Benzotrithiophenes vs. Benzo/Naptha-dithiophenes: The Effect of Star-Shaped versus Linear Conjugation on Their Electronic Structures

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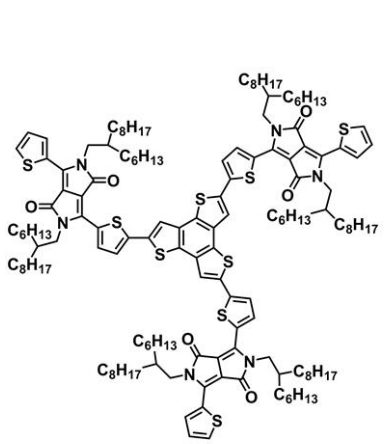
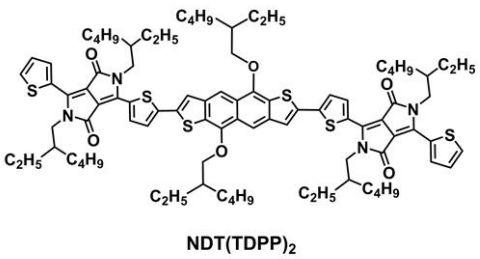
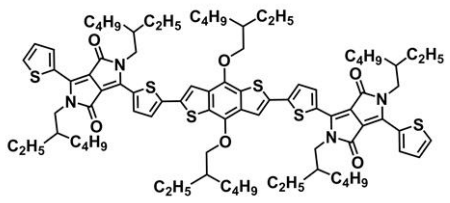
Star-shaped complexes of π-conjugated chromophores are currently of great interest for use in optoelectronic devices.[1] Recently, different planar central cores involving three thiophene rings fused to a benzenic ring (BTTs) have been described. In these systems, the coplanarity and extended π-conjugation of the BTT skeleton should promote intermolecular π-stacking, which would induce strong aggregation and enhanced packing in the solid state of BTT-containing molecules. We propose here the study of a BTT conjugated system with DPPT fragments, in which three DPP2T units are linked to a central rigid trithienobenzene core. Comparison with homologous linear systems, based on the benzodithiophene (BDT) unit and the naphtodithiophene (NDT) unit,[2] will be carried out in order to elucidate the effect of star-shaped configuration versus linear conformation on the optical and electrical properties.



BTT-3DPP



NDT(TDPP)$_2$



BDT(TDPP)$_2$

1. (a) Kanibolotsky, A. L.; Perepichka, I. F.; Skabara, P. J. *Chem. Soc. Rev.* **2010**, *39*, 2695. (b) Lin, Y.; Zhang, Z.-G.; Bai, H.; Li, Y.; Zhan, X. Chem. Comm. **2012**, *48*, 9655. (c) Lin, Y.; Wang, H.; Li, Y.; Zhu, D.; Zhan, X. Journal of Materials Chemistry A **2013**, *1*, 14627.

2. (a) Loser, S.; Bruns, C. J.; Miyauchi, H.; Ortiz, R. P.; Facchetti, A.; Stupp, S. I.; Marks, T. J. J. Am. Chem. Soc. 2011, 133, 8142. (b) Loser, S.; Miyauchi, H.; Hennek, J. W.; Smith, J.; Huang, C.; Facchetti, A.; Marks, T. J. Chem. Comm. **2012**, *48*, 8511.(c)Guerrero, A.; Loser, S.; Garcia-Belmonte, G.; Bruns, C. J.; Smith, J.; Miyauchi, H.; Stupp, S. I.; Bisquert, J.; Marks, T. J. Phys. Chem. Chem. Phys. **2013**, 15, 16456.