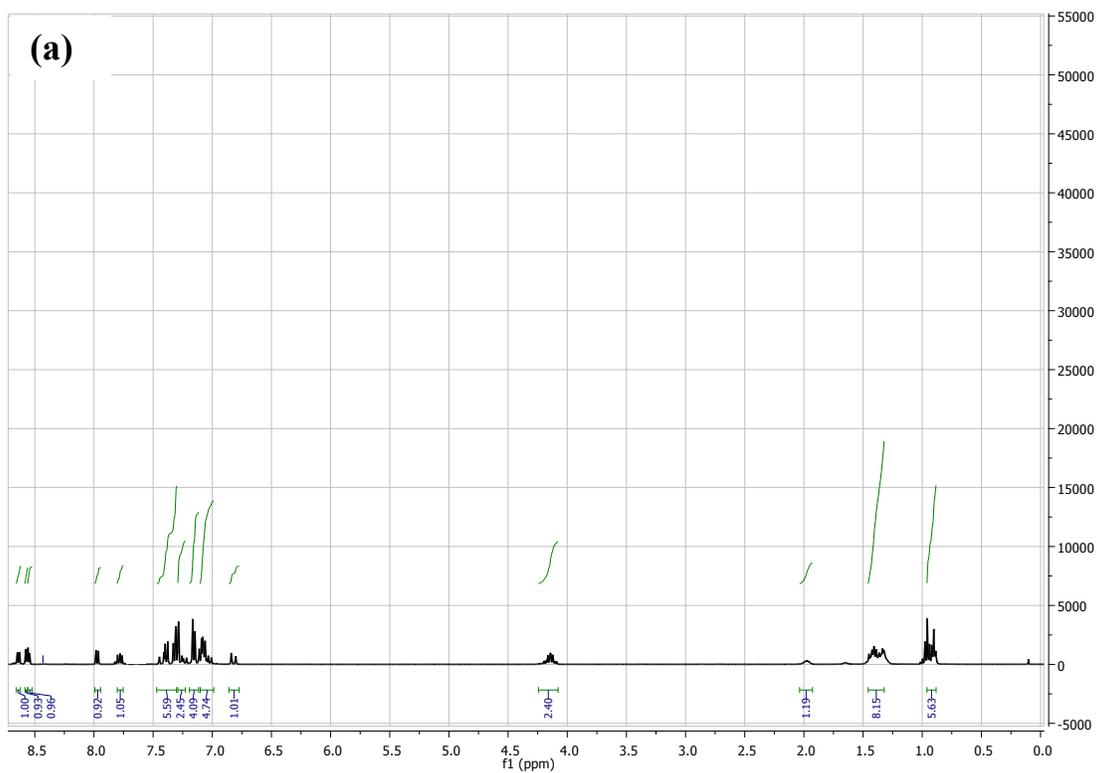


Figure S1. ^1H NMR spectra of compound 4 (a) and compound 5 (b).

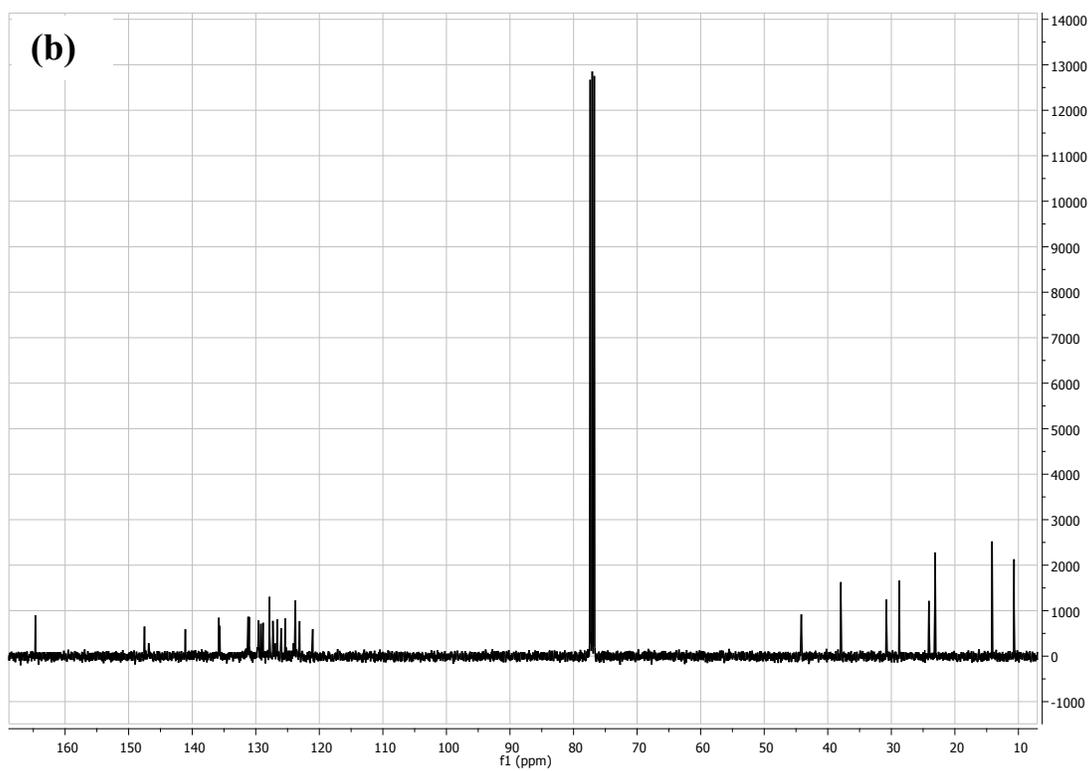
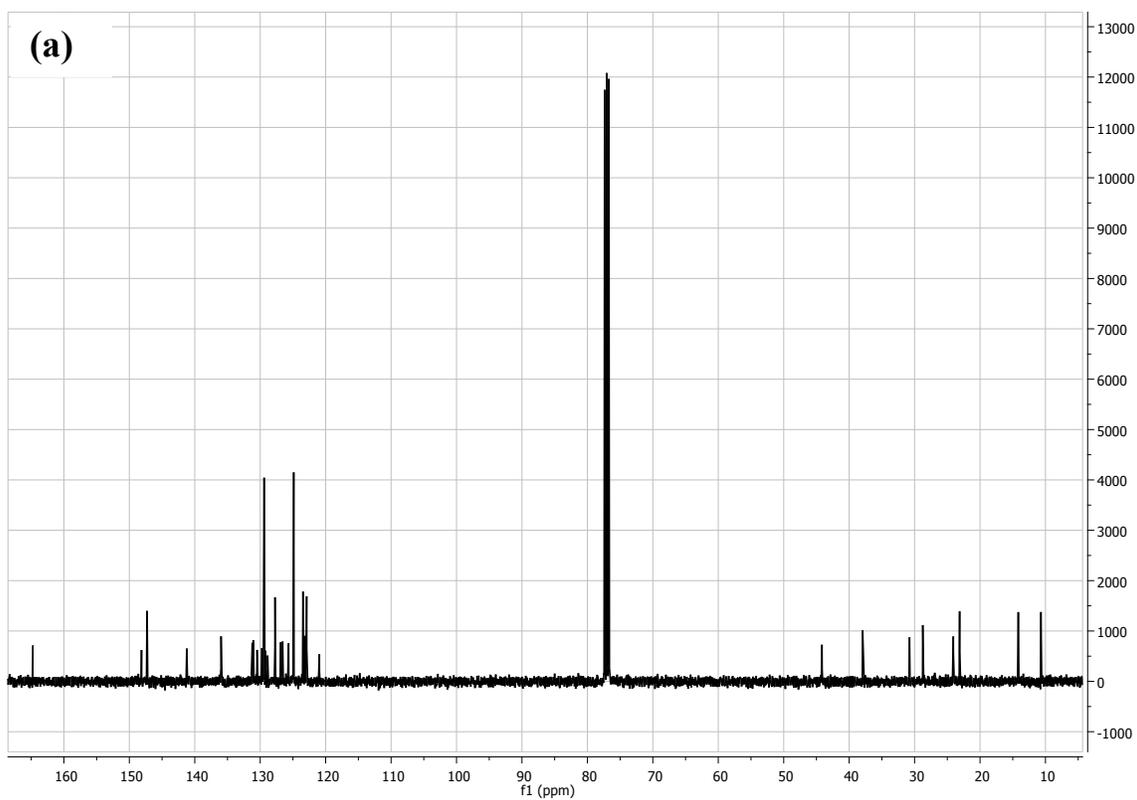
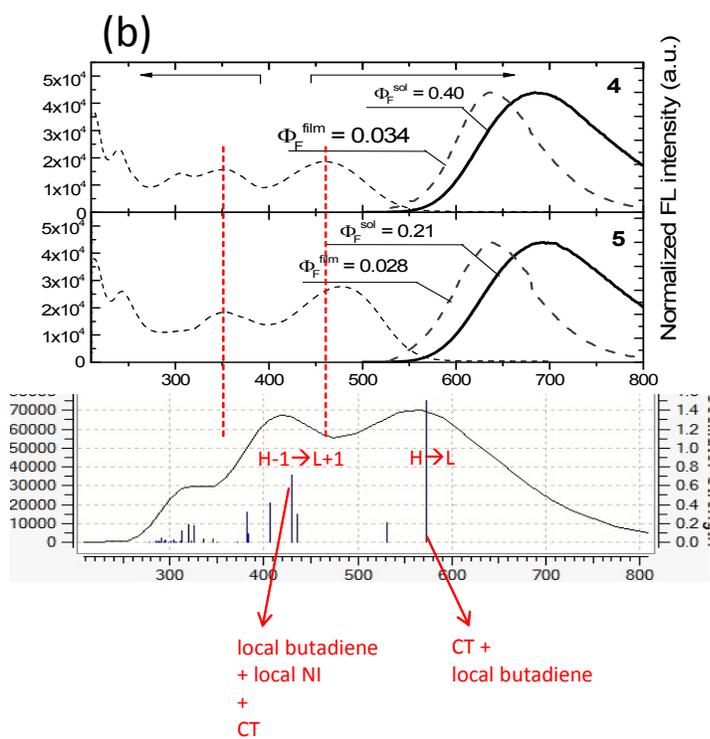
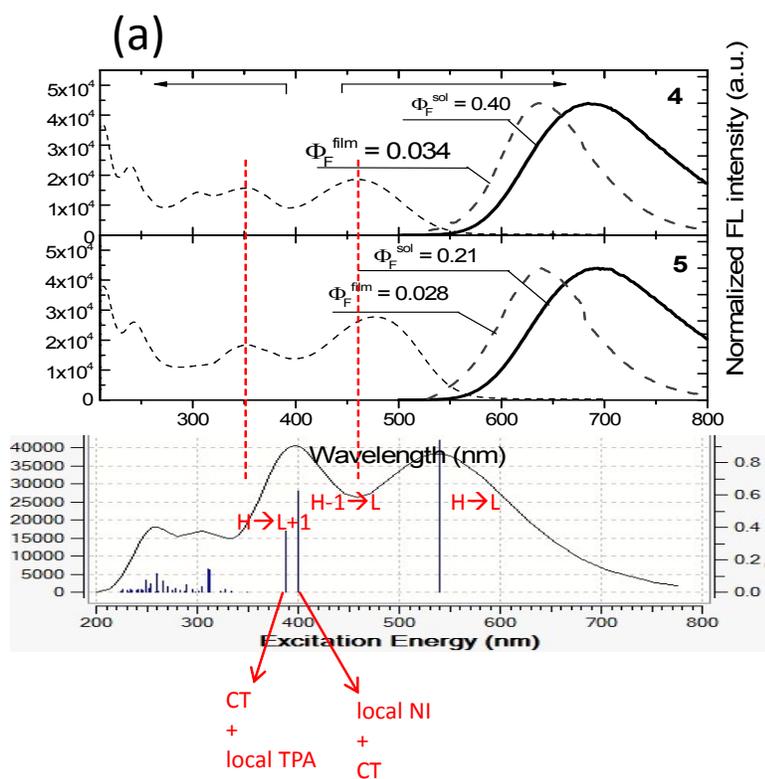


Figure S2. ^{13}C NMR spectra of compound 4 (a) and compound 5 (b).



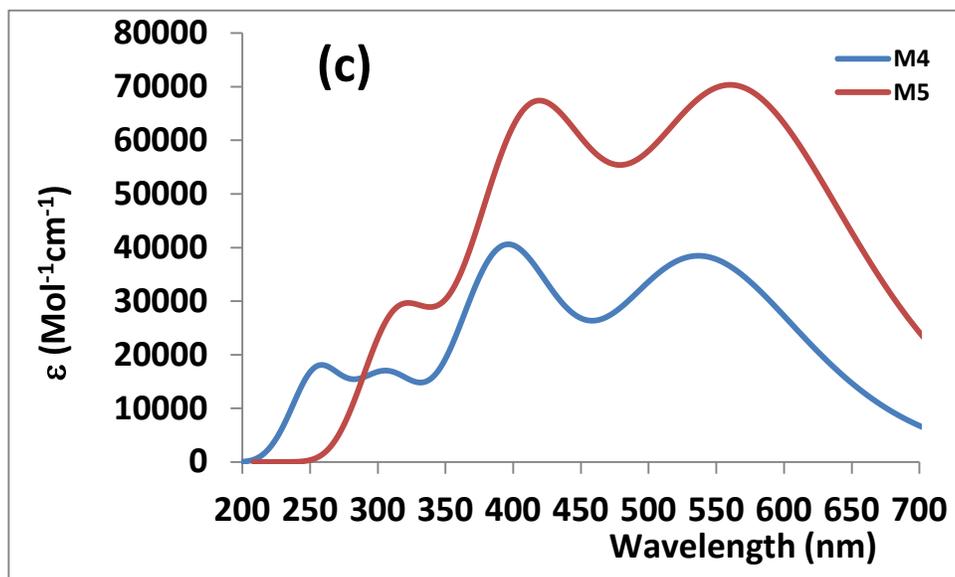
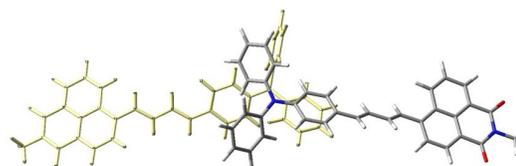


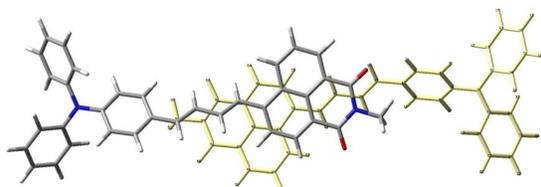
Figure S3. Theoretical absorption spectra of model compounds (a) **M4** and (b) **M5**, along with their comparison in (c). The spectra are obtained at the TD-B3LYP/6-31G(d,p) level in gas phase. B3LYP (and other functionals containing low % of hartree-fock exchange) is known to badly perform for the description of the charge transfer states (important red-shift). It is however sufficient for the comparison of the absorption spectra across the series of compounds **4**, **5**. The theoretical absorption bands were obtained by considering a band half-width at half-maximum of 0.2 eV.



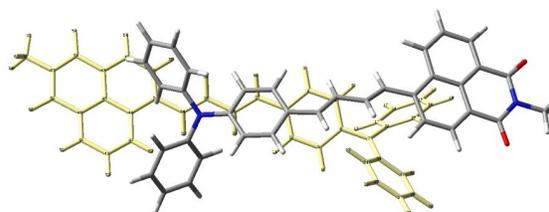
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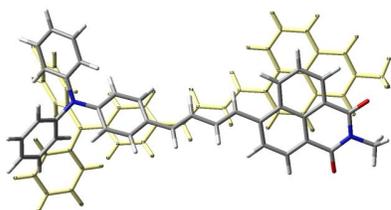
M4-dimer-TPA-over-TPA



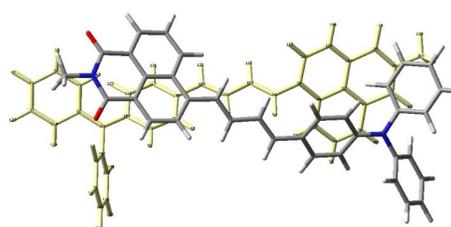
M4-dimer-NI-over-bridge



M4-dimer-TPA-over-bridge



M4-dimer-cofacial



M4-dimer-NI-over-TPA

Figure S4. Selected choice of dimers constructed from the model compound **M4**, obtained at the ω B97XD/6-31G(d,p) level in gas phase. The dimer indicated as „naphthalimide-over-bridge“, for instance, corresponds to naphthalimide moiety over the butadiene one.